Summary of the course

Advanced Quantum Theory | $\mathcal{AQT}$

Lecture notes by Noa Goedee

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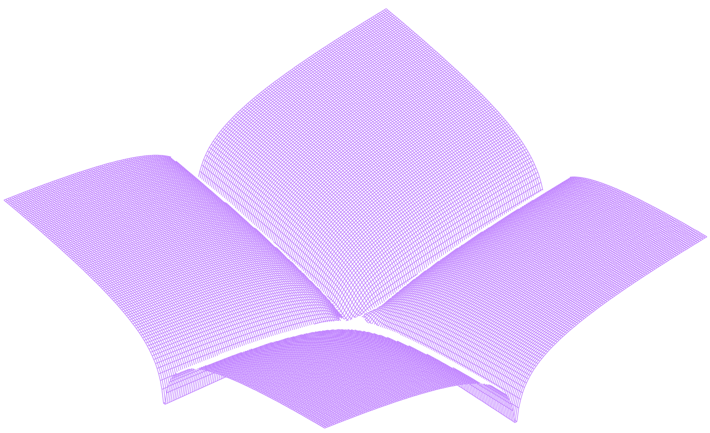


These notes are based on the lecture held by Prof. Manuel Drees and further sources which are not always mentioned specifically.

Introduction

This document is composed of lecture notes for the Advanced Quantum Theory (AQT) course, which was taught by Professor Manuel Drees at Bonn University during the Fall term of 2024-2025. Compiled and expanded upon by Noa Goedee, the notes seek to provide a comprehensive overview of advanced topics in quantum mechanics, including its foundational postulates, path integral formulations, scattering theory, and the principles of second quantization. The material also delves into specialised topics such as gauge invariance, the Aharonov-Bohm effect, and Bell's inequality, offering theoretical insights and practical applications.

Intended for advanced students of physics, this document bridges classical and modern quantum mechanics, laying the groundwork for further exploration into quantum field theory and related disciplines. While not exhaustive, these notes serve as a supplementary resource, capturing key concepts and methodologies discussed in the lectures.

Contents

Review of Quantum Mechanics

Postulates of Quantum Mechanics

- Each system of particles, moving under the influence of internal and/or external forces, can be described by a complex wave function $\psi(\vec{x}_i, t)(i = 1, \dots, N =$ number of particles). ψ contains <u>all</u> the information about the system.

- Each physical observable Q (coordinate, energy, ...) is associated with a hermitian operator $\hat{Q}$. A measurement of Q yields one of the eigenvalues q_n of $\hat{Q}$, defined via

$$\hat{Q}\psi_n(\vec{x}_i, t) = q_n\psi_n(\vec{x}_i, t) \tag{1}$$

  Measurement implies interaction between (quantum) system and (classical) measuring device. If $\psi = \psi_n$ before the measurement, measurement of $\hat{Q}$ always (with probabilty = 1) yields q_n. Otherwise, i.e. $\psi \neq \psi_n\ \forall n$, the outcome can <u>not</u> be predicted with certainty. Just <u>after</u> the measurement yielding $q_n : \psi = \psi_n$.

- The (often infinite) set of linearly independend eigenfunctions ψ_n, with $\hat{Q}\psi_n = q_n\psi_n$ for some hermitian operator $\hat{Q}$, can be used to descibe all physically meaningful wavefunctions.

$$\text{sum: } \psi(\vec{x}_i, t) = \sum_n u_n(t)\psi_n(\vec{x}_i)\ \forall \vec{x}_i, u_n(t) \in \mathbb{C}. \tag{2}$$

  If $\hat{Q}$ has a continuous spectrum of eigenvalues

$$\text{integral: } \psi(\vec{x}_i, t) = \int \mathrm{d}q u(q,t)\psi_q(\vec{x}_i) \tag{3}$$

  The eigenfunctions of a hermitian operator are (or can be chosen) orthogonal

$$\Rightarrow \qquad u_n(t) = \int \mathrm{d}^3x_1 \dots \mathrm{d}^3x_N \psi_n^\star(\vec{x}_i, t) \tag{4}$$

- Given a wavefunction $\psi(\vec{x}_i, t)$, the expectation value (in statistical sense) of observable Q is

$$\langle Q \rangle = \int \mathrm{d}^3x_1 \dots \mathrm{d}^3x_N \psi_n^\star(\vec{x}_i, t) \tag{5}$$

  If $\psi(\vec{x}_i, t) = \sum_n u_n(t)\psi_n(\vec{x}_i) + \int \mathrm{d}q u(q,t)\psi_q(\vec{x}_i)$, with

$$\sum_n |u_n(t)|^2 + \int \mathrm{d}q |u(q,t)|^2 = 1 \tag{6}$$

$$\Rightarrow \qquad \langle \hat{Q} \rangle = \sum_n q_n |u_n(t)|^2 + \int \mathrm{d}q q |u(q,t)|^2 \tag{7}$$

- Lacking external influence (e.g. measurement), the time evolution of the wavefunction is given by Schrödinger‘s equation:

$$i\hbar \frac{\partial \psi(\vec{x}_i, t)}{t} = \hat{H}(\vec{x}_i, t)\psi(\vec{x}_i, t). \tag{8}$$

  $\hat{H}$ can be obtained from classical Hamilton functions by replacing all classical generalized coordinates and canonically conjugated momenta by the corresponding hermitian operators.

- The commutation of operators describing physical observables can be derived from the Poisson bracket of these classical observables.

$$\left[\hat{Q}, \hat{R}\right] = \hat{Q}\hat{R} - \hat{R}\hat{Q} = i\hbar \left\{\hat{Q}, \hat{R}\right\}\Big|_{\text{observables}\to\text{operators}} \tag{9}$$

$$\text{Poisson bracket: } \{Q, R\} = \sum_K \left(\frac{\partial Q}{\partial q_K}\frac{\partial R}{\partial p_K} - \frac{\partial Q}{\partial p_K}\frac{\partial R}{\partial q_K} \right) \tag{10}$$

$$p_K = \frac{\partial L}{\partial \dot{q}_K}, \quad L: \text{ Lagrangefunction}$$

- Possible wavefunctions are elements of physical Hilbert space: differentiable complex functions, possible of many variables, which can be normalised (to unity, for discrete spectrum of eigenvalues; to δ-“function”, for continuous spectrum). Relevant operators act on this Hilbert space, and are linear: $\hat{Q}(a\psi_1 + b\psi_2) = a\hat{Q}\psi_1 + b\hat{Q}\psi_2$, if $a, b \in \mathbb{C}$ are constants. Hilbert space is (often ∞-dimensional) linear vector space.

Examples of operators and eigenfunctions

$$\text{Linear momentum: } \hat{\vec{p}} = -i\hbar\vec{\nabla}, \quad \hat{p}_K = -i\hbar\frac{\partial}{\partial x_K}, x_K: \text{ cartesian coordinates} \tag{11}$$

$$\text{Eigenfunctions: plane wave, } \frac{1}{(2\pi)^{3/2}}e^{\vec{K}\cdot\vec{x}}, \qquad \text{eigenvalues } \hbar\vec{K} \tag{12}$$

Coordinate: $\hat{\vec{x}} = \vec{x}$, eigen“function” $= \delta(\vec{x} - \vec{x_0})$, eigenvalue $\vec{x}_0$

$$\text{Orbital angular momentum: } \hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}} \tag{13}$$

$$\Rightarrow \hat{L_x} = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right); \hat{L_y} = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right); \hat{L_z} = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{14}$$

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \text{ and cyclical permutations} \tag{15}$$

$$\hat{L}^2 = \hat{L}\cdot\hat{L}: \text{ eigenvalues } \hat{L}^2\psi_{lm} = \hbar^2 l\,(l+1)\,\psi_{lm}; \hat{L}_z\psi_{lm} = \hbar m\psi_{lm} \tag{16}$$

Eigenfunctions in spherical coordinates $(r,\theta,\phi): \hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2 + \cot(\theta)\frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}}\right) \tag{17}$$

$$\psi_{lm} = \frac{e^{im\phi}}{\sqrt{2\pi}}\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)\,(l+m)}{2\,(l-m)!}}\frac{1}{(\sin(\theta))^m}\left(\frac{\mathrm{d}}{\mathrm{d}\cos(\theta)}\right)^{l-m}\left(1-\cos^2(\theta)\right)^l \tag{18}$$

(18) are the spherical harmonics.
Raising and lowering operators (<u>not</u> hermitian): $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$: raise/ lower m by 1, leave l such.

$$\text{Harmonic oscillator (1-dim): } \hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{C}{2}\hat{x}^2 \tag{19}$$

$$\text{Raising \& lowering (“ladder”) operators: } \hat{a}_\pm = \frac{1}{\sqrt{2m}}p_x \pm i\sqrt{\frac{C}{2}}\hat{x} \tag{20}$$

$$[\hat{a}_+, \hat{a}_-] = -\hbar\omega_0, \omega_0 = \sqrt{\frac{C}{m}} \tag{21}$$

$$\left[\hat{H}, \hat{a}_\pm\right] = \pm\hbar\omega_0\hat{a}_\pm \tag{22}$$

$$\hat{H} = \hat{a}_+\hat{a}_- + \frac{\hbar\omega_0}{2} \tag{23}$$

$$\tag{24}$$

Often: dimensionless $b_\pm = \frac{\hat{a}_\pm}{\sqrt{\hbar\omega_0}} \Rightarrow \hat{H} = \hbar\omega_0\left(\hat{b}_+\hat{b}_- + \frac{1}{2}\right)$.

$$\text{Energies: } E_n = \hbar\omega_0\left(n + \frac{1}{2}\right), n = 0,1,2,\ldots \tag{25}$$

$$\text{Eigenfunctions: } u_0(x) = \left(\frac{C}{\hbar\omega_0\pi}\right)^{\frac{1}{4}} e^{-Cx^2/2\hbar\omega_0}, u_n(x) = \frac{1}{(\hbar\omega_0)^n}\frac{1}{n!}\hat{a}_+^n u_0(x) \tag{26}$$

Basis states, matrix representation, pertubation theory

$|i\rangle$: Describes state $i, \psi = \psi_i$: (state) vector Hilbert space
$\langle K|$: corresponds to ψ_K^*

$$\langle K|i\rangle = \int \mathrm{d}^3x_1\ldots\mathrm{d}^3x_N\psi_K^*(\vec{x}_l)\psi_i(\vec{x}_l), \langle i|i\rangle: \text{ Norm of } |i\rangle \tag{27}$$

$$\langle K|\hat{Q}|i\rangle = \int \mathrm{d}^3x_1\ldots\mathrm{d}^3x_N\psi_K^*(\vec{x}_l)\hat{Q}\psi_i(\vec{x}_l) =: (O^{\leftrightsquigarrow})_{ki} \tag{28}$$

(27) is the matrix representation of operator Q, if $|i\rangle, |K\rangle$ are elements of a basis of Hilbert space, matrix representation is basis dependent! Useful e.g. in time-independend pertubation theory: $\hat{H} = \hat{H}_0 + \lambda\hat{H}_1 : \lambda\hat{H}_1$: small pertubation

$$\hat{H}_0 u_K = E_k^{(0)} u_K \tag{29}$$

assumed to be knwon, $\hat{H}_0$ is hermitian $\Rightarrow u_K$ forms basis state $|K\rangle_0$: wave function $\psi = u_K$ of unpertubated system ($\lambda = 0$)

$$E_K = E_K^{(0)} + \lambda E_K^{(1)} + \lambda^2 E_K^{(2)} + \dots, \qquad E_K^{(1)} = {}_0\langle K|\hat{H}_1|K\rangle_0 \tag{30}$$

$$E_K^{(2)} = \sum_{i\neq K} \frac{\left|{}_0\langle i|\hat{H}_1|K\rangle_0\right|^2}{E_K^{(0)} - E_i^{(0)}} \tag{31}$$

$$\text{Wavefunction: } \psi_K = \underbrace{\psi_K^{(0)}}_{u_K} + \lambda\psi_K^{(1)} + \lambda^2\psi_K^{(2)} + \dots, \psi_K^{(l)} = \sum_i c_{Ki}^{(l)} u_K \tag{32}$$

$$\Rightarrow c_{K1}^{(1)} = \frac{\left|{}_0\langle i|\hat{H}_1|K\rangle_0\right|^2}{E_K^{(0)} - E_i^{(0)}} \tag{33}$$

[07.10.2024, Lecture 1]

[09.10.2024, Lecture 2]

Transformation and Symmetries

In Hamiltononian classical mechanics

The hamilton function is a function of $2N$ phase space coordinates q_i, p_i for system with N degrees of freedom can define a transformation of variables describing phase space:

$$q_i \to \bar{q}_i(q_k, p_k); p_i \to \bar{p}_i(q_k, p_k). \tag{34}$$

General transformation does not leave the equation of motion (e.o.m.) form invariant. The e.o.m. are form invariant, if (34) is canonical, i.e. it satisfies

$$\{\bar{q}_i, \bar{q}_k\} = \{\bar{p}_i, \bar{p}_k\} \tag{35}$$

$$\{\bar{q}_i, \bar{p}_k\} = \delta_{ik} \tag{36}$$

Canonical transformations leave arbitrary Poisson brackets invariant:

$$\text{let } A(q_k,p_k), B(q_k,p_k);\text{ then } \left\{\underbrace{A(q_k,p_k), B(q_k,p_k)}_{functions\ of\ q_k,p_k}\right\}_{(q,p)} = \left\{\underbrace{A(\bar{q}_k,\bar{p}_k), B(\bar{q}_k,\bar{p}_k)}_{functions\ of\ \bar{q}_k,\bar{p}_k}\right\}_{(\bar{q},\bar{p})} \tag{37}$$

Examples

(i)

$$\bar{q}_i = -p_i;\ \bar{p}_i = q_i \tag{38}$$

$$\{\bar{q}_i, \bar{q}_k\} \overset{38}{=} \{-p_i, -p_k\} = \{p_i, p_k\} = 0$$
$$\{\bar{p}_i, \bar{p}_k\} \overset{38}{=} \{q_i, q_k\} = 0$$
$$\{\bar{q}_i, \bar{p}_k\} \overset{38}{=} \{-p_i, q_k\} = -\{p_i, q_k\} = \{q_k, p_i\} = \delta_{ik}$$

Physical application: work in Fourier space!

(ii)

$$\text{“point transformation”: } q_i \to \bar{q}_i(q_k) \tag{39}$$

Is change of coordinates $\Rightarrow$ e.o.m. in Lagrange formulation are form invariant $\Rightarrow$ e.o.m. in Hamilton formalism should also be form invariant. Have to find transformation law of momenta that follows from (39):

$$\bar{p}_i = \frac{\partial L(\bar{q}_i, \dot{\bar{q}}_i)}{\partial \dot{\bar{q}}_i} = \sum_k \frac{\partial L(q_k, \dot{q}_k)}{\partial \dot{q}_k}\frac{\partial \dot{q}_k}{\partial \dot{\bar{q}}_i} = \sum_k p_k \frac{\partial \dot{q}_k}{\partial \dot{\bar{q}}_i} \tag{40}$$

$$\dot{\bar{q}}_i = \frac{\mathrm{d}\bar{q}_i}{\mathrm{d}t} = \sum_l \frac{\partial \bar{q}_i}{\partial q_l}\frac{\mathrm{d}q_l}{\mathrm{d}t} = \sum_l \frac{\partial \bar{q}_i}{\partial q_l}\dot{q}_l \quad \Rightarrow \quad \frac{\partial \dot{\bar{q}}_i}{\partial \dot{q}_l} = \frac{\partial \bar{q}_i}{\partial q_l} \tag{41}$$

$$\text{(40) implies: } \frac{\partial \bar{p}_i}{\partial p_l} = \frac{\partial q_l}{\partial \bar{q}_i} \tag{42}$$

$$\frac{\partial \bar{p}_i}{\partial q_l} = \sum_k p_k \frac{\partial}{\partial q_l}\frac{\partial q_k}{\partial \bar{q}_i} = \sum_k p_k \frac{\partial}{\partial \bar{q}_i}\underbrace{\frac{\partial q_k}{\partial q_l}}_{\delta_{lk}} = 0 \tag{43}$$

$$\{\bar{q}_i, \bar{q}_k\} = 0;\ \{\bar{p}_i, \bar{p}_k\} = 0 \text{ from (43)}$$

$$\{\bar{q}_i, \bar{q}_k\} = \sum_l \left(\frac{\partial \bar{q}_i}{\partial q_l}\frac{\partial \bar{p}_k}{\partial p_l} - \frac{\partial \bar{q}_i}{\partial p_l}\frac{\partial \bar{p}_k}{\partial q_l}\right) \overset{42}{=} \sum_l \frac{\partial \bar{q}_i}{\partial q_l}\frac{\partial q_l}{\partial \bar{q}_k} = \frac{\partial \bar{q}_i}{\partial \bar{q}_k} = \delta_{ik}$$

Active vs. passive transformations

(34) always makes sense as a passive transformation: change of variables, such $\{q_i, p_i\}$ and $\{\bar{q}_i, \bar{p}_i\}$ refer to the same physical point in phase space.
(34) is called regular if the $\bar{q}_i, \bar{p}_i$ lie in the same range of values as original q_i, p_i. E.g. rotation of axes, or translation, are regular; going from cartesian to cylindrical coordinates is not.
A regular transformation of the form (34) can be interpreted as an active transformation, $\{q_i, p_i\}$ and $\{\bar{q}_i, \bar{p}_i\}$ refer to different points of phase space.
A quantity $A(q_i, p_i)$ is invariant under an active transformation, if

$$A(q_i, p_i) = A(\bar{q}_i, \bar{p}_i) \qquad \text{Always true for passive transformation} \tag{44}$$

[09.10.2024, Lecture 2]

[14.10.2024, Lecture 3]

A systematic way to produce (infinitesimal) canonical transformations is via a smooth generating function (generator) $g(q_i, p_i)$:

$$q_i \to \bar{q}_i = q_i + \underbrace{\varepsilon \frac{\partial g}{\partial p_i}}_{\delta q_i}; p_i \to \bar{p}_i = p_i + \underbrace{\varepsilon \frac{\partial g}{\partial q_i}}_{\delta p_i} \tag{45}$$

Let us check that is canonical transformation:

$$\begin{aligned}
\{\bar{q}_i, \bar{q}_k\} &= \left\{q_i + \varepsilon\frac{\partial g}{\partial p_i}, q_k + \varepsilon\frac{\partial g}{\partial p_k}\right\} = \underbrace{\{q_i, q_k\}}_{0} + \varepsilon\left[\left\{q_i, \frac{\partial g}{\partial p_k}\right\} + \left\{\frac{\partial g}{\partial p_i}, q_k\right\}\right] + \underbrace{\mathcal{O}(\varepsilon^2)}_{\text{ignore}} \\
&= \varepsilon \sum_l \left(\underbrace{\frac{\partial q_i}{\partial q_l}}_{\delta_{il}}\frac{\partial^2 g}{\partial p_l \partial p_k} - \cancelto{0}{\frac{\partial q_i}{\partial p_l}}\frac{\partial^2 g}{\partial q_l \partial p_k} + \frac{\partial^2 g}{\partial q_l \partial p_i}\cancelto{0}{\frac{\partial q_k}{\partial p_l}} - \frac{\partial^2 g}{\partial p_l \partial p_i}\underbrace{\frac{\partial q_k}{\partial q_l}}_{\delta_{kl}}\right) \\
&= \varepsilon\left(\frac{\partial^2 g}{\partial p_i \partial p_k} - \frac{\partial^2 g}{\partial p_k \partial p_i}\right) = 0; \{\bar{q}_i, \bar{q}_k\} = 0 \text{ analogously} \\
\{\bar{q}_i, \bar{p}_k\} &= \left\{q_i + \varepsilon\frac{\partial g}{\partial p_i}, p_k - \varepsilon\frac{\partial g}{\partial q_k}\right\} = \{q_i, p_k\} + \varepsilon\left[\left\{\frac{\partial g}{\partial p_i}, p_k\right\} - \left\{q_i, \frac{\partial g}{\partial q_k}\right\}\right] + \underbrace{\mathcal{O}(\varepsilon^2)}_{\text{ignore}} \\
&= \delta_{ik} + \varepsilon\sum_l \left(\frac{\partial^2 g}{\partial q_l \partial p_i}\underbrace{\frac{\partial p_k}{\partial p_l}}_{\delta_{kl}} - \underbrace{\frac{\partial q_i}{\partial q_l}}_{\delta_{il}}\frac{\partial^2 g}{\partial p_l \partial q_k}\right) = \delta_{ik} + \varepsilon\left(\frac{\partial^2 g}{\partial q_k \partial p_i} - \frac{\partial^2 g}{\partial p_i \partial q_k}\right) = \delta_{ik}
\end{aligned}$$

Theorem: If the Hamilton function $H(q_i, p_i)$ is invariant under the active transformation (45), then the generator g is conserved (independend of time).

Proof: H is invariant if the $\mathcal{O}(\varepsilon)$ change $\delta H = 0$. From (45):

$$\delta H = \sum_l \left(\frac{\partial H}{\partial q_l} \delta q_l + \frac{\partial H}{\partial p_l} \delta p_l \right) = \varepsilon \sum_l \left(\frac{\partial H}{\partial q_l} \frac{\partial g}{\partial p_l} + \frac{\partial H}{\partial p_l} \frac{\partial g}{\partial q_l} \right) = \varepsilon \{H, g\} \stackrel{!}{=} 0 \tag{46}$$

$$\{H, g\} = 0 \text{ iff } H \text{ is invariant under the transformation generated by } g$$

For arbitrary function $g(q_i, p_i)$:

$$\frac{\mathrm{d}g}{\mathrm{d}t} = \sum_l \left(\frac{\partial g}{\partial q_l} \dot{q}_l + \frac{\partial g}{\partial p_l} \dot{p}_l \right) \stackrel{e.o.m.}{=} \sum_l \left(\frac{\partial g}{\partial q_l} \frac{\partial H}{\partial p_l} - \frac{\partial g}{\partial p_l} \frac{\partial H}{\partial q_l} \right) = \{g, H\}$$
$$\Rightarrow \delta H = 0 \text{ implies } \dot{g} = 0, \text{ i.e. } g \text{ is conserved.}$$

$$\text{In general: Any function } A(q_i, p_i) \underset{g}{\to} A + \varepsilon \{A, g\} \tag{47}$$

Theorem: If H is invariant under a regular canonical transformation (34), and if $(q_i(t), p_i(t))$ is a valid trajectory (solution of e.o.m.), then $(\bar{q}_i(t), \bar{p}_i(t))$ is also a solution of e.o.m.
Given the infinitesimal transformation (45), one can obtain a finite transformation by integrating 1^{st} order differential equation:

$$\frac{\partial \bar{q}_i}{\partial \xi} = \frac{\partial g}{\partial \bar{p}_i} = \{\bar{q}_i, g\}\,; \frac{\partial \bar{p}_i}{\partial \xi} = -\frac{\partial g}{\partial \bar{q}_i} = \{\bar{p}_i, g\} \tag{48}$$

Formally identical to Hamiltononian e.o.m., with $t \to \xi, H \to g$.

Examples: (i)

$$\underline{g = p_k} \stackrel{45}{\Rightarrow} \delta q_i = \epsilon \delta_{ik}; \delta p_i = 0 \tag{49}$$

p_k generates a shift (translation) in the associated coordinate.
For cartesian coordinates: translational invariance $\Leftrightarrow$ conservation of linear momentum (classical Noether's theorem). To a get finite transformation:

$$q_i \to \bar{q}_i = q_i + \xi \delta_{ik}; p_i \to \bar{p}_i = p_i, \qquad \xi \in \mathbb{R} \text{ arbitrary}$$

(49) changes a single p_k. For a N-particle system invariant under a shift in z direction, need $g = \sum_{n=1}^{N} (\vec{p}_n)_z$ if component of total linear momentum conserved.
(ii) N particles in $dim \geq 2$ dimensions; cartesian coordinates

$$g = \sum_{n=1}^{N} (x_n p_{y_n} - y_n p_{x_n}) = \left(\vec{L}\right)_z \tag{50}$$

$$\Rightarrow \delta x_n = \varepsilon \frac{\partial g}{\partial p_{x_n}} = -\varepsilon y_n; \delta y_n = \varepsilon \frac{\partial g}{\partial p_{y_n}} = \varepsilon x_n; \delta p_{x_n} = \varepsilon \frac{\partial g}{\partial x_n} = -\varepsilon p_{y_n}; \delta p_{y_n} = \varepsilon \frac{\partial g}{\partial y_n} = -\varepsilon p_{x_n} \tag{51}$$

Finite transformation: $\frac{\partial \bar{x}_n}{\partial \xi} = -\bar{y}_n; \frac{\partial \bar{y}_n}{\partial \xi} = \bar{x}_n$

$$\Rightarrow \frac{\partial^2 \bar{x}_n}{\partial \xi^2} = -\frac{\partial \bar{y}_n}{\partial \xi} = -\bar{x}_n \quad \Rightarrow \quad \bar{x}_n(\xi) = A_n \cos(\xi) + B_n \sin(\xi) \quad \wedge \quad \bar{y}_n(\xi) = C_n \cos(\xi) + D_n \sin(\xi)$$

$$\bar{x}_n(\xi = 0) = x_n \Rightarrow A_n = x_n; \quad \left.\frac{\partial \bar{x}_n}{\partial \xi}\right|_{\xi=0} = -y_n \Rightarrow B_n = -y_n, \quad C_n = y_n, \quad D_n = x_n$$

$$\Rightarrow \begin{pmatrix} \bar{x}_n \\ \bar{y}_n \end{pmatrix} = \underbrace{\begin{pmatrix} \cos(\xi) & -\sin(\xi) \\ \sin(\xi) & \cos(\xi) \end{pmatrix}}_{\text{Rotation matrix}} \begin{pmatrix} x_n \\ y_n \end{pmatrix} \tag{52}$$

$\Rightarrow g = L_z$ generates rotations around the z-axis!
(iii)

$$\underline{g = H} \tag{53}$$

Only works if H has no explicit time dependence

$$\{H, H\} = 0 \Rightarrow H \text{ is conserved: } \dot{H} = 0$$
$$\delta q_i = \varepsilon \frac{\partial H}{\partial p_i} = \varepsilon \dot{q}_i, \delta p_i = -\varepsilon \frac{\partial H}{\partial q_i} = \varepsilon \dot{p}_i : \text{ corresponds to time translation,}$$
$$t \to t + \varepsilon, \text{ for } (q_i(t), p_i(t)) \text{ forming trajectory. } H \text{ generates time translation!}$$

Canonical transformation & symmetries in quantum mechanics

Cannot simultanously determine (generalized) coordinate and (conjugated) momentum $\Rightarrow$ transformation (34), (45) cannot directly be applied to quantum mechanics. However, can define transformation such that (34) holds for expectation values! For infinitesimal transformation (45), demand:

$$\langle \hat{q}_i \rangle \to \langle \hat{q}_i \rangle + \varepsilon \langle \frac{\partial g}{\partial p_i}\Big|_{\text{observables}\to\text{operators}} \rangle ; \langle \hat{p}_i \rangle \to \langle \hat{p}_i \rangle - \varepsilon \langle \frac{\partial g}{\partial q_i}\Big|_{\text{observables}\to\text{operators}} \rangle \tag{54}$$

Def.: Expectation value $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$
Shift $\langle \hat{A} \rangle \to \langle \hat{A} \rangle + \delta_A$ can be obtained in two ways:

$$\underline{\text{Active transformation :}}\ \psi \to \psi_j = \psi + \delta_g \psi ; \hat{A} \to \hat{A} \tag{55}$$

Changes state vector: corresponds to changing phase space point in classical mechanics.

$$\underline{\text{Passive transformation :}}\ \psi \to \psi ; \hat{A} \to \hat{A} + \delta_g \hat{A} \tag{56}$$

leaves state unchanged, changes dependence of $\hat{A}$ on coordinates & momenta. Transformation $\psi \to \psi_g$ must be uniform, so that ψ_g is still normalized

$$\Rightarrow \psi_g = \hat{U}_g \psi, \text{ for some } \underline{\text{unitary}} \text{ operator } \hat{U}_g \left(\hat{U}^\dagger{}_g = \left(\hat{U}_g \right)^{-1} \right) \tag{57}$$

Implies:

$$\langle \psi | \hat{A} | \psi \rangle \to \langle \psi_g | \hat{A} | \psi_g \rangle \overset{57}{=} \langle \psi | \hat{U}^\dagger{}_g \hat{A} \hat{U}_g | \psi \rangle \tag{58}$$

$$\Rightarrow \text{ Passive transformation is given by } \hat{A} \to \hat{U}^\dagger{}_g \hat{A} \hat{U}_g \tag{59}$$

For infinitesimal transformation, write:

$$\hat{U}_g = 1 - \frac{i\varepsilon}{\hbar} \hat{G} \tag{60}$$

$$\Rightarrow \hat{U}^\dagger{}_g = 1 + \frac{i\varepsilon}{\hbar} \hat{G}^\dagger \Rightarrow \hat{U}_g \hat{U}^\dagger{}_g = 1 - \frac{i\varepsilon}{\hbar} \left(\hat{G} - \hat{G}^\dagger \right) + \mathcal{O}(\varepsilon^2) \overset{!}{=} 1$$
$$\Rightarrow \hat{G} = \hat{G}^\dagger \Rightarrow \hat{G} \text{ is hermitian!}$$

$$\text{Suggests } \hat{G} = \hat{g}, \text{ operator version of classical generator } g(q_i, p_i) \tag{61}$$

Check:

$$\langle \hat{q}_i \rangle = \langle \psi | \hat{q}_i | \psi \rangle \to \langle \psi_g | \hat{q}_i | \psi_g \rangle \overset{57,60,61}{=} \langle \psi | \left(1 + \frac{i\varepsilon}{\hbar}\hat{g}\right) \hat{q}_i | \left(1 - \frac{i\varepsilon}{\hbar}\hat{g}\right) \psi \rangle$$

$$= \langle \hat{q}_i \rangle + \frac{i\varepsilon}{\hbar} \langle \psi | [\hat{g}, \hat{q}_i] \psi \rangle + \underbrace{\cancel{\mathcal{O}(\varepsilon^2)}}_{\text{ignore}}$$

$$= \langle \hat{q}_i \rangle + \frac{i\varepsilon}{\hbar} i\hbar \langle \{g, q_i\} \Big|_{\text{observables}\to\text{operators}} \rangle$$

$$= \langle \hat{q}_i \rangle - \varepsilon \langle \sum_l \left(\frac{\partial g}{\partial q_l} \underbrace{\frac{\partial q_i}{\partial p_l}}_{\delta_{il}} - \frac{\partial g}{\partial p_l} \underbrace{\frac{\partial q_i}{\partial q_l}}_{\delta_{il}} \right) \Big|_{\text{observables}\to\text{operators}} \rangle = \langle \hat{q}_i \rangle + \varepsilon \langle \frac{\partial g}{\partial p_i} \Big|_{\text{observables}\to\text{operators}} \rangle$$

$$\langle \hat{p}_i \rangle \to \langle \hat{p}_i \rangle - \varepsilon \langle \{g, p_i\} \Big|_{\text{observables}\to\text{operators}} \rangle$$

$$= \langle \hat{p}_i \rangle - \varepsilon \langle \sum_l \left(\frac{\partial g}{\partial q_l} \underbrace{\frac{\partial p_i}{\partial p_l}}_{\delta_{il}} - 0 \right) \rangle = \langle \hat{p}_i \rangle - \varepsilon \langle \frac{\partial g}{\partial q_i} \Big|_{\text{observables}\to\text{operators}} \rangle$$

For a finite transformation:

$$(60), (61) \Rightarrow \hat{U}_g(\xi) = e^{-\frac{i\xi}{\hbar}\hat{g}} \tag{62}$$

✶ Reproduces (60), with $\hat{G} = \hat{g}$, for $\xi = \varepsilon$ with $|\varepsilon| << 1$
✶ For suitable ξ, write $\xi = N\varepsilon, |\varepsilon| << 1, N >> 1$: one finite transformation via $N >> 1$ tiny steps

$$\text{Use } \lim_{N\to\infty} \left(1 - \frac{z}{N}\right)^N = e^{-z} \forall z \in \mathbb{C} \tag{63}$$

Here needeed with $z = \frac{i\xi}{\hbar}\hat{g}$: is a operator, but commutes with itself: (63) works

[14.10.2024, Lecture 3]

[16.10.2024, Lecture 4]

Examples:
(i) $g = p_k$: generates shift in q_k, cf. (49)

$$\text{Expect } \hat{U}_g \psi(q_i) = \psi(q_1, \dots, q_k - \xi, \dots, q_N) = \psi_g(q_i) \tag{64}$$

$$\text{Since: } \psi_g(q_k + \xi) = \psi(q_k), \text{ check with (62) with } \hat{p}_k = -i\hbar \frac{\partial}{\partial q_k} \Rightarrow \hat{U}_g = e^{-\xi \frac{\partial}{\partial q_k}} \tag{65}$$

$$\hat{U}_g \psi(q_k) = \sum_{n=0}^{\infty} \frac{\left(-\xi \frac{\partial}{\partial q_k}\right)^n}{n!} \psi(q_k) = \psi(q_k) - \xi \frac{\partial \psi(q_k)}{\partial q_k} + \frac{1}{2}\xi^2 \frac{\partial^2 \psi(q_k)}{\partial q_k^2} + \dots$$

Is Taylor expansion of $\psi(q_k - \xi)$ aroung q_k

(ii) $g = L_z$: generates solutions around the z-axis
In spherical coordinates: $\hat{L}_z \overset{33}{=} -i\hbar \frac{\partial}{\partial \phi}$, is special case of (i), with

$$q_k = \phi : e^{-\frac{i\phi_0}{\hbar}\hat{L}_z} \psi(\phi) = \psi(\phi - \phi_0) \tag{66}$$

(iii) $g = \hat{H}$: time translation ($\hat{H}$ has no explicit time dependence); note: $\hat{H}\psi = +i\hbar \frac{\partial \psi}{\partial t}$

$$e^{-\frac{i}{\hbar}T\hat{H}} \psi(q_i, t) = \psi(q_i, t + T) \tag{67}$$

Note: Can use similar formalism also for regular canonical transformations that do not have an infinitesimal limit, e.g. parity: $\vec{x}_i \to -\vec{x}_i, \quad \vec{p}_i \to -\vec{p}_i$

Invariance: A system is invariant under some transformation generated by g, if $\langle \hat{H} \rangle$ is unchanged:

$$\langle \psi | \hat{H} | \psi \rangle = \langle \psi_g | \hat{H} | \psi_g \rangle \forall \psi \tag{68}$$

Since this must hold $\forall \psi$, it is a statement on $\hat{H}$. From (56,60,61):

$$\begin{aligned}\langle \psi_g | \hat{H} | \psi_g \rangle &= \langle \psi | (1 + \frac{i\epsilon}{\hbar}\hat{g}) \hat{H} (1 - \frac{i\epsilon}{\hbar}\hat{g}) | \psi \rangle \\ &= \langle \psi | \hat{H} | \psi \rangle + \frac{i\epsilon}{\hbar} \langle \psi | [\hat{g}, \hat{H}] | \psi \rangle \stackrel{!}{=} \langle \psi | \hat{H} | \psi \rangle \quad \forall \psi\end{aligned}$$

$$\Rightarrow [\hat{g}, \hat{H}] = 0 \quad \text{cf. (46)} \tag{69}$$

$$\text{Ehrenfest theorem then implies } \frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{g} \rangle = 0 : \tag{70}$$

analog of $\dot{g} = 0$ if $g, H = 0$.

Gauge invariance & Aharnov-Bohm effet

Classical electrodynamics can be formulated in terms of electric field $\vec{E}(\vec{x}, t)$ and magnetic field $\vec{B}(\vec{x}, t)$, which can be computed from the vector potential $\vec{A}(\vec{x}, t)$ and scalar potential $V(\vec{x}, t)$:

$$\vec{B} = \nabla \times \vec{A} \quad ; \quad \vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t} \tag{71}$$

Note: "Gauge transformation"

$$\vec{A}(\vec{x}, t) \to \vec{A}(\vec{x}, t) + \nabla \lambda(\vec{x}, t) \quad ; \quad V(\vec{x}, t) \to V(\vec{x}, t) - \frac{\partial \lambda(\vec{x}, t)}{\partial t} \tag{72}$$

leaves $\vec{E}$ and $\vec{B}$ unchanged, for a real function $\lambda(\vec{x}, t)$. Hence, the equations of motion of classical electromagnetism are gauge invariant.

In quantum mechanics (as opposed to quantum field theory): $\vec{E}, \vec{B}, \vec{A}, V$ are treated as classical fields. The interaction of a particle with extended fields is given by

$$\hat{H} = \underbrace{\frac{1}{2M} \left(\hat{\vec{P}} - q\vec{A} \right)^2}_{E_{kin}} + qV \tag{73}$$

M mass of particle, q its charge, $\hat{\vec{P}} = -i\hbar\nabla$ is the canonical momentum,

$$\vec{p} = M\dot{\vec{x}} + q\vec{A} \tag{74}$$

(73) is not gauge invariant. But the Schrödinger equation can be "gauge invariant", if, in addition to $\vec{A} \to \vec{A}'$, $V \to V'$, we also transform: $\psi \to \psi'$, so that

$$\hat{H}\psi(\vec{x}, t) = i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} \quad \text{should imply:} \quad \hat{H}'\psi'(\vec{x}, t) = i\hbar \frac{\partial \psi'(\vec{x}, t)}{\partial t}$$

The gauge-transformed wave function solves the Schrödinger equation with gauge-transformed Hamiltonian. Physics then remains gauge invariant: I can trade

$$(\vec{A}, V, \psi) \to (\vec{A}', V', \psi')$$

[16.10.2024, Lecture 4]

[21.10.2024, Lecture 5]

Want:

$$\hat{H}\psi(\vec{x}, t) = i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t}$$

implies

$$\hat{H}'\psi'(\vec{x},t) = i\hbar\frac{\partial\psi'(\vec{x},t)}{\partial t}$$

$$\frac{1}{2M}\left(-i\hbar\nabla - q\vec{A}\right)^2\psi + qV\psi = i\hbar\frac{\partial\psi}{\partial t} = \left(i\hbar\frac{\partial}{\partial t} - qV\right)\psi$$

Gauge transformation:

$$\frac{1}{2M}\left(-i\hbar\nabla - q\vec{A}'\right)^2\psi' = \left(i\hbar\frac{\partial}{\partial t} - qV'\right)\psi' \tag{75}$$

Suggestion:

$$\psi'(\vec{x},t) = e^{i\alpha(\vec{x},t)}\psi(\vec{x},t)$$

Unitary for real α, has one free function α, related to $\lambda(\vec{x},t)$.
Want:

$$\left(-i\hbar\nabla - q\vec{A} - q\nabla\lambda\right)^2 e^{i\alpha}\psi = e^{i\alpha}\left(-i\hbar\nabla - q\vec{A}\right)^2\psi \tag{76}$$

$$\text{and}\quad \left(i\hbar\frac{\partial}{\partial t} - qV + q\frac{\partial\lambda}{\partial t}\right)e^{i\alpha}\psi = e^{i\alpha}\left(i\hbar\frac{\partial}{\partial t} - qV\right)\psi \tag{77}$$

Since then (75) implies:

$$e^{i\alpha}\frac{1}{2M}\left(-i\hbar\nabla - q\vec{A}\right)^2\psi = e^{i\alpha}\left(i\hbar\frac{\partial}{\partial t} - qV\right)\psi \tag{78}$$

Is $e^{i\alpha}$ times the original Schrödinger equation. (77) holds if:

$$\left[-i\hbar\nabla - q\vec{A}, e^{i\alpha}\right]e^{i\alpha} = qe^{i\alpha}\nabla\lambda$$

$$\Rightarrow \left(-i\hbar\nabla - q\vec{A} - q\nabla\lambda\right)\left(-i\hbar\nabla - q\vec{A} - q\nabla\lambda\right)e^{i\alpha} = e^{i\alpha}\left(-i\hbar\nabla - q\vec{A}\right)^2 \quad \text{as needed for (78)}$$

Second equation (77):

$$\left(i\hbar\frac{\partial}{\partial t} - qV + q\frac{\partial\lambda}{\partial t}\right)e^{i\alpha}\psi = e^{i\alpha}\left(i\hbar\frac{\partial}{\partial t} - qV\right)\psi$$

implies

$$e^{i\alpha}\left(i\hbar\frac{\partial}{\partial t} - qV\right)\psi = e^{i\alpha}\left(i\hbar\frac{\partial}{\partial t} - \hbar\frac{\partial\alpha}{\partial t} - qV + q\frac{\partial\lambda}{\partial t}\right)\psi$$

$$\Rightarrow -\hbar\frac{\partial\alpha}{\partial t} + q\frac{\partial\lambda}{\partial t} \overset{!}{=} 0 \Leftrightarrow \alpha = \frac{q}{\hbar}\lambda \tag{79}$$

Check the first equation (77):

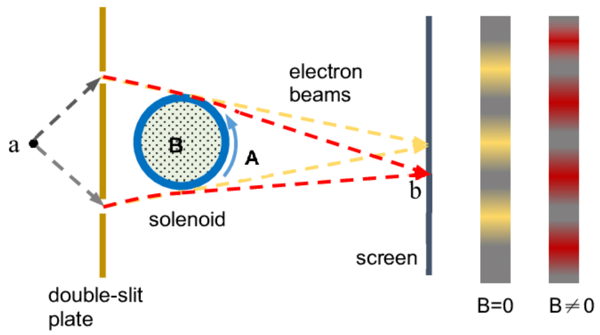
$$\left(-i\hbar\nabla - q\vec{A} - q\nabla\lambda\right)e^{i\alpha}\psi = e^{i\frac{q\lambda}{\hbar}}\left(-i\hbar\nabla - q\vec{A}\right)\psi$$

The equation holds as expected.
Altogether, gauge transformation in quantum mechanics:

$$\vec{A}(\vec{x},t) \to \vec{A}(\vec{x},t) + \nabla\lambda(\vec{x},t), \quad V(\vec{x},t) \to V(\vec{x},t) - \frac{\partial\lambda(\vec{x},t)}{\partial t}, \quad \psi(\vec{x},t) \to e^{\frac{iq}{\hbar}\lambda(\vec{x},t)}\psi(\vec{x},t) \tag{80}$$

Note: (last equation (80)) allows "local" phase transformations of all changed ψ (dependent on $\vec{x},t$), as opposed to "global" transformations $\psi \to e^{i\beta}\psi$ with constant $\beta \in \mathbb{R}$, if and only if simultaneously the potentials $\vec{A}$ and V are changed. In particular, a local phase transformation, starting with $\vec{A} = V = 0$, gives non-vanishing $\vec{A}, V$, but $\vec{E} = \vec{B} = 0$.

Local phase transformation can change interference patterns. "pure gauge" chaos of $\vec{A}, V$: (i.e. with



$\vec{E}, \vec{B} = 0$) can be physical!?

Aharnov-Bohm effect
(One view: "hole" in phase space; has non-trivial topology: "topological phase". If $\vec{A}$ is pure phase, it can be gauged away $\Rightarrow \oint \vec{A} d\vec{s}$ cannot be non zero.)

Near both classical paths $\vec{B} = 0$. Nevertheless the observed interference pattern can change when current in the coil is turned on.

$$\vec{B} = 0 \quad \text{for both paths} \quad \Rightarrow \nabla \times \vec{A} = 0 \quad \text{everywhere accessible}$$

$$\Rightarrow \exists \lambda \quad \text{such that: } \vec{A}(\vec{x}) = \nabla \lambda(\vec{x}) : \tag{81}$$

is pure gauge. Consider steady state $\Rightarrow$ no time dependence ($\Rightarrow V$ remains zero)

$$\Rightarrow \lambda(\vec{x}) = \int_{\vec{x}_0}^{\vec{x}} d\vec{s} \cdot \vec{A}(\vec{s}) \tag{82}$$

Is independent of path as long as $\nabla \times \vec{A} = 0$ everywhere along the path. Changing $\vec{x}_0$ does not change $\vec{x}$-dependence $\Rightarrow$ take $\vec{x}_0 = \vec{x}_s$ (location of source)

Let $\psi_{\substack{I\\II},0}(\vec{x}, t)$: The wave function along path I and II for $\vec{B} = 0$ in solenoid
$\psi_{\substack{I\\II}}(\vec{x}, t)$: The wave function along path I and II for $\vec{B} \neq 0$ in solenoid From (80):

$$\psi_I(\vec{x}, t) = e^{\frac{iq}{\hbar} \int_{\vec{x}_s}^{\vec{x}} d\vec{s}_I \cdot \vec{A}(\vec{s})} \psi_{I,0}(\vec{x}, t)$$
$$\psi_{II}(\vec{x}, t) = e^{\frac{iq}{\hbar} \int_{\vec{x}_s}^{\vec{x}} d\vec{s}_{II} \cdot \vec{A}(\vec{s})} \psi_{II,0}(\vec{x}, t)$$

Total wave function at detector:

$$\psi(\vec{x}_d) = \psi_I(\vec{x}) + \psi_{II}(\vec{x}) = e^{\frac{iq}{\hbar} \int_{\vec{x}_s}^{\vec{x}_d} d\vec{s}_I \cdot \vec{A}} \left[\psi_{I,0}(\vec{x}, t) + \psi_{II,0}(\vec{x}, t) e^{\frac{iq}{\hbar} \left(\int_{\vec{x}_s}^{\vec{x}_d} d\vec{s}_{II} \cdot \vec{A} - \int_{\vec{x}_s}^{\vec{x}_d} d\vec{s}_I \cdot \vec{A} \right)} \right]$$

$$\int_{\vec{x}_s}^{\vec{x}_d} d\vec{s}_{II} \cdot \vec{A}(\vec{s}) + \int_{\vec{x}_d}^{\vec{x}_s} d\vec{s}_I \cdot \vec{A}(\vec{s}) = \oint_{I+II} d\vec{s} \cdot \vec{A}(\vec{s}) \overset{Stokes}{=} \int_{\text{encl. area}} d\vec{a} \cdot \vec{B} = \Phi \quad \text{(magnetic flux)}$$

Thus,

$$\psi(\vec{x}_d) = e^{\frac{iq}{\hbar} \int_{\vec{x}_s}^{\vec{x}_d} d\vec{s}_I \cdot \vec{A}(\vec{s})} \left[\psi_{I,0}(\vec{x}_I) + \psi_{II,0}(\vec{x}_{II}) e^{\frac{iq\Phi}{\hbar}} \right] \tag{83}$$

The relative phase does matter, but interference pattern does not change if:

$$\frac{q\Phi}{\hbar} = 2\pi n \quad \Rightarrow \Phi = n\frac{h}{q} = n\Phi_0 \tag{84}$$

where Φ_0 is the flux quantum (for flux quantization in superconductors see Flux Quantization in Superconductors).

The path integral formulation of Quantum Mechanics

The Propagator

Any wave function $\psi(\vec{x},t)$ can be expanded (Postulate III):

$$\psi(\vec{x},t) = \sum_n u_n(t)\psi_n(\vec{x}), \text{ with } \hat{H}\psi_n(\vec{x}) = E_n\psi_n(\vec{x}) \tag{85}$$

Assumption: $\hat{H}$ has no explicit time dependence. If $\psi(\vec{x},t)$ is a solution of the Schrödinger equation.

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} \overset{85}{=} \sum_n i\hbar\frac{du_n(t)}{dt}\psi_n(\vec{x})$$

$$\hat{H}\psi(\vec{x},t) \overset{85}{=} \sum_n u_n(t)\hat{H}\psi_n(\vec{x}) = \sum_n u_n(t)E_n\psi_n(\vec{x})$$

$$\Rightarrow i\hbar\frac{\mathrm{d}u_n(t)}{\mathrm{d}t} = E_n u_n(t) \Rightarrow u_n(t) = u_n(t_0)e^{-iE_n(t-t_0)/\hbar} \tag{86}$$

$$u_n(t_0) = \int \mathrm{d}^3x'\psi_n^*(\vec{x}')\ \psi(\vec{x}',t_0)$$

$$\Rightarrow \psi(\vec{x},t) = \sum_n \int \mathrm{d}^3x'\ \psi_n^*(\vec{x}')\ \psi(\vec{x}',t_0)\ e^{-iE_n(t-t_0)/\hbar}\ \psi_n(\vec{x}) \tag{87}$$

Formally:

$$\underbrace{|\psi(t)\rangle}_{\text{state vector at } t} = \sum_n e^{-iE_n(t-t_0)/\hbar} \underbrace{|n\rangle\langle n|}_{\text{basis states}} \underbrace{\psi(t_0)\rangle}_{\text{state vector at } t_0} \tag{88}$$

The time evolution operator:

$$\hat{U}(t,t_0) = \sum_n e^{-iE_n(t-t_0)/\hbar}|n\rangle\langle n| \tag{89}$$

Evolves the state vector:

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \tag{90}$$

In coordinate space, the time evolution operator:

$$\hat{U}(\vec{x},t;\vec{x}',t_0) = \langle\vec{x}|\hat{U}(t,t_0)|\vec{x}'\rangle \overset{88}{=} \sum_n e^{-iE_n(t-t_0)/\hbar}\langle\vec{x}|n\rangle\langle n|\vec{x}'\rangle \tag{91}$$

$$= \sum_n e^{-iE_n(t-t_0)/\hbar}\psi_n(\vec{x})\psi_n^*(\vec{x}') \tag{92}$$

Thus, the wave function at time t:

$$\psi(\vec{x},t) = \int \mathrm{d}^3x'\ \hat{U}(\vec{x},t;\vec{x}',t_0)\ \psi(\vec{x}',t_0) \tag{93}$$

$\Rightarrow$ Any quantum mechanical problem can be solved if $\psi(t_0)$ and propagator $U(\vec{x},\vec{x}',t,t_0)$ are known!
Example: Propagator of free particle in 1 dimension. Use eigenfunctions of momentum, which are eigenfunctions of:

$$\hat{H} = \frac{p^2}{2m}, \quad E = \frac{p^2}{2m}$$

The propagator is:

$$U(x,x',t,t_0) = \int_{-\infty}^{\infty}\mathrm{d}p\ e^{\frac{-ip^2(t-t_0)}{2m\hbar}}\langle x|p\rangle\langle p|x'\rangle$$

$$= \int_{-\infty}^{\infty}\mathrm{d}p\ e^{\frac{-ip^2(t-t_0)}{2m\hbar}}\ \frac{e^{\frac{ipx}{\hbar}}}{\sqrt{2\pi\hbar}}\ \frac{e^{\frac{-ipx'}{\hbar}}}{\sqrt{2\pi\hbar}}$$

$$= \int_{-\infty}^{\infty}\mathrm{d}p\ e^{\frac{-ip^2(t-t_0)}{2m\hbar}}\ \frac{e^{\frac{ip(x-x')}{\hbar}}}{2\pi\hbar}$$

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}p\ \exp\left[-\frac{i}{\hbar}\left(\frac{p^2(t-t_0)}{2m}+p(x'-x)\right)\right]$$

Use:

$$\int_{-\infty}^{\infty}\mathrm{d}x\ e^{-ax^2+bx}=e^{\frac{b^2}{4a}}\sqrt{\frac{\pi}{a}}\quad ,\text{if } \Re(a)>0 \tag{94}$$

Here:

$$a=\frac{i(t-t_0)}{2m\hbar},\quad b=\frac{i(x-x')}{\hbar},\quad \frac{b^2}{4a}=\frac{i(x-x')^2m}{2\hbar(t-t_0)}$$

Thus:

$$U(x,x',t,t_0)=\sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}e^{\frac{i(x-x')^2m}{2\hbar(t-t_0)}} \tag{95}$$

[21.10.2024, Lecture 5]

[23.10.2024, Lecture 6]

Definition of path integral

Recipe:

* Consider all trajectories $x(t)$ (paths) that go from $x_0(t_0)$ to $x_N(t_N)$.
* For each path, compute the classical action:

$$S(x(t))=\int_{t_0}^{t_N}L(x(t),\dot{x}(t),t)\mathrm{d}t \tag{96}$$

  where $L(x(t),\dot{x}(t),t)$ is the Lagrangian.
* The propagator is obtained by integrating over all paths:

$$U(x_N,x_0,t_N,t_0)=A\int\mathcal{D}x(t)\ e^{\frac{i}{\hbar}S(x(t))} \tag{97}$$

  where A is a normalization constant.

It may appear that all paths contribute with equal weight. But most paths will average out via rapidly fluctuating exponential. Exception: paths near classical path, where the action is stationary. As a rough estimate, a path contributes if:

$$|S(x(t))-S(x_{\mathrm{cl}}(t))|\lesssim\pi\hbar$$

A path is an (infinite) collection of points, thus the path integral involves (infinitely many) integrals over these points.
The integral defining the action S is also discretized:

$$S=\sum_{i=1}^{N-1}L\left(x_i,\frac{x_{i+1}-x_i}{\varepsilon},t_i\right)\cdot\varepsilon \tag{98}$$

where $\frac{x_{i+1}-x_i}{\varepsilon}$ is the discrete version of $\dot{x}(t_i)$.

Propagator of a Free Particle:

$$U_{\mathrm{free}}(x_N,x_0,t_N,t_0)=A\lim_{N\to\infty,\ \varepsilon\to0}\int_{-\infty}^{\infty}\mathrm{d}x_1\cdots\int_{-\infty}^{\infty}\mathrm{d}x_{N-1}\exp\left[\frac{i}{\hbar}\frac{m}{2}\sum_{k=0}^{N-1}\frac{(x_{k+1}-x_k)^2}{\varepsilon}\right] \tag{99}$$

Let $y_k=\sqrt{\frac{m}{2\hbar\varepsilon}}\ x_k$.

$$U_{\mathrm{free}}(x_N,x_0,t_N,t_0)=A\lim_{N\to\infty,\ \varepsilon\to0}\left(\frac{2\hbar\varepsilon}{m}\right)^{\frac{N-1}{2}}\int_{-\infty}^{\infty}\mathrm{d}y_1\cdots\int_{-\infty}^{\infty}\mathrm{d}y_{N-1}\exp\left[\frac{i}{\hbar}\sum_{k=0}^{N-1}(y_{k+1}-y_k)^2\right] \tag{100}$$

To do the integral over y_1, we apply:

$$\int_{-\infty}^{\infty} \mathrm{d}y_1 \ \exp\left\{i\left[(y_1-y_0)^2+(y_2-y_1)^2\right]\right\} = \int_{-\infty}^{\infty} \mathrm{d}y_1 \ \exp\left\{i\left[2y_1^2-2y_1(y_0+y_2)+y_0^2+y_2^2\right]\right\}$$

Using the Gaussian integral formula:

$$\sqrt{\frac{i\pi}{2}} \ \exp\left\{i\left[y_0^2+y_2^2-\frac{1}{2}(y_2+y_0)^2\right]\right\} = \sqrt{\frac{i\pi}{2}} \ \exp\left[\frac{i(y_0-y_2)^2}{2}\right]$$

This indicates:

$$I_n = \int_{-\infty}^{\infty} \mathrm{d}y_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}y_n \ \exp\left[i\sum_{k=0}^{n}(y_{k+1}-y_k)^2\right] = \sqrt{\frac{(i\pi)^n}{n+1}} \exp\left[\frac{i(y_{n+1}-y_0)^2}{n+1}\right] \tag{101}$$

Proof by induction: Step $n-1 \to n$ (already proven for $n=1$):

$$I_n = \sqrt{\frac{(i\pi)^{n-1}}{n}} \int_{-\infty}^{\infty} \mathrm{d}y_n \ \exp\left[\frac{i(y_n-y_0)^2}{n}\right] \exp\left[i(y_{n+1}-y_n)^2\right]$$

This leads to:

$$I_n = \sqrt{\frac{(i\pi)^{n-1}}{n}} \int_{-\infty}^{\infty} \mathrm{d}y_n \ \exp\left\{i\left[y_n^2\left(1+\frac{1}{n}\right)-2y_n\left(\frac{y_0}{n}+y_{n+1}\right)+\frac{y_0^2}{n}+y_{n+1}^2\right]\right\}$$

Using (94) with $a=-i\left(n+\frac{1}{n}\right)$ and $b=-2i\left(\frac{y_0}{n}+y_{n+1}\right)$, we get:

$$I_n = \underbrace{\sqrt{\frac{(i\pi)^{n-1}}{n}} \cdot \sqrt{\frac{i\pi}{1+\frac{1}{n}}}}_{\sqrt{\frac{(i\pi)^n}{n+1}}} \cdot \exp\left\{i\left(\frac{y_0^2}{n}+y_{n+1}^2-\frac{1}{1+\frac{1}{n}}\left(\frac{y_0}{n}+y_{n+1}\right)^2\right)\right\}$$

where:

$$\frac{b^2}{4a} = \frac{1}{1+\frac{1}{n}}\left(\frac{y_0}{n}+y_{n+1}\right)^2$$

Expanding:

$$\frac{y_0^2}{n}\left(\frac{n}{n+1}\right)+\frac{y_{n+1}^2}{n+1}-\frac{2y_0y_{n+1}}{n+1}$$

Simplifying:

$$I_n = \sqrt{\frac{(i\pi)^n}{n+1}} \exp\left[\frac{i(y_0-y_{n+1})^2}{n+1}\right]$$

[23.10.2024, Lecture 6]

[28.10.2024, Lecture 7]

Hence:

$$\begin{aligned} U_{\mathrm{free}}(x_N,x_0,t_N,t_0) &= A \lim_{N\to\infty}\left(\frac{2\hbar\varepsilon}{m}\right)^{\frac{N-1}{2}} \cdot \frac{(i\pi)^{\frac{N-1}{2}}}{\sqrt{N}} \cdot e^{\frac{(x_N-x_0)^2}{N}} \\ &= A \lim_{\substack{N\to\infty \\ \varepsilon\to 0 \\ N\varepsilon=t_N-t_0}} \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{\frac{N}{2}} \cdot \underbrace{\sqrt{\frac{m}{2\pi i\hbar\varepsilon N}} \cdot e^{i\frac{m(x_N-x_0)^2}{2\hbar\varepsilon N}}}_{\overset{95}{=}U(x_N,x_0,t_n,t_0)} \end{aligned}$$

$$\to A = \lim N \underset{\varepsilon\to 0}{\to} \infty \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{-\frac{N}{2}} \equiv B^{-N}, \text{ with } B=\sqrt{\frac{2\pi i\hbar\varepsilon}{m}} \tag{102}$$

One B^{-1} per $\mathrm{d}x_k$ integral, one overall B^{-1}

$$\int \mathcal{D}x = \lim_{\substack{N\to\infty \\ \varepsilon\to 0 \\ N\varepsilon=t_N-t_0}} \frac{1}{B}\int_{-\infty}^{\infty}\frac{\mathrm{d}x_1}{B}\cdots\frac{\mathrm{d}x_{N-1}}{B} \tag{103}$$

Equivalence to Schrödinger

Prove that the propagator from the path integral reproduces the time evolution of the wave function according to the Schrödinger equation, for one infinitesimal time step:

$$\psi(x,t=\varepsilon)-\psi(x,0)\overset{Taylor}{=}\varepsilon\left.\frac{\partial\psi(x,t)}{\partial t}\right|_{t=0}+\mathcal{O}(\varepsilon^2) \tag{104}$$

$$=-i\frac{\varepsilon}{\hbar}\hat{H}\psi(x,0)=-i\frac{\varepsilon}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,0)\right)\psi(x,0) \tag{105}$$

Same result should follow from propagator:

$$\psi(x,\varepsilon)=\int_{-\infty}^{\infty}U(x,x',\varepsilon,0)\,\psi(x',0)\,\mathrm{d}x' \tag{106}$$

Propagation from path integral. Note: have single (infinitesimal) time step ⇒ no intermediate x_n or t_n:

$$U(x,x',\varepsilon,0)=\underbrace{\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{1/2}}_{1/B}\exp\left\{i\underbrace{\left[\frac{m(x'-x)^2}{2\varepsilon\hbar}-\frac{\varepsilon}{\hbar}V\left(\frac{x+x'}{2},0\right)\right]}_{\text{discretized action}}\right\} \tag{107}$$

Substitute (107) into (106):

$$\psi(x,\varepsilon)=\sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\int_{-\infty}^{\infty}\mathrm{d}x'\quad\underbrace{\exp\left[\frac{im(x-x')^2}{2\varepsilon\hbar}\right]}_{\text{oscillates quickly, unless } x\approx x'}\quad\exp\left[-i\frac{\varepsilon}{\hbar}V\left(\frac{x+x'}{2},0\right)\right]\psi(x',0) \tag{108}$$

$$\Rightarrow\ \text{need } |\eta|=|x-x'|\lesssim\sqrt{\frac{2\varepsilon\hbar\pi}{m}},\eta\text{ is }\mathcal{O}(\sqrt{\varepsilon})$$

Want to compute to first order in ε ⇒ need to expand to second order in η:

$$\psi(x',0)=\psi(x+\eta,0)=\psi(x,0)+\eta\frac{\partial\psi(x,0)}{\partial x}+\frac{1}{2}\eta^2\frac{\partial^2\psi(x,0)}{\partial x^2}+O(\eta^3)$$

$$\exp\left[-\frac{i\varepsilon}{\hbar}V\left(x+\frac{\eta}{2},0\right)\right]=1-\frac{i\varepsilon}{\hbar}\left[V(x,0)+\underbrace{\frac{\eta}{2}\frac{\partial V(x,0)}{\partial x}+\dots}_{\text{ignore}}\right]+\mathcal{O}(\varepsilon^2)$$

Substitute into (108):

$$\psi(x,\varepsilon)=\sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\int_{-\infty}^{\infty}\mathrm{d}\eta e^{\frac{im\eta^2}{2\varepsilon\hbar}}\left[\psi(x,0)+\cancelto{0}{\eta\frac{\partial\psi(x,0)}{\partial x}}+\frac{1}{2}\eta^2\frac{\partial^2\psi(x,0)}{\partial x^2}-\frac{i\varepsilon}{\hbar}V(x,0)\psi(x,0)\right]+\mathcal{O}(\varepsilon\eta,\varepsilon^2,\eta^3)$$

(94) with $a=-\frac{im}{2\varepsilon\hbar},b=0$; and $\int_{-\infty}^{\infty}\mathrm{d}x\,x^2e^{-ax^2}=\frac{1}{2}\sqrt{\frac{\pi}{a^3}}$

$$\Rightarrow\psi(x,\varepsilon)=\sqrt{\frac{m}{2\pi i\hbar\varepsilon}}\left\{\psi(x,0)\left(1-\frac{i\varepsilon}{\hbar}V(x,0)\right)\cdot\sqrt{\frac{2i\pi\varepsilon\hbar}{m}}+\frac{1}{4}\frac{\partial^2\psi(x,0)}{\partial x^2}\cdot\sqrt{\frac{8\pi\varepsilon^3\hbar^3i^3}{m^3}}\right\}$$

$$=\psi(x,0)-\frac{i\varepsilon}{\hbar}V(x,0)\psi(x,0)+\frac{\hbar\varepsilon i}{2m}\frac{\partial^2\psi(x,0)}{\partial x^2}:\quad\text{agrees with (105)}$$

Path Integral Treatment of Aharonov-Bohm Effect

$$S=\int_{t_s}^{t_d}L(t)\mathrm{d}t=\int_{t_s}^{t_d}\left(\frac{1}{2}m\dot{\vec{x}}^2+q\dot{\vec{x}}\cdot\vec{A}-qV\right)\mathrm{d}t \tag{109}$$

Gauge transformation:

$$\vec{A} \to \vec{A}_\lambda = \vec{A} + \nabla\lambda, \quad V \to V_\lambda = V - \frac{\partial\lambda}{\partial t} \tag{110}$$

$$S \to S_\lambda = S + \int_{t_s}^{t_d} \left(q\dot{\vec{x}} \cdot \nabla\lambda + q\frac{\partial\lambda}{\partial t} \right) \mathrm{d}t = S + q\int_{t_s}^{t_d} \frac{\mathrm{d}\lambda}{\mathrm{d}t}\mathrm{d}t \tag{111}$$

$$= S + [\lambda(\vec{x}_d, t_d) - \lambda(\vec{x}_s, t_s)]\, q \tag{112}$$

This does not change classical e.o.m., since in δS, $(\vec{x}_d, t_d)$ and $(\vec{x}_s, t_s)$ are fixed.
The change of action in Eq. (112) gives a change of the path-integral representation of the propagator: $U \sim e^{-\frac{S}{\hbar}}$

$$U(\vec{x}_d, \vec{x}_s, t_d, t_s) \to U_\lambda(\vec{x}_d, \vec{x}_s, t_d, t_s) = U(\vec{x}_d, \vec{x}_s, t_d, t_s) \cdot e^{\frac{iq}{\hbar}[\lambda(\vec{x}_d, t_d) - \lambda(\vec{x}_s, t_s)]} \tag{113}$$

Since

$$U(\vec{x}_d, \vec{x}_s, t_d, t_s) = \langle \vec{x}_d | U(t_d, t_s) | \vec{x}_s \rangle$$

(113) is equivalent to

$$|\vec{x}\rangle \to |\vec{x}\rangle_\lambda = e^{-\frac{iq\lambda(\vec{x},t)}{\hbar}} |\vec{x}\rangle \quad \text{new basis of coordinate state with phase}$$

Or

$$\psi(\vec{x}, t) = \langle \vec{x} | \psi(t) \rangle \to e^{\frac{iq\lambda(\vec{x},t)}{\hbar}} \psi(\vec{x}, t) \quad \text{agrees with (79)}$$

For the Aharonov-Bohm experiment: From (109), turning on $\vec{B} \neq 0$ inside the coil leaves $V, \dot{\vec{x}}$ unchanged, but does change $\vec{A}$.
Thus, the propagator, and hence the wavefunction, gains an extra phase factor.

$$\exp\left[\frac{iq}{\hbar}\int_{t_s}^{t_d} \dot{\vec{x}} \cdot \vec{A}\,\mathrm{d}t\right] = \exp\left[\frac{iq}{\hbar}\int_{\vec{x}_s}^{\vec{x}_d} \vec{A} \cdot \mathrm{d}\vec{x}\right], \quad \text{for a given path.}$$

$$\int_{\vec{x}_s}^{\vec{x}_d} \vec{A} \cdot \mathrm{d}\vec{x} \,\text{is independent of path, if it does not enter an area where}\, \nabla \times \vec{A} = \vec{B} \neq 0.$$

Therefore, for all paths I we get the same phase factor, as do all paths II, but these two paths differ, with

$$\int_{\vec{x}_s}^{\vec{x}_d} \vec{A} \cdot \mathrm{d}\vec{x}_I - \int_{\vec{x}_s}^{\vec{x}_d} \vec{A} \cdot \mathrm{d}\vec{x}_{II} = \oint \vec{A} \cdot \mathrm{d}\vec{x} = \Phi, \text{ as in (83)}$$

The Phase space path integral

Yields definition of path integral. Consider Hamiltonian

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{x}) \tag{114}$$

Has no explicit time dependence. Therefore:

$$\hat{U}(t, t_0) = e^{-i\frac{\hat{H}(t-t_0)}{\hbar}} \text{.c.f. (??)}$$

$$\Rightarrow U(x, x', t) = \langle x | e^{-i\frac{\hat{H}t}{\hbar}} | x' \rangle \tag{115}$$

Write

$$e^{-i\frac{\hat{H}t}{\hbar}} = \left[e^{-i\frac{\hat{H}\varepsilon}{\hbar}}\right]^N, t = N\varepsilon \tag{116}$$

Thus:

$$e^{-i\frac{\hat{H}\varepsilon}{\hbar}} = e^{-i\frac{\varepsilon}{\hbar}\left[\frac{\hat{P}^2}{2m} + V(\hat{x})\right]} = e^{-i\frac{\varepsilon}{\hbar}\frac{\hat{P}^2}{2m}} \cdot e^{-i\frac{\varepsilon}{\hbar}V(\hat{x})} \tag{117}$$

Since

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]} + \mathcal{O}([\hat{A},\hat{B}])$$

If $\hat{A},\hat{B}$ are both $\mathcal{O}(\varepsilon)$ the commutators are $\mathcal{O}(\varepsilon^2)$ at least: ignore!

$$U(x,x';t) = \langle x|\underbrace{e^{-\frac{i\varepsilon\hat{P}^2}{2m\hbar}}e^{-\frac{i\varepsilon V(\hat{x})}{\hbar}}}_{N \text{ factors}}\ldots|x'\rangle \tag{118}$$

Alternatively, using the completeness relation in coordinate space:

$$1 = \int_{-\infty}^{\infty} \mathrm{d}x|x\rangle\langle x| \tag{119}$$

And (modified) p-space:

$$1 = \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar}|p\rangle\langle p| \tag{120}$$

With

$$\langle x|p\rangle = e^{\frac{ipx}{\hbar}} \tag{121}$$

$$U(x,x',t) \overset{N=3}{=} \int \langle x|e^{-\frac{i\varepsilon\hat{P}^2}{2m\hbar}}|p_3\rangle\frac{\mathrm{d}p_3}{2\pi\hbar}\langle p_3|e^{-\frac{i\varepsilon V(\hat{x})}{\hbar}}|x_2\rangle dx_2\langle x_2|e^{-\frac{i\varepsilon\hat{P}^2}{2m\hbar}}|p_2\rangle\frac{\mathrm{d}p_2}{2\pi\hbar}$$
$$\langle p_2|e^{-\frac{i\varepsilon V(\hat{x})}{\hbar}}|x_1\rangle\mathrm{d}x_1\langle x_1|e^{-\frac{i\varepsilon\hat{P}^2}{2m\hbar}}|p_1\rangle\frac{\mathrm{d}p_1}{2\pi\hbar}\langle p_1|e^{-\frac{i\varepsilon V(\hat{x})}{\hbar}}|x'\rangle$$

For N steps, we have N integrals:

$$\int\frac{\mathrm{d}p_k}{2\pi\hbar} \quad \text{and} \quad N-1 \text{ integrals } \int \mathrm{d}x_k$$

Use

$$e^{-\frac{i\epsilon\hat{P}^2}{2m\hbar}}|p_k\rangle = |p_k\rangle e^{-\frac{i\epsilon p_k^2}{2m\hbar}} \tag{122}$$
$$e^{-\frac{i\epsilon V(\hat{x})}{\hbar}}|x_k\rangle = |x_k\rangle e^{-\frac{i\epsilon V(x_k)}{\hbar}} \tag{123}$$

Thus,

$$U(x,x',t) \underset{\substack{\lim_{N\to\infty}\\ N\epsilon=t}}{=} \int\prod_{K=1}^{N}\frac{\mathrm{d}p_K}{2\pi\hbar}\int\prod_{K=1}^{N-1}\mathrm{d}x_K e^{-\frac{i\varepsilon}{2m\hbar}\sum_{K=1}^N p_K^2}e^{-\frac{i\varepsilon}{\hbar}\sum_{K=1}^N V(x_{K-1})}\cdot e^{\frac{i}{\hbar}\sum_{K=1}^N p_K(x_K-x_{K-1})} \tag{124}$$

where $x \equiv x_N, x' \equiv x_0$
Exponent is quadratic in p_K, so <u>all</u> p_K integrals can be performed explicitly.

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Continuum limit:

$$\sum_{K=1}^N p_K(x_K - x_{K-1}) = \varepsilon\sum_{K=1}^N p(t_K)\frac{x(t_K)-x(t_{K-1})}{\varepsilon} = \varepsilon\sum_{K=1}^N p(t_K)\frac{x(t_K)-x(t_K-\varepsilon)}{\varepsilon} \underset{\substack{\varepsilon\to 0\\ N\to\infty}}{\to} \int_0^t \mathrm{d}t'\, p(t_K)\dot{x}(t_K)$$

$$U(x,x',t) = \int \underbrace{\tilde{\mathcal{D}}x}_{\text{no } \frac{1}{B} \text{ factors cf.103}} \underbrace{\tilde{\mathcal{D}}p}_{\frac{1}{2\pi\hbar} \text{ per integral}} e^{\frac{i}{\hbar}\int_0^t \mathrm{d}t'(p\dot{x}-H(x,p))} \tag{125}$$

Remarks:

- Integrand in exponential is Lagrange function, expressed in terms of x, p.
- (125) looks nicer, but is defined by (124).
- Re-establishes formal equivalence between coordinate and its conjugate momentum.
- Many different forms of path integral are possible by using different completeness relations in (119, 120).

Time-Dependent Perturbation Theory

Formalism

Consider Hamiltonian

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t), \tag{126}$$

where $\hat{H}_0$ is independent of time; assume eigenvalues and eigenfunctions of $\hat{H}_0$ are known.

$$\hat{H}_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \tag{127}$$

Perturbation $\hat{H}_1(t)$ does have time dependence. If $[\hat{H}_0, \hat{H}_1(t)] \neq 0$ for some t, $\hat{H}_1(t)$ can induce transitions between the $|n^{(0)}\rangle$: Let $|\psi(t_0)\rangle = |i^{(0)}\rangle$, then at $t > t_0$ there can be a non-vanishing probability to have $|\psi(t)\rangle = |f^{(0)}\rangle$, with $i \neq f$. We want to compute this probability. Note: Are only considering transitions between eigenstates of $\hat{H}_0$! Is relevant if either

- $\hat{H}_1(t) \ll \hat{H}_0 \forall t$: $\hat{H}_1$ is always a small perturbation, i.e. $\left|n^{(0)}\right\rangle$ are a good approximation of the eigenstates of $\hat{H}$.
- or, $\hat{H}_1(t) \to 0$ for both $t \to -\infty$ and $t \to +\infty$: prepare the system in $\left|i^{(0)}\right\rangle$ at $t \to -\infty$; switch on pertubation for finite time; observe the system at $t \to +\infty$.

For a more general case: consider $|\psi_f(t)\rangle = \sum_K c_K(t)\left|K^{(0)}\right\rangle$.
The problem can be tackled using the interaction picture propagator!

In the Schrödinger picture, we have:

$$|\psi_S(t)\rangle = \hat{U}_S(t, t_0)\,|\psi_S(t_0)\rangle \tag{128}$$

where $\hat{U}_S(t, t_0)$ is the time-evolution operator in the Schrödinger picture.
Differentiating with respect to time, we get:

$$i\hbar\frac{d}{dt}\,|\psi_S(t)\rangle \overset{\text{Schrödinger eq.}}{=} \hat{H}_S\,|\psi_S(t)\rangle$$

Thus with (128),

$$i\hbar\frac{\partial \hat{U}_S(t, t_0)}{\partial t}\,|\psi_S(t_0)\rangle = \hat{H}_S\hat{U}_S(t, t_0)\,|\psi_S(t_0)\rangle$$

for any initial state $|\psi_S(t_0)\rangle$.
Therefore, we have:

$$i\hbar\frac{\partial \hat{U}_S(t, t_0)}{\partial t} = \hat{H}_S\hat{U}_S(t, t_0) \tag{129}$$

Consider (129) with $\hat{H}_S = \hat{H}_{0,S}$, defining the unperturbed Schrödinger-picture propagator:

$$i\hbar\frac{\partial \hat{U}_S^{(0)}(t, t_0)}{\partial t} = \hat{H}_{0,S}\hat{U}_S^{(0)}(t, t_0) \Rightarrow \hat{U}_S^{(0)}(t, t_0) = e^{-i\hat{H}_{0,S}(t-t_0)/\hbar} \tag{130}$$

since $\hat{H}_0$ has no time dependence.
Define the interaction-picture state vector:

$$|\psi_I(t)\rangle = \left[\hat{U}_S^{(0)}(t, t_0)\right]^\dagger |\psi_S(t)\rangle \tag{131}$$

This inverse propagator implies that in the limit $\hat{H}_1 \to 0$, $|\psi_I(t)\rangle$ is independent of time!
At the same time:

$$\hat{O}_I(t) = \left[\hat{U}_S^{(0)}(t, t_0)\right]^\dagger \hat{O}_S(t)\hat{U}_S^{(0)}(t, t_0) \tag{132}$$

The operator can be time-dependent in the interaction picture, even if $\hat{O}_S$ is independent of time.
Expectation values are same in both pictures:

$$\langle \hat{O}_S(t)\rangle = \langle \psi_S(t)|\hat{O}_S(t)|\psi_S(t)\rangle \overset{131}{=} \langle \psi_I(t)|\underbrace{\left[\hat{U}_S^{(0)}(t,t_0)\right]^\dagger \hat{O}_S(t)\hat{U}_S^{(0)}(t,t_0)}_{\hat{O}_I(t)}|\psi_I(t)\rangle$$

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Taking the hermitian conjugate of (130) we get:

$$-i\hbar\frac{\partial}{\partial t}\left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger = \left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger \hat{H}_{0,S} \tag{133}$$

$$\Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_I(t)\rangle \overset{131}{=} i\hbar\left\{\frac{\partial}{\partial t}\left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger|\psi_S(t)\rangle + \left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger\frac{\partial}{\partial t}|\psi_S(t)\rangle\right\} \tag{134}$$

$$\overset{133}{=} \left\{\cancelto{0}{-\left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger \hat{H}_{0,S}} + \left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger\left(\cancelto{0}{\hat{H}_{0,S}} + \hat{H}_{1,S}\right)|\psi_S(t)\rangle\right\} \tag{135}$$

$$= \underbrace{\left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger \hat{H}_{1,S}(t)\hat{U}_S^{(0)}(t,t_0)}_{\hat{H}_{1,I}(t)}\underbrace{\left(\hat{U}_S^{(0)}(t,t_0)\right)^\dagger|\psi_S(t)\rangle}_{|\psi_I(t)\rangle} = \hat{H}_{1,I}(t)|\psi_I(t)\rangle \tag{136}$$

Definition: Interaction picture propagator satisfies

$$|\psi_I(t)\rangle = \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle \tag{137}$$

$$\Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_I(t)\rangle = i\hbar\frac{\partial \hat{U}_I(t,t_0)}{\partial t}|\psi_I(t_0)\rangle$$

Since

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_I(t)\rangle \overset{136}{=} \hat{H}_{1,I}(t)|\psi_I(t)\rangle$$

we have

$$\hat{H}_{1,I}(t)|\psi_I(t)\rangle \overset{137}{=} \hat{H}_{1,I}(t)\hat{U}_I(t,t_0)|\psi_I(t_0)\rangle$$

$\forall|\psi_I(t_0)$

$$i\hbar\frac{\partial \hat{U}_I(t,t_0)}{\partial t} = \hat{H}_I(t)\hat{U}_I(t,t_0) \tag{138}$$

$\hat{H}_{1,I}$ has explicit time dependence: $[\hat{H}_{1,I}(t_1), \hat{H}_{1,I}(t_2)] \neq 0$ in general

$$\Rightarrow \hat{U}_I(t,t_0) \neq e^{-i\hbar\hat{H}_{1,I}(t)(t-t_0)}$$

Formal solution of (138):

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}_{1,I}(t')\hat{U}_I(t',t_0)\,\mathrm{d}t' \tag{139}$$

Implicit solution: $\hat{U}_I$ appears on right hand side. But allows perturbative expansion in powers of $\hat{H}_{1,I}$.

Zeroth order: No $\hat{H}_{1,I}$ allowed. $\Rightarrow \hat{U}_I^{(0)}(t,t_0) = 1$ trivial.
If $\hat{H}_{1,I}(t) = 0$: $|\psi_I(t)\rangle$ does not depend on t.

First order: Insert zeroth order solution for U_I in r.h.s. of (139).

$$\hat{U}_I^{(1)}(t,t_0) = 1 - \frac{1}{i\hbar}\int_{t_0}^{t}\hat{H}_{1,I}(t')\,\mathrm{d}t' \tag{140}$$

Second order: Insert (140) in r.h.s. of (139).

$$\hat{U}_I^{(2)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} \hat{H}_{1,I}(t')\,\mathrm{d}t' + \left(-\frac{i}{\hbar}\right)^2 \underbrace{\int_{t_0}^{t}\mathrm{d}t' \int_{t_0}^{t'}\mathrm{d}t''\, \hat{H}_{1,I}(t')\hat{H}_{1,I}(t'')}_{\text{time-ordered product: later time} t'>t'' \text{ to the left}} \tag{141}$$

n-th order:

$$\begin{aligned}\hat{U}_I^{(n)}(t,t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\, \hat{H}_{1,I}(t') + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}t' \int_{t_0}^{t'}\mathrm{d}t''\, \hat{H}_{1,I}(t')\hat{H}_{1,I}(t'') + \dots \qquad (142)\\ &+ \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \dots \int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, \hat{H}_{1,I}(t_1)\hat{H}_{1,I}(t_2)\dots\hat{H}_{1,I}(t_n) \qquad (143)\end{aligned}$$

Recall: We want to compute transition probabilites between eigenstates of $\hat{H}_0$! For an unpertubated system: time-dependent states $|i_S^{(0)}(t)\rangle = e^{-iE_i^{(0)}(t-t_0)/\hbar}|i^{(0)}\rangle$, where $|i^{(0)}\rangle$ are the eigenstates of $\hat{H}_0$

$$\Rightarrow \text{ final state } \langle f_S^{(0)}(t)| = \langle f^{(0)}|e^{iE_f^{(0)}(t-t_0)/\hbar} \tag{144}$$

Transition probability from $|i_S^{(0)}(t_0)\rangle$ to $\langle f_S^{(0)}(t)|$ is:

$$\mathcal{P}_{i\to f}(t) = \left|\langle f_S^{(0)}(t)|i_S(t)\rangle\right|^2 \tag{145}$$

where $|i_S(t)\rangle$ is the state that was $|i^{(0)}\rangle$ at $t = t_0$.

$\Rightarrow$ Need $\langle f_S^{(0)}(t)|i_S(t)\rangle \overset{144}{\underset{128}{=}} \langle f^{(0)}|e^{iE_f^{(0)}(t-t_0)/\hbar}\hat{U}_S(t,t_0)|i^{(0)}\rangle$, where $\langle f^{(0)}|$ and $|i^{(0)}\rangle$ are time-independent basis states and $|i^{(0)}\rangle = |i_S^{(t_0)}\rangle = |i_I^{(0)}\rangle$

$$= \langle f^{(0)}|\underbrace{\left(\hat{U}_S^{(0)}\right)^\dagger(t,t_0)\hat{U}_S(t,t_0)}_{\hat{U}_I(t,t_0)}|i^{(0)}\rangle = \langle f^{(0)}|\hat{U}_I(t,t_0)|i^{(0)}\rangle \equiv \mathcal{A}_{fi} \tag{146}$$

Used:

$$\begin{aligned}|\psi_I(t)\rangle &\overset{137}{=} \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle \overset{131}{=} \hat{U}_I(t,t_0)|\psi_S(t_0)\rangle\\ \left(\hat{U}_S^{(0)}\right)^\dagger(t,t_0)|\psi_S(t)\rangle &\overset{128}{=} \left(\hat{U}_S^{(0)}\right)^\dagger(t,t_0)\hat{U}_S(t,t_0)|\psi_S(t_0)\rangle \quad \forall|\psi_S(t_0)\end{aligned}$$

(146) is exact. n-th order approximation for $\mathcal{A}_{fi}(t)$ results by using n-th order approximation for $\hat{U}_I$.
To 1^{st} order:

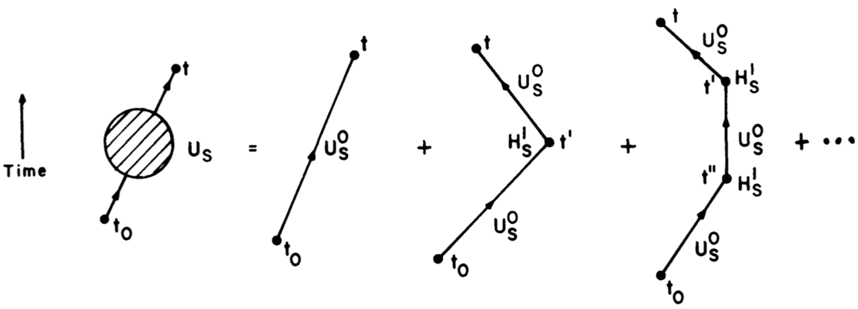
$$\begin{aligned}\mathcal{A}_{fi}^{(1)}(t) &= \langle f^{(0)}|\hat{U}_I^{(1)}(t,t_0)|i^{(0)}\rangle \qquad (147)\\ &= \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\langle f^{(0)}|\hat{H}_{1,I}(t')|i^{(0)}\rangle \qquad (148)\\ &= \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\, e^{i(E_f^{(0)}-E_i^{(0)})(t'-t_0)/\hbar}\langle f^{(0)}|\hat{H}_{1,S}|i^{(0)}\rangle \qquad (149)\\ \Rightarrow \mathcal{A}_{fi}^{(1)}(t) &= \delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\, e^{i\omega_{fi}(t'-t_0)}\langle f^{(0)}|\hat{H}_{1,S}|i^{(0)}\rangle, \quad \omega_{fi} = \frac{E_f^{(0)}-E_i^{(0)}}{\hbar} \qquad (150)\end{aligned}$$

Agrees with result from ansatz $|\psi(t)\rangle = \sum_n c_n(t)|n^{(0)}$
Multiply (143) with $\hat{U}_S^{(0)}(t,t_0)$ replace $\hat{H}_{1,I} \to \hat{H}_{1,S}$ everywhere gives the propagator in Schrödinger picture:

$$\begin{aligned}\hat{U}_S^{(0)}(t,t_0)\hat{U}_I^{(n)}(t,t_0) &= \hat{U}_S^{(n)}(t,t_0)\\ &= \hat{U}_S^{(0)}(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t}\hat{U}_S^{(0)}(t,t_0)\overbrace{\left[\hat{U}_S^{(0)}(t',t_0)\right]^\dagger \hat{H}_{1,S}(t')\hat{U}_S^{(0)}(t',t_0)}^{\hat{H}_{1,I}(t')}\mathrm{d}t'\\ &+ \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{U}_S^{(0)}(t,t_0)\left[\hat{U}_S^{(0)}(t',t_0)\right]^\dagger\hat{H}_{1,S}(t')\hat{U}_S^{(0)}(t',t_0)\\ &\cdot\left[\hat{U}_S^{(0)}(t'',t_0)\right]^\dagger\hat{H}_{1,S}(t'')U_S^{(0)}(t'',t_0) + \dots\end{aligned}$$

$$\hat{U} \text{ is unitary } \Rightarrow \left[\hat{U}(t,t_0)\right]^{\dagger} = \left[\hat{U}(t,t_0)\right]^{-1} = \hat{U}(t,t_0) \tag{151}$$
$$\text{Also: } \hat{U}(t_1,t_2)\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3) \tag{152}$$

$$\Rightarrow \hat{U}_S^{(n)}(t,t_0) = \hat{U}_S^{(0)}(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} \hat{U}_S^{(0)}(t,t')\hat{H}_{1,S}(t')\hat{U}_S^{(0)}(t',t_0)\,\mathrm{d}t' \tag{153}$$
$$+\cdots+\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{U}_S^{(0)}(t,t_1)\hat{H}_{1,S}(t_1)\hat{U}_S^{(0)}(t,t_2)\cdots \tag{154}$$
$$\hat{U}_S^{(0)}(t_{n-1},t_n)\hat{H}_{1,S}(t_n)\hat{U}_S^{(0)}(t_n,t_0) \tag{155}$$



Transition matrix element in *Schrödinger* picture:

$$\begin{aligned}\tilde{\mathcal{A}}_{fi}^{(1)}(t) &= \langle f^{(0)}|\hat{U}_S^{(1)}(t,t_0)|i^{(0)}\\ &= \delta_{fi}e^{-iE_f^{(0)}(t-t_0)/\hbar} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\langle f^{(0)}|\hat{U}_S^{(0)}(t,t')\hat{H}_{1,S}(t')\hat{U}_S^{(0)}(t',t_0)|i^{(0)}\rangle\end{aligned}$$

Use

$$\hat{U}_S^{(0)}(t_1,t_2)|\kappa^{(0)}\rangle = e^{-iE_\kappa^{(0)}(t_1-t_2)/\hbar}|\kappa^{(0)}\rangle;\quad \langle\kappa^{(0)}|\hat{U}_S^{(0)}(t_2,t_1) = \langle\kappa^{(0)}|e^{-iE_\kappa^{(0)}(t_2-t_1)/\hbar}$$

Hence

$$\begin{aligned}\tilde{\mathcal{A}}_{fi}^{(n)}(t) = e^{-iE_f^{(0)}(t-t_0)/\hbar}\cdot&\left\{\delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\langle f^{(0)}|\hat{H}_{1,S}(t')|i^{(0)}\rangle e^{\frac{i}{\hbar}\left[E_f^{(0)}(t'-t+t-t_0)-E_i^{(0)}(t'-t_0)\right]}\right\}\\ &+\left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,e^{-iE_f^{(0)}(t'-t_0)/\hbar}\langle f^{(0)}|\hat{H}_{1,S}(t')\hat{U}_S^{(0)}\sum_n|n^{(0)}\rangle\langle n^{(0)}|(t',t'')\\ &\cdot\hat{H}_{1,S}(t'')|i^{(0)}\rangle e^{-iE_i^{(0)}(t''-t_0)/\hbar}\end{aligned}$$

$$\Rightarrow \tilde{A}_{fi}(t) = e^{-iE_f^{(0)}(t-t_0)/\hbar}\left\{\delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\langle f^{(0)}|\hat{H}_{1,S}(t')|i^{(0)}\rangle e^{i\omega_{fi}(t'-t_0)}\right\} \tag{156}$$
$$+\left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\sum_n\langle f^{(0)}|\hat{H}_{1,S}(t')|n^{(0)}\rangle\langle n^{(0)}|\hat{H}_{1,S}(t'')|i^{(0)}\rangle \tag{157}$$
$$\cdot\exp\left\{\underbrace{\frac{i}{\hbar}\left(E_f^{(0)}-E_n^{(0)}\right)(t'-t_0)}_{i\omega_{fn}(t'-t_0)} + \underbrace{\frac{i}{\hbar}\left(E_n^{(0)}-E_i^{(0)}\right)(t''-t_0)}_{i\omega_{ni}(t''-t_0)}\right\}+\ldots \tag{158}$$

$$\omega_{fi} = \frac{E_f^{(0)}-E_i^{(0)}}{\hbar},\quad \omega_{fn} = \frac{E_f^{(0)}-E_n^{(0)}}{\hbar},\quad \omega_{ni} = \frac{E_n^{(0)}-E_i^{(0)}}{\hbar} \tag{159}$$

- 1^{st} order term: direct $i^{(0)} \to f^{(0)}$ transition
- 2^{nd}x order term: transition $i^{(0)} \to n^{(0)} \to f^{(0)}$

[04.11.2024, Lecture 9]

[06.11.2024, Lecture 10]

Applications

(i) Sudden Perturbation

A perturbation is sudden if its rise time

$$\delta t \ll \frac{1}{\omega_{fi}} \tag{160}$$

where $\frac{1}{\omega_{fi}}$ is the intrinsic time scale of the system.
This does not immediately change the state of the system: If change happens at $t = 0$:

$$|\psi(t = +\varepsilon/2)\rangle - |\psi(t = -\varepsilon/2)\rangle = -\frac{i}{\hbar} \underbrace{\int_{-\varepsilon/2}^{\varepsilon/2} \hat{H}(t')\,|\psi(t')\rangle\,\mathrm{d}t'}_{\underset{\varepsilon\to 0}{\to 0};\text{ if } \hat{H}(t') \text{ remains finite}} \tag{161}$$

Example: β^--decay of a nucleus $(A, Z) \to (A, Z+1) + e^- + \bar{\nu}_e$: Increase charge of nucleus by 1 unit. Emitted electron is relativistic:

$$v(e_{\text{emit}}) \simeq c;\; v(e_{\text{atom}}) \lesssim Z\alpha_{em}c, \quad \text{if } Z\alpha_{em} \ll 1:\; v(e_{\text{emit}}) \gg v(\text{eatom}), \quad \alpha_{em} \simeq \frac{1}{137}:\text{ fine structue constant}$$

The wave functions of bound electrons need time to adjust; they are in an excited state of the new atom. De-excitation mostly through photon emission (see **??**).

(ii) Adiabatic Perturbation

Change is so slow that the system is always in an eigenstate of $\hat{H}(t)$, if $|\psi(t_0)$ is eigenstate of $\hat{H}(t_0)$. In this sense: no transitions! For sufficiently slow time dependence we recover the time-independend pertubation theory, where sufficiently means that

$$\tau \gg \frac{1}{\omega_{\text{min}}} \tag{162}$$

$$\text{where } \tau \text{ is the time scale and } \omega_{\text{min}} = \frac{\Delta E_{\text{min}}}{\hbar} \tag{163}$$

and ΔE_{min} is the smallest relevant energy distance between states.
Let

$$\hat{H}(t) = \begin{cases} \hat{H}_0 + e^{t/\tau}\hat{H}_1, & -\infty < t \leq 0 \\ \hat{H}_0 + \hat{H}_1 \quad , & t > 0, \end{cases}$$

where $\hat{H}_1$ has no time dependence.
Insert into (150) (1^{st} order), $f \neq i$:

$$\begin{aligned} A_{fi}^{(1)}(t=0) &= -\frac{i}{\hbar}\int_{-\infty}^{0} \mathrm{d}t\, e^{i\omega_{fi}t} e^{t/\tau} \langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \\ &= -\frac{i}{\hbar}\frac{1}{\frac{1}{\tau} + i\omega_{fi}}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \underset{\tau \gg \frac{1}{\omega_{fi}}}{\to} -\frac{1}{\hbar\omega_{fi}}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \\ &= \frac{1}{E_i^{(0)} - E_f^{(0)}}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \equiv c_{fi} \end{aligned}$$

Reproduces result of time-independent perturbation theory for first-order change of wave function,

$$|\psi^{(1)}\rangle = |i^{(0)}\rangle + \sum_{f \neq i} c_{fi}|f^{(0)}\rangle$$

(iii) Periodic Perturbations: Fermi's Golden Rule

$$\hat{H}_1(t) = \hat{H}_1 e^{-i\omega t}\theta(t) \quad \text{(Should consider real part!)} \tag{164}$$

where $\hat{H}_1$ is constant and $\theta(t)$ is switched on at $t = 0$.
Insert into (158) (1^{st} order only), $f \neq i$:

$$A_{fi}^{(1)}(t) = -\frac{i}{\hbar}\int_0^t \mathrm{d}t' \underbrace{\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle}_{independend of time} e^{i(\omega_{fi}-\omega)t'} \tag{165}$$

$$= -\frac{i}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \frac{1}{i(\omega_{fi}-\omega)}\left[e^{i(\omega_{fi}-\omega)t} - 1\right]$$

$$\Rightarrow P_{fi}^{(1)}(t) = \frac{1}{\hbar^2}\left|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle\right|^2 \frac{1}{(\omega_{fi}-\omega)^2}\underbrace{\left[2 - \underbrace{e^{i(\omega_{fi}-\omega)t} - e^{-i(\omega_{fi}-\omega)t}}_{2\cos((\omega_{fi}-\omega)t)}\right]}_{4\sin^2\left(\frac{(\omega_{fi}-\omega)t}{2}\right)}$$

$$\Rightarrow P_{fi}^{(1)}(t) = \left|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle\right|^2 \frac{t^2}{\hbar^2}\left(\frac{\sin\left(\frac{(\omega_{fi}-\omega)t}{2}\right)}{\frac{(\omega_{fi}-\omega)t}{2}}\right)^2 \tag{166}$$

$\left(\frac{\sin x}{x}\right)^2$ is peaked at $x = 0$; width (1^{st} zero) at $x = \pi$
$\Rightarrow$ only states with $|\omega_{fi} - \omega| \lesssim \frac{2\pi}{t}$ are populated!

[06.11.2024, Lecture 10]

[11.11.2024, Lecture 11]

Peaks at $\omega = \omega_{fi}$; width:

$$|\omega_{fi} - \omega| \lesssim \frac{2\pi}{t} \tag{167}$$

required for sizable transition probability or

$$E_{fi}^{(0)} - E_i^{(0)} \in \left[\hbar\omega\left(1 - \frac{2\pi}{\omega t}\right), \hbar\omega\left(1 + \frac{2\pi}{\omega t}\right)\right]$$

something like energy-time uncertainty.
If t becomes large: go back to (165)

$$\begin{aligned}\mathcal{A}_{fi}(t) &= -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \int \mathrm{d}t' e^{i(\omega_{fi}-\omega)t'}, \text{ use } t'' = t' - \frac{t}{2} \\ &= -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \int_{-t/2}^{t/2} \mathrm{d}t'' e^{i(\omega_{fi}-\omega)\frac{t}{2}} e^{i(\omega_{fi}-\omega)t''} \\ &\underset{t\to\infty}{\to} -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle e^{i(\omega_{fi}-\omega)\frac{t}{2}} \cdot 2\pi\delta(\omega_{fi}-\omega)\end{aligned}$$

$$P_{fi}(t\to\infty) \to \left(\frac{2\pi}{\hbar}\right)^2 \left|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle\right|^2 \left[\delta(\omega_{fi}-\omega)\right]^2 \tag{168}$$

Square of δ-“fct”.

$$\left[\delta(\omega_{fi}-\omega)\right]^2 = \delta(\omega_{fi}-\omega)\cdot\frac{1}{2\pi}\lim_{T\to\infty}\int_{-T/2}^{T/2}\mathrm{d}t' e^{i(\omega_{fi}-\omega)t'} = \delta(\omega_{fi}-\omega)\cdot\lim_{T\to\infty}\frac{T}{2\pi} \tag{169}$$

where $(\omega_{fi}-\omega)t' = 0$ (from $1^{st}\delta$-“fct”)
Transition probability becomes very large as $T \to \infty$; however, transition <u>rate</u> ≡ transition probability per unit time remains small.

$$R_{fi}^{(1)} = \lim_{t\to\infty}\frac{P_{fi}^{(1)}(t)}{t} = \frac{2\pi}{\hbar^2}\left|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle\right|^2 \delta\left(\underbrace{\frac{E_f^{(0)} - E_i^{(0)}}{\hbar}}_{\omega_{fi}} - \omega\right), \quad \text{use } \delta(ax) = \frac{1}{a}\delta(x)$$

$$R_{fi}^{(1)} = \frac{2\pi}{\hbar}\left|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle\right|^2 \delta\left(E_f^{(0)} - E_i^{(0)} - \hbar\omega\right) \tag{170}$$

"Fermi's Golden Rule"

Remarks

* Applicable only after (∞) many oscillations of perturbation.
* To make $\hat{H}_1$ real (hermitian): we have to add a term with $\omega \to -\omega$.
  For $\omega > 0$: (170) describes absorption of energy by the system ($E_f^{(0)} > E_i^{(0)}$);
  term with $\omega \to -\omega$ describes (stimulated) emission, ($E_f^{(0)} < E_i^{(0)}$): not possible if system is initially in the ground state
* δ-fct in energy or ω needs to be "used up" by integration
  - → spectrum of pertubations: $\int \mathrm{d}\omega I(\omega)$, where I is the intensity
  - → introduce finite line width (intrinsic width; Doppler broadening; collisional broadening)
  - → integrate over continuum of final states (e.g. ionisation of atom)

Radiative transitions in atoms

Assume the infinite mass limit of the nucleus and a single electron (Hydrogen-like ion).

$$(72) \text{ with } q = -e : \hat{H}(\hat{\vec{x}}, t) = \frac{1}{2m_e}\left(\hat{\vec{P}} + e\vec{A}(\hat{\vec{x}}, t)\right) - eV(\hat{\vec{x}}) \tag{171}$$

Total electromagnetic field: static electric potential $V(\hat{\vec{x}})$ due to the nucleus, plus radiation field, for which we assume a monochromatic plane wave:

$$\vec{A}_{\text{rad}}(\vec{x}, t) = \underbrace{\vec{A}_0}_{const.} e^{i(\vec{k}\cdot\vec{x} - \omega t)} + \text{c.c.}; \quad V_{\text{rad}} = 0 \tag{172}$$

Electromagnetic radiation is transverse $\Rightarrow \vec{k}\cdot\vec{A}_0 \Rightarrow \nabla\cdot\vec{A}_{\text{rad}} = 0$

$$\Rightarrow [\hat{\vec{P}}, \vec{A}_{\text{rad}}] = [\hat{\vec{P}}, \vec{A}] = 0 \tag{173}$$

Recall:

$$\vec{B} = \vec{\nabla}\times\vec{A} \Rightarrow \vec{B}_{\text{rad}} = i\vec{k}\times\vec{A}_0 e^{i(\vec{k}\cdot\vec{x}-\omega t)} + \text{c.c.}$$
$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} \Rightarrow \vec{E}_{\text{rad}} = -i\omega\vec{A}_0 e^{i(\vec{k}\cdot\vec{x}-\omega t)} + \text{c.c.}$$

Propagating wave with velocity $c = \frac{\omega}{|\vec{k}|}$.

$\Rightarrow$ (Average) energy in electromagnetic radiation in volume V (SI units):

$$E = \frac{\varepsilon_0}{2}\int_V \mathrm{d}^3x \left(|\vec{E}|^2 + c^2|\vec{B}|^2\right) = \frac{\varepsilon_0}{2}|\vec{A}_0|^2 V[2\omega^2 + 2\underbrace{|\vec{k}|^2c^2}_{\omega^2}]$$

$$E = 2\varepsilon_0|\vec{A}_0|^2 V\omega^2 \stackrel{!}{=} N_\gamma\hbar\omega$$

where N_γ is the number of photons in the volume.

$$\Rightarrow |\vec{A}_0|^2 = \frac{N_\gamma\hbar}{2\varepsilon_0 V\omega} \tag{174}$$

$$\Rightarrow \vec{A}_{\text{rad}}^{(\text{abs})}(\vec{x}, t) = \sqrt{\frac{N_\gamma\hbar}{2\varepsilon_0 V\omega}}\,\vec{\varepsilon}\, e^{i(\vec{k}\cdot\vec{x}-\omega t)} \tag{175}$$

where $\vec{\varepsilon}$ is the polarization vector (unit vector).

To correct for the absorption of a photon; for emission we need $N_\gamma \to N_\gamma + 1$:

$$\vec{A}_{\text{rad}}^{(\text{em})} = \sqrt{\frac{(N_\gamma + 1)\hbar}{2\varepsilon_0 V\omega}}\,\vec{\varepsilon}\, e^{i(\vec{k}\cdot\vec{x}-\omega t)} \tag{176}$$

For spontaneous emission, $N_\gamma = 0$ in the initial state, from (171), (173), (176):

$$\hat{H}_1(\hat{\vec{x}}, t) = \frac{e}{M_e}\sqrt{\frac{\hbar}{2\varepsilon_0 V\omega}}\, e^{-i(\vec{k}\cdot\vec{x}-\omega t)}\, i\hbar\vec{\varepsilon}\cdot\vec{\nabla} \tag{177}$$

to leading order. Note: $\vec{A}^2$-term is second order in e!
$\Rightarrow$ Transition rate from (170):

$$R_{fi} = \frac{2\pi}{\hbar}\frac{e^2\hbar}{M_e^2}\frac{1}{2\varepsilon_0 V\omega}\left|\langle f|e^{-i\vec{k}\cdot\vec{x}}\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle\right|^2 \delta(E_f - E_i + \hbar\omega) \tag{178}$$

where $E_f = E_i - \hbar\omega$: emission.
Describe transition $|i\rangle \to |f, \gamma(\vec{k})\rangle$:

- $|i\rangle$: Atomic excited state
- $|f, \gamma(\vec{k})\rangle$: Atom in state $|f\rangle$ plus photon with wave vector $\vec{k}$

Two tasks remaining:

(i) Integrate over photon phase space to derive atomic total transition rate: gets rid of δ-"fct", $\frac{1}{V}$ factor

(ii) Evaluate atomic matrix element

(i) Phase space integration First, we need to count the number of photonic states with wave vectors between $\vec{k}$ and $\vec{k} + \mathrm{d}\vec{k}$. To that end, consider a cubical box of length L. Use periodic boundary conditions:

$$\vec{A}(x+L, y, z, t) = \vec{A}(x, y+L, z, t) = \vec{A}(x, y, z+L, t) = \vec{A}(x, y, z, t)$$

$$\underset{176}{\Rightarrow} e^{-ik_xL} = e^{-ik_yL} = e^{-ik_zL} = 1 \Rightarrow k_x = \frac{2\pi}{L}n_x, \quad k_y = \frac{2\pi}{L}n_y, \quad k_z = \frac{2\pi}{L}n_z$$

where $n_x, n_y, n_z \in \mathbb{Z}$.

$$\Rightarrow \mathrm{d}^3k = \mathrm{d}k_x\,\mathrm{d}k_y\,\mathrm{d}k_z = \left(\frac{2\pi}{L}\right)^3 \Delta n_x\,\Delta n_y\,\Delta n_z \tag{179}$$

$$\omega = |\vec{k}|c = \frac{2\pi c}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}$$

Total atomic transition rate obtained by summing over all possibilities for the photon:

$$\Gamma_{fi} = \sum_{n_x, n_y, n_z} R_{fi} \xrightarrow{L\to\infty} \int \mathrm{d}^3n\, R_{fi} \underset{179}{=} \left(\frac{L}{2\pi}\right)^3 \int \mathrm{d}^3k\, R_{fi} = V\int \frac{\mathrm{d}^3p_\gamma}{(2\pi\hbar)^3} R_{fi} \tag{180}$$

Used 3-momentum of photon:

$$\vec{p}_\gamma = \hbar\vec{k} \tag{181}$$

Use spherical coordinates:

$$\mathrm{d}^3p_\gamma = \mathrm{d}\Omega_\gamma |\vec{p}_\gamma|^2 \mathrm{d}|\vec{p}_\gamma| = \mathrm{d}\Omega_\gamma \left(\frac{\hbar\omega}{c}\right)^2 \mathrm{d}\left(\frac{\hbar\omega}{c}\right) \tag{182}$$

Substitute (182) and (178) in (180):

$$\begin{aligned}
\Gamma_{fi} &= V\frac{\pi e^2}{M_e^2\varepsilon_0 V}\hbar\int \frac{\mathrm{d}\Omega_\gamma}{(2\pi\hbar)^3}\frac{1}{c^3}\int \mathrm{d}(\hbar\omega)\,\delta(E_f - E_i - \hbar\omega)\,(\hbar\omega)^2\left|\langle f|e^{-i\vec{k}\cdot\vec{x}}\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle\right|^2 \\
&= \frac{e^2\hbar\omega_{if}}{\varepsilon_0 M_e^2}\frac{\hbar}{8\pi^2c^3}\int \mathrm{d}\Omega_\gamma \left|\langle f|e^{-i\vec{k}\cdot\vec{x}}\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle\right|^2 \\
\Rightarrow \Gamma_{fi} &= \frac{\alpha_{\mathrm{em}}}{2\pi}\omega_{fi}\int \mathrm{d}\Omega_\gamma \left|\frac{\hbar}{M_ec}\langle f|e^{-i\vec{k}\cdot\vec{x}}\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle\right|^2
\end{aligned}$$

where

$$\alpha_{\text{em}} = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137} \quad \text{(fine structure constant)}$$

Note: "phase space element"

$$d^3n = V\frac{\mathrm{d}^3p}{(2\pi\hbar)^3} \tag{183}$$

can be applied to any particle with a plane wave as wave function! But: relation between $|\vec{p}|$ (or $|\vec{k}|$) and energy (or ω) depends on the particle's mass.

(ii) Calculation of the matrix element
Need

$$\mathcal{M}_{fi} = \frac{\hbar}{M_e c}\langle f|e^{-i\vec{k}\cdot\vec{x}}\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle \tag{184}$$

with

$$|\vec{k}| = \frac{\omega}{c} = \frac{E_i - E_f}{\hbar c} \tag{185}$$

Order of magnitude: $|\vec{x}| \sim a_B$ (Bohr radius) $= \frac{\hbar}{Z\alpha M_e c}$, where Z is the charge of the nucleus.

$$E_i - E_f \sim \frac{1}{2}M_e c^2(Z\alpha)^2 \quad \text{(Rydberg energy)}$$

$$|\vec{k}||\vec{x}| \sim \frac{\frac{1}{2}(Z\alpha)^2 M_e c^2}{\hbar c}\frac{\hbar}{Z\alpha M_e c} = \frac{1}{2}Z\alpha \ll 1 \quad \left(\alpha = \frac{1}{137}\right)$$

$$\Rightarrow \text{to } 1^{st} \text{ approximation:} \quad e^{-i\vec{k}\cdot\vec{x}} = 1 \quad \text{("electric dipole transition")}$$

$$\Rightarrow \mathcal{M}_{fi} \simeq \frac{\hbar}{M_e c}\langle f|\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle = -\frac{i}{M_e c}\langle f|\vec{\varepsilon}\cdot\hat{\vec{P}}_e|i\rangle \tag{186}$$

where $\hat{\vec{P}}_e$ is the mom. of an electron.

[11.11.2024, Lecture 11]

[13.11.2024, Lecture 12]

Had:

$$\hat{H}_0 = \frac{\hat{\vec{P}}_e^2}{2M_e} - eV(\vec{x}_e) \quad \Rightarrow \quad [\hat{\vec{x}}_e, \hat{H}_0] = \frac{1}{2M_e}[\hat{\vec{x}}_e, \hat{\vec{P}}_e^2] \quad \text{(considering the } x\text{-component)}$$

(e stands for electron)

$$[\hat{x}_e, \hat{\vec{P}}_e^2] = [\hat{x}_e, \hat{P}_{x_e}^2 + \hat{P}_{y_e}^2 + \hat{P}_{z_e}^2] = [\hat{x}_e, \hat{P}_{x_e}^2] = \hat{x}_e\hat{P}_{x_e}\hat{P}_{x_e} - \hat{P}_{x_e}\hat{P}_{x_e}\hat{x}_e$$

$$= \left(\cancel{\hat{P}_{x_e}\hat{x}_e} + \underbrace{[\hat{x}_e, \hat{P}_{x_e}]}_{i\hbar}\right)\hat{P}_{x_e} - \hat{P}_{x_e}\left(\cancel{\hat{x}_e\hat{P}_{x_e}} + \underbrace{[\hat{P}_{x_e}, \hat{x}_e]}_{-i\hbar}\right) = 2i\hbar\hat{P}_{x_e}$$

$$\Rightarrow [\hat{\vec{x}}_e, \hat{H}_0] = i\frac{\hbar}{M_e}\hat{\vec{P}}_e \quad \Rightarrow \quad \hat{\vec{P}}_e = -iM_e\frac{[\hat{\vec{x}}_e, \hat{H}_0]}{\hbar} \tag{187}$$

$$\Rightarrow M_{fi} = \frac{-i}{M_e c}\left\langle f\left|\vec{\varepsilon}\cdot\left(\hat{\vec{x}}_e\hat{H}_0 - \hat{H}_0\hat{\vec{x}}_e\right)\right|i\right\rangle = -\frac{1}{\hbar c}(E_i - E_f)\left\langle f\left|\vec{\varepsilon}\cdot\hat{\vec{x}}_e\right|i\right\rangle$$

$$\Rightarrow M_{fi} = -\frac{\omega_{if}}{c}\left\langle f\left|\vec{\varepsilon}\cdot\hat{\vec{x}}_e\right|i\right\rangle \tag{188}$$

Selection rules:
Write

$$\vec{\varepsilon}\cdot\vec{x}_e = r_e\sum_{m=-1}^{1} c_m Y_{1m}(\theta,\varphi) \tag{189}$$

where c_m depends on $\vec{\varepsilon}$.
$\Rightarrow \vec{\varepsilon}\cdot\vec{x}_e$ has the same angular dependence as an $\ell = 1$ state.
Let ℓ_i be the angular momentum of the initial state. Then $\vec{\varepsilon}\cdot\vec{x}_e|i\rangle$ has the angular dependence of a state with $\ell_f = \ell_i - 1, \ell_i$, or $\ell_i + 1$.

$$\vec{x}_e \text{ has odd parity } \Rightarrow |f\rangle, |i\rangle \text{ must have opposite parity, otherwise } \langle f|\vec{x}_e|i\rangle = 0. \text{ (Includes } \int d^3x_e) \tag{190}$$

If state $|n\rangle$ has parity $(-1)^{\ell_n}$, then $|i\rangle, |f\rangle$ must have different ℓ.

$$\Rightarrow |\Delta\ell| = 1 \quad \text{for electric dipole transitions} \tag{191}$$

Similarly,

$$\Delta m \in \{-1, 0, 1\} \tag{192}$$

E.g.: $(2s)$-state cannot decay into $(1s)$ state; $(2p)\to(1s)$ is allowed. (189) and (192) hold only for electric dipole 1st order transitions. Transitions violating either rule are "forbidden". Higher order terms in expansion:

$$e^{-i\vec{k}\cdot\vec{x}} = 1 - i\cdot\underbrace{\vec{k}\cdot\vec{x}}_{\substack{\uparrow\\|\Delta\ell|,|\Delta m|\le 2}} - \frac{1}{2}\cdot\underbrace{(\vec{k}\cdot\vec{x})^2}_{\substack{\uparrow\\|\Delta\ell|,|\Delta m|\le 3}} + \ldots$$

where $\vec{k}$ is $\mathcal{O}\left(\frac{1}{2}Z\alpha_{\text{em}}\right)$.
Transitioning between $J = 0$ ($J \stackrel{?}{=} L\cdot S$) states are strictly forbidden in 1st order pertubation theory.
Reason: $\hat{H}_1$ is linear in $\vec{A}$, i.e. $\hat{H}_1 = \vec{A}\cdot\hat{\vec{v}}$ for some vector $\hat{\vec{v}}$. Since states with $J = 0$ have full spherical symmetry, the matrix element $\langle f|\hat{\vec{v}}|i\rangle$ must vanish for such states. These transitions are allowed in higher order in pertubation theory: contain more factors of $\vec{A}$, i.e. corresponds to emission or absorption of several photons.
Numerical estimate for allowed transitions:

$$\langle f|\vec{\varepsilon}\cdot\vec{x}_e|i\rangle \simeq a_B = \frac{\hbar}{Z\alpha_{\text{em}}M_e c}; \quad \omega_{if} \lesssim \frac{E_{\text{Ryd}}}{\hbar} = \frac{1}{2}\frac{M_e c^2 (Z\alpha_{\text{em}})^2}{\hbar}$$

$$\Rightarrow \Gamma_{fi} \approx \frac{\alpha_{\text{em}}}{2\pi}\cdot\left[\frac{1}{2}M_e c^2\left(\frac{Z\alpha_{\text{em}}}{\hbar}\right)^2\right]^3 \frac{\hbar^2}{(Z\alpha_{\text{em}}M_e c)^2} = \frac{1}{4}Z^4\alpha_{\text{em}}^5\frac{M_e c^2}{\hbar} \approx Z^4\cdot 4\times 10^9/\text{s}$$

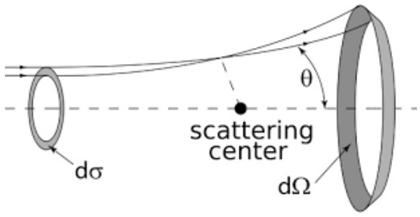
with $\hbar \approx 6.6\times 10^{-22}\,\text{MeV s}$ and $M_e c^2 = 0.511\,\text{MeV}$.

[13.11.2024, Lecture 12]

[18.11.2024, Lecture 13]

Scattering Theory

Problem: Beam of (parallel) particles impacts on "scattering center" finite region of space with potential $V(\vec{x}) \neq 0$. Place a detector far from scattering center at an angle to incoming beam. How many particles reach the detector?



Scattering center is static and scattering is elastic. Transverse diameter of beam $\gg$ extension of scattering center. Measuring the flux of scattered particles yields information about the structure of the scattering center. Examples: electron scattering on nuclei; neutron scattering on matter; etc.

Formalism

At the initial time t_0:

$$\psi_i(\vec{x}, t_0) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} a(\vec{k}) e^{i\vec{k}\cdot\vec{x}} \tag{193}$$

If $a(\vec{k})$ is peaked at $\vec{k} = \vec{k}_0$, the wave packet propagates with velocity:

$$\vec{v}_0 = \frac{\hbar\vec{k}_0}{m}$$

where m is the mass of the particle. Expand this in eigenstates of the <u>total</u> Hamiltonian, $\psi_{\vec{k}}(\vec{x})$, with:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\psi_{\vec{k}}(\vec{x}) = E_{\vec{k}}\psi_{\vec{k}}(\vec{x}) \tag{194}$$

$$E_{\vec{k}} = \frac{\hbar^2\vec{k}^2}{2m} \tag{195}$$

In terms of these:

$$\psi_i(\vec{x}, t_0) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \psi_{\vec{k}}(\vec{x}) A(\vec{k}) \tag{196}$$

$$\Rightarrow \text{ Full time-dependent: } \psi(\vec{x}, t) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \psi_{\vec{k}}(\vec{x}) A(\vec{k}) e^{-iE_{\vec{k}}(t-t_0)/\hbar} \tag{197}$$

Let's solve the time-dependent *Schrödinger* equation (194) using Green's function $G_+(\vec{x})$, where the + means outgoing.

$$\left[\nabla^2 + k^2\right] G_+(\vec{x}) = \delta^{(3)}(\vec{x}) \tag{198}$$

Thus, the formal solution:

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \frac{2m}{\hbar^2}\int \mathrm{d}^3x' G_+(\vec{x}-\vec{x}')V(\vec{x}')\psi_{\vec{k}}(\vec{x}') \tag{199}$$

Because:

$$\begin{aligned}
\left[\nabla^2 + k^2\right]\psi_{\vec{k}}(\vec{x}) &\overset{199}{=} \left[\nabla^2 + k^2\right] e^{i\vec{k}\cdot\vec{x}} + \frac{2m}{\hbar^2}\int \mathrm{d}^3x' \left[\nabla^2 + k^2\right] G_+(\vec{x}-\vec{x}')V(\vec{x}')\psi_{\vec{k}}(\vec{x}') \\
&\overset{198}{=} 0 + \frac{2m}{\hbar^2}\int \mathrm{d}^3x' \delta^{(3)}(\vec{x}-\vec{x}')V(\vec{x}')\psi_{\vec{k}}(\vec{x}') \\
&= \frac{2m}{\hbar^2}V(\vec{x})\psi_{\vec{k}}(\vec{x}).
\end{aligned}$$

Green's function via Fourier transform:

$$(198) \Rightarrow \frac{1}{(2\pi)^{3/2}}\int e^{-i\vec{q}\cdot\vec{x}}\left[\nabla^2 + k^2\right] G_+(\vec{x})\mathrm{d}^3x = \frac{1}{(2\pi)^{3/2}}\int e^{-i\vec{q}\cdot\vec{x}}\delta^{(3)}(\vec{x})\mathrm{d}^3x$$

$$\underset{\text{apply } \nabla^2 \text{ to the left (hermitian!)}}{\Rightarrow} \left(\vec{k}^2 - \vec{q}^2\right) \underbrace{\frac{1}{(2\pi)^{3/2}} \int e^{-i\vec{q}\cdot\vec{x}} G_+(\vec{x}) \mathrm{d}^3x}_{G_+(\vec{q})} = \frac{1}{(2\pi)^{3/2}}$$

$$\Rightarrow G_+(\vec{q}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\vec{k}^2 - \vec{q}^2} \tag{200}$$

Notes:
- $G_+(\vec{q})$ has a pole at $q^2 = k^2$, since $\nabla^2 + k^2$ has vanishing eigenvalues: <u>not</u> invertible!
- Fix: Let $k^2 \to k^2 + i\varepsilon$, with $\varepsilon \to 0$ (real, infinitesimal). This regularizes the integral.

Take $\varepsilon \to 0$ at the end. Hence, by inverse Fourier transform:

$$G_+(\vec{x}) = \frac{1}{(2\pi)^3} \int e^{i\vec{q}\cdot\vec{x}} \frac{1}{k^2 + i\varepsilon - q^2} \mathrm{d}^3q$$

Switching to spherical coordinates:

$$\begin{aligned} G_+(\vec{x}) &= \frac{1}{(2\pi)^3} \int e^{i|\vec{q}||\vec{x}|\cos\theta} \frac{1}{k^2 + i\varepsilon - |\vec{q}|^2} |\vec{q}|^2 \mathrm{d}|\vec{q}| \, \mathrm{d}\cos\theta \, \mathrm{d}\varphi \\ &= \frac{1}{(2\pi)^2} \int_0^\infty \frac{|\vec{q}|^2 \mathrm{d}|\vec{q}|}{k^2 + i\varepsilon - |\vec{q}|^2} \int_{-1}^{1} e^{i|\vec{q}||\vec{x}|\cos\theta} \mathrm{d}\cos\theta \end{aligned}$$

The angular integral evaluates to:

$$\int_{-1}^{1} e^{i|\vec{q}||\vec{x}|\cos\theta} \mathrm{d}\cos\theta = \frac{e^{i|\vec{q}||\vec{x}|} - e^{-i|\vec{q}||\vec{x}|}}{i|\vec{q}||\vec{x}|}.$$

Substituting:

$$G_+(\vec{x}) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{q^2 \mathrm{d}q}{iq|\vec{x}|} \frac{e^{iq|\vec{x}|}}{k^2 + i\varepsilon - |\vec{q}|^2}. \tag{201}$$

Now, use Cauchy's residue theorem for the complex integral:

$$\oint f(t)\mathrm{d}t = 2\pi i \sum \mathrm{Res}(f(z_e)), \tag{202}$$

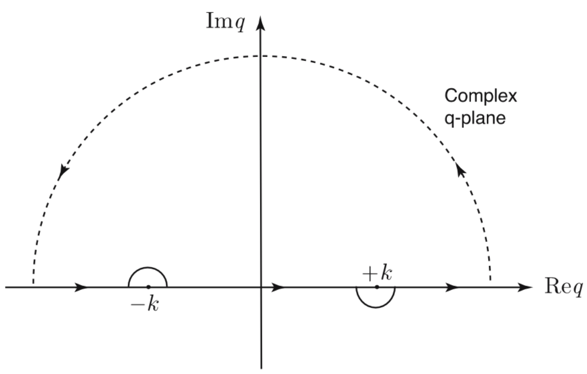
where z_e are the poles of $f(t)$. Let $f(t)$ be a complex function of $z \in \mathbb{C}$. If z_e is a pole, then:

$$\mathrm{Res}(f, z_e) = \lim_{z \to z_e} (z - z_e) f(z).$$

The equation:

$$\left(|\vec{k}|^2 + i\varepsilon - q^2\right) = \left(|\vec{k}| + i\eta + q\right)\left(|\vec{k}| + i\eta - q\right) \simeq \vec{k}^2 + 2i|\vec{k}|\eta - q^2,$$

where $\eta = \frac{\varepsilon}{2|\vec{k}|}$.



Poles are located at:

$$q = \pm|\vec{k}| \pm i\eta.$$

For large q, where $|q| \to \infty$, the integral vanishes, since:

$$\lim_{|q|\to\infty} e^{iq|\vec{x}|} \to 0.$$

The Green's function is given by:

$$\begin{aligned} G_+(\vec{x}) &= -\frac{i}{4\pi^2|\vec{x}|} \oint q\mathrm{d}q \frac{e^{iq|\vec{x}|}}{(|\vec{k}| + i\eta + q)(|\vec{k}| + i\eta - q)} \\ &= -\frac{i}{4\pi^2|\vec{x}|} \cdot 2\pi i \cdot \frac{e^{i|\vec{k}|\cdot|\vec{x}|}}{2|\vec{k}} \cdot (-1) \cdot |\vec{k}| \end{aligned}$$

$$G_+(\vec{x}) = -\frac{e^{i|\vec{k}||\vec{x}|}}{4\pi|\vec{x}|}. \tag{203}$$

Key Notes:

- No angular dependence, since $\nabla^2 + k^2$ doesn't have any either.
- The solution corresponds to an outgoing spherical wave.

Multiplying with the time-dependent term: $e^{-i\frac{E_k t}{\hbar}}$ leads to total phase: $\frac{E_k t}{\hbar} - |\vec{k}||\vec{x}|$, ensuring a positive time step. For $t \to t + \mathrm{d}t$, we require $|\vec{x}| \to |\vec{x}| + |\mathrm{d}\vec{x}|$ to keep the phase constant. $\varepsilon \to -\varepsilon$ gives incoming wave. Inserting (203) into (199):

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \frac{2m}{\hbar^2} \int \mathrm{d}^3x' \frac{e^{i|\vec{k}||\vec{x}-\vec{x}'|}}{4\pi|\vec{x} - \vec{x}'|} V(\vec{x}')\psi_k(\vec{x}'). \tag{204}$$

Let the origin lie inside the scattering center ($V(0) \neq 0$). We are interested in the wave function at $|\vec{x}| \gg |\vec{x}'|$, where:

$$\frac{1}{|\vec{x} - \vec{x}'|} \approx \frac{1}{|\vec{x}|} \quad \text{is sufficient.}$$

$$|\vec{k}||\vec{x} - \vec{x}'| = |\vec{k}|\sqrt{\vec{x}^2 + \vec{x}'^2 - 2\vec{x}\vec{x}'} \simeq |\vec{k}||\vec{x}|\left(1 - \frac{\vec{x}\cdot\vec{x}'}{|\vec{x}|^2}\right) \equiv |\vec{k}||\vec{x}| - \vec{k}'\vec{x}',$$

where $\hat{k}' = |\vec{k}|\frac{\vec{x}}{|\vec{x}|}$: points from scattering center to detector. For large distances $|\vec{x}| \to \infty$, we observe that:

$$\psi_k(\vec{x}) \underset{|\vec{x}|\to\infty}{\longrightarrow} e^{i\vec{k}\cdot\vec{x}} - \frac{e^{i|\vec{k}||\vec{x}|}}{4\pi|\vec{x}|}\frac{2m}{\hbar^2} \int \mathrm{d}^3x' e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}')\psi_{\vec{k}}(\vec{x}').$$

Alternatively, it can be written as:

$$\psi_{\vec{k}}(\vec{x}) \underset{|\vec{x}|\to\infty}{\longrightarrow} e^{i\vec{k}\cdot\vec{x}} + \frac{e^{i|\vec{k}||\vec{x}|}}{|\vec{x}|} f_{\vec{k}}(\theta, \varphi), \tag{205}$$

where:

$$f_k(\theta, \varphi) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}^3x' e^{-i|\vec{k}|\hat{x}\cdot\frac{\vec{x}\vec{x}'}{|\vec{x}|}} V(\vec{x}')\psi_{\vec{k}}(\vec{x}').$$

Here, $f_k(\theta, \varphi)$ is the scattering amplitude.
Remarks on $f_{\vec{k}}(\theta, \varphi)$
The scattering amplitude $f_{\vec{k}}(\theta, \varphi)$ does not depend on $|\vec{x}|$. The wave function $\psi_{\vec{k}}(\vec{x})$ is a sum of the incoming plane wave and an outgoing spherical wave modulated by $f_{\vec{k}}(\theta, \varphi)$.

- (205) works for short-range potentials: Assumes $|\vec{x}| \gg |\vec{x}'|$.
- Works for a wave packet (single-mode approximation) if:

  $$\delta_{\vec{k}} \frac{\partial f_{\vec{k}}}{\partial \vec{k}} \ll |f_{\vec{k}}|,$$

  where $\delta_{\vec{k}}$ is the width of the wave packet.

Differential and Total Scattering Cross Section

Definition: Differential cross section

$$\frac{\mathrm{d}\sigma(\theta,\varphi)}{\mathrm{d}\Omega}\underbrace{\mathrm{d}\Omega}_{=\mathrm{d}\varphi\mathrm{d}\cos\theta} = \frac{\text{number of particles scattered into d}\Omega\text{ per time}}{\text{incident flux of particles}} \tag{206}$$

Flux = $\frac{\#\text{ of particles}}{\text{time}\cdot\text{area}}$.
Total cross section:

$$\sigma_{\text{tot}} = \int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}(\cos\theta)\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}. \tag{207}$$

For a simple mode: (205)

$$\psi_{\vec{k}}(\vec{x})\xrightarrow[|\vec{x}|\to\infty]{} e^{i\vec{k}\cdot\vec{x}} + \frac{e^{i\vec{k}\cdot\vec{x}}}{|\vec{x}|}f_{\vec{k}}(\theta,\varphi).$$

Probabilty current (= number current, up to normalization):

$$\vec{J}_P = \frac{\hbar}{2m}\left[-i\psi^*\vec{\nabla}\psi + \text{h.c.}\right]. \tag{208}$$

where h.c. stands for hermitian conjugate. ψ is normalized to $\delta^{(3)}$, not to 1.

- incoming current:

$$\psi_{\text{in}} = e^{i\vec{k}\cdot\vec{x}} = \vec{J}_{P,\text{in}} = \frac{\hbar}{2m}\left(\vec{k}+\text{h.c.}\right) = \frac{\hbar\vec{k}}{m} = \vec{v}_{\text{gr}}. \tag{209}$$

- scattering current:

$$\psi_{\text{sc}} = \frac{e^{i|\vec{k}||\vec{x}|}}{|\vec{x}|}f_{\vec{k}}(\theta,\varphi);$$

  use spherical coordinates for $\vec{\nabla}$

$$\vec{\nabla} = \vec{e}_r\frac{\partial}{\partial r} + \underbrace{\vec{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \vec{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}}_{\xrightarrow[|\vec{x}|=r\to\infty]{}0}.$$

$$\begin{aligned}\vec{J}_{P,\text{sc}} \xrightarrow[r\to\infty]{} &\vec{e}_r\frac{\hbar}{2m}\left(-i\frac{e^{-i|\vec{k}|r}}{r}\frac{\partial}{\partial r}\frac{e^{i|\vec{k}|r}}{r}|f_{\vec{k}}|^2 + \text{h.c.}\right)\\ =&\vec{e}_r\frac{\hbar}{2m}\left(\left(\frac{|\vec{k}|}{r^2}+\frac{i}{r^3}\right)|f_{\vec{k}}|^2 + \text{h.c.}\right)\end{aligned}$$

$$\vec{J}_{P,\text{sc}} = \frac{\vec{e}_r}{r^2}\frac{\hbar|\vec{k}|}{m}|f_{\vec{k}}(\theta,\varphi)|^2.$$

Probabilty flow into $\mathrm{d}\Omega : R(\mathrm{d}\Omega) = \vec{J}_P\cdot\vec{e}_r r^2\mathrm{d}\Omega = \frac{\hbar|\vec{k}|}{m}|f_{\vec{k}}(\theta,\varphi)|^2\mathrm{d}\Omega$

$$\Rightarrow\quad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{R(\mathrm{d}\Omega)}{|\vec{J}_{\text{in}}|} = |f_{\vec{k}}(\theta,\varphi)|^2 \tag{210}$$

Modulation of outgoing spherical wave immediately gives the cross section!

[18.11.2024, Lecture 13]

[20.11.2024, Lecture 14]

The Born Approximation

Born approximation: Use the 0^{th} order result for $\psi_{\vec{k}}$ in the integral, i.e. keep only linear order in V when computing $f_{\vec{k}}$.

$$f_{\vec{k}}^{(\text{Born})}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int \mathrm{d}^3x' e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}'}V(\vec{x}'),\ \text{where } \vec{q} = \vec{k}' - \vec{k} \tag{211}$$

This is basically the Fourier transform of the scattering potential V.

$$|\vec{q}|^2 = |\vec{k}-\vec{k}'|^2 = k^2 + k'^2 - 2|\vec{k}||\vec{k}'|\cos\theta = 2|\vec{k}|^2(1-\cos\theta) = 4|\vec{k}|^2\sin^2\left(\frac{\theta}{2}\right) \tag{212}$$

where θ is the scattering angle.
If the potential has spherical symmetry, $V(\vec{x}') = V(|\vec{x}'|)$, we use spherical coordinates with the z'-axis aligned along $\vec{q}$.

$$f_{\vec{k}}^{(\text{Born})}(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int e^{-i|\vec{q}|r'\cos\theta'}V(r')\mathrm{d}\cos\theta'\mathrm{d}\varphi r'^2\mathrm{d}r' = -\frac{m}{\hbar^2}\int_0^\infty r'^2\mathrm{d}r'\frac{1}{-i|\vec{q}|r'}\underbrace{\left(e^{-i|\vec{q}|r'} - e^{i|\vec{q}|r'}\right)}_{-2i\sin(|\vec{q}r'|)}V(r')$$

Simplifying with spherical symmetry:

$$f_{\vec{k}}^{(\text{Born})}(\theta,\varphi) = -\frac{2m}{\hbar^2|\vec{q}|}\int_0^\infty r'\mathrm{d}r'\sin(|\vec{q}|r')V(r') \tag{213}$$

Remarks:

* To this order, the cross section does not depend on the sign of V. The same cross section is obtained for attractive and repulsive potentials (of given strength).
* The cross section does not depend on φ since there is only one relevant angle in the problem. This is no longer true if incoming particles are transversely polarized. In that case, a second direction is defined, leading to φ dependence.

Example: The Yukawa potential is given by:

$$V(r) = g\frac{e^{-\mu r}}{r}.$$

The scattering amplitude in the Born approximation is:

$$f_{\vec{k}}^{(\text{Born})}(\theta) = -\frac{2m}{|\vec{q}|\hbar^2}g\int_0^\infty r'\mathrm{d}r'\left(\frac{e^{i|\vec{q}|r'} - e^{-i|\vec{q}|r'}}{2i}\right)\frac{e^{-\mu r'}}{r}.$$

Simplifying further:

$$= \frac{img}{|\vec{q}|\hbar^2}\int_0^\infty \mathrm{d}r'\left(e^{r'(i|\vec{q}|-\mu)} - e^{-r'(i|\vec{q}|+\mu)}\right).$$
$$= \frac{img}{|\vec{q}|\hbar^2}\left[-\frac{1}{i|\vec{q}|-\mu} - \frac{1}{i|\vec{q}|+\mu}\right].$$

Simplifying further:

$$f_{\vec{k}}^{(\text{Born})}(\theta) = -\frac{2mg}{\hbar^2\left(|\vec{q}|^2+\mu^2\right)}$$

The differential cross-section is given by:

$$\frac{d\sigma^{(\text{Born})}}{d\Omega} = \frac{4m^2g^2}{\hbar^4\left(4|\vec{k}|^2\sin^2\frac{\theta}{2}+\mu^2\right)^2}. \tag{214}$$

Remarks

* As $\vec{k}^2\sin^2\frac{\theta}{2} \ll \mu^2$, the cross-section approaches a constant value:

$$\frac{4m^2g^2}{\hbar^4\mu^4}.$$

* For a fixed scattering angle θ, the differential cross-section $\frac{d\sigma}{d\Omega}$ drops as:

$$\frac{1}{|\vec{k}|^4}, \quad \text{for } |\vec{k}|^2 \gg \frac{\mu}{\sin^2\frac{\theta}{2}}.$$

Reason: The drop in the differential cross-section for large $|\vec{k}|$ is due to many oscillations within the effective range $r_0 = \frac{1}{\mu}$, leading to large cancellations in the integral (213).
If we take $\mu \to 0$, we obtain the Coulomb scattering case with:

$$g = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0},$$

where Z_1, Z_2 are the charges of the particles.
The differential cross-section in the Born approximation becomes:

$$\left(\frac{d\sigma^{(\text{Born})}_{\text{Coulomb}}}{d\Omega}\right) = \frac{m^2c^2}{4|\vec{k}|^4\sin^4\frac{\theta}{2}\hbar^2}\underbrace{\left(\frac{Z_1Z_2e^2}{4\pi\epsilon_0\hbar c}\right)^2}_{(Z_1Z_2\alpha_{\text{em}})^2} = \frac{c^2\hbar^2Z_1^2Z_2^2(\alpha_{\text{em}})^2}{16E^2\sin^4\frac{\theta}{2}}. \tag{215}$$

where E is the energy of the incoming particle:

$$E = \frac{\hbar^2|\vec{k}|^2}{2m}.$$

<u>Remarks:</u>

* The cross-section becomes badly divergent as $\theta \to 0$. Recall:

$$\int \mathrm{d}\cos\theta = \int \sin\theta\,\mathrm{d}\theta \underset{\theta\ll 1}{\simeq} \int \theta\mathrm{d}\theta$$

Thus:

$$\Rightarrow \sigma_{\text{tot}} \sim \int \frac{d\theta}{\theta^3}.$$

* Strictly speaking, this formalism is not applicable when the potential has infinite range. However, the result is still correct.

* $\theta \to 0$ implies $|\vec{q}| \to 0$: probe large r' ($e^{i|\vec{q}|r'} \simeq 1$ out to large r). At some point, likely gets shielded (e.g. by electrons in the atom).

* Was used by Rutherford to prove the existence of "pointlike" nuclei.

[20.11.2024, Lecture 14]

[25.11.2024, Lecture 15]

Partial Wave Expansion

For spherically symmetric potential, $V(\vec{x}) = V(|\vec{x}|) \Rightarrow f_{\vec{k}}(\theta,\phi)$ has <u>no</u> ϕ dependence

$$\Rightarrow f_{\vec{k}}(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)a_\ell(|\vec{k}|)P_\ell(\cos\theta) \tag{216}$$

where P_ℓ is the Legendre Polynomial:

$$P_\ell = \sqrt{\frac{4\pi}{2\ell+1}}\cdot Y_{\ell 0}(\theta).$$

$a_\ell(|\vec{k}|)$: ℓ-th partial wave amplitude; $(2\ell+1)$: convention. Examples:

- $\ell = 0$: S-wave
- $\ell = 1$: P-wave

- $\ell = 2$: D-wave
- $\ell = 3$: F-wave, etc.

For incident plane wave, for $\vec{k} = (0, 0, |\vec{k}|)$ (in $+z$-direction).

$$e^{i\vec{k}\cdot\vec{x}} = e^{i|\vec{k}||\vec{x}|\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) j_\ell(|\vec{k}||\vec{x}|) P_\ell(\cos\theta) \tag{217}$$

$j_\ell(z)$: spherical Bessel functions:

$$j_\ell(z) = (-z)^\ell \left(\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^\ell \frac{\sin z}{z} \tag{218}$$

$$j_0(t) = \frac{\sin t}{t}, \quad j_1(t) = \frac{\sin t}{t^2} - \frac{\cos t}{t}, \quad j_2(t) = \left(\frac{3}{t^2} - 1\right)\frac{\sin t}{t} - \frac{3\cos t}{t^2}, \dots \tag{219}$$

Recursively, $j_\ell(t) = \left(1 - t\frac{1}{t}\frac{d}{dt}\right) j_{\ell-1}(t)$. Asymptotically:

$$j_\ell(z) \xrightarrow{z\to\infty} \frac{\sin\left(z - \ell\frac{\pi}{2}\right)}{z} \tag{220}$$

Recall:

$$\sin\left(z - \frac{\pi}{2}\right) = -\cos z, \quad \sin(z - \pi) = -\sin z, \quad \sin\left(z - \frac{3\pi}{2}\right) = \cos z.$$

(216) trades out $f_{\vec{k}}(\theta)$ of two continuous variables $(|\vec{k}|, \theta)$.
For an infinite (discrete) sum (over ℓ) of functions of one variable $|\vec{k}|$.
It is useful at low $|\vec{k}|$, since then only a few ℓ-values contribute;
Semi-classically, $\hbar|\vec{k}|r_0 \simeq \hbar\ell_{\max}$

$$\implies \ell \lesssim |\vec{k}|r_0, \text{ where } r_0 \text{ is the range of } V \tag{221}$$

Asymptotically: (220) in (217):

$$e^{i\vec{k}\cdot\vec{x}} \xrightarrow{|\vec{x}|\to\infty} \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) \frac{\sin(|\vec{k}||\vec{x}| - \ell\pi/2)}{|\vec{k}||\vec{x}|} P_\ell(\cos\theta)$$

$$e^{i\vec{k}\cdot\vec{x}} \xrightarrow{|\vec{x}|\to\infty} \frac{1}{2i|\vec{k}|} \sum_{\ell=0}^{\infty} \Bigg(\underbrace{e^{i\frac{\pi}{2}}}_{\ell}\Bigg)^\ell (2\ell+1) \frac{e^{i(|\vec{k}||\vec{x}|-\ell\pi/2)} - e^{-i(|\vec{k}||\vec{x}|-\ell\pi/2)}}{|\vec{x}|} P_\ell(\cos\theta) \tag{222}$$

$$= \frac{1}{2i|\vec{k}|} \sum_{\ell=0}^{\infty} (2\ell+1) \frac{e^{i(|\vec{k}||\vec{x}|)} - e^{-i(|\vec{k}||\vec{x}|-\ell\pi)}}{|\vec{x}|} P_\ell(\cos\theta) \tag{223}$$

Is the sum of outgoing (1st term) and incoming (2nd term) spherical waves, with equal amplitudes (up to sign),
$\Rightarrow$ no net scattering, as expected for plane waves!
Asymptotically, the total wave function (with $V \neq 0$) must also be a free-particle solution, possible with phase shift and free normalization:

$$\psi_{\vec{k}}(\vec{x}) \xrightarrow{|\vec{x}|\to\infty} \sum_{\ell=0}^{\infty} A_\ell P_\ell(\cos\theta) \frac{e^{i(|\vec{k}||\vec{x}|-\ell\pi/2+\delta_\ell)} - e^{-i(|\vec{k}||\vec{x}|-\ell\pi/2+\delta_\ell)}}{|\vec{x}|} \tag{224}$$

Scattered part only contains <u>outgoing</u> spherical wave $\Rightarrow$ incoming spherical wave, 2nd term in (224), must be entirely due to plane wave: must agree with 2^{nd} term in (223).

$$\Rightarrow A_\ell e^{-i(\delta_\ell - \ell\pi/2)} = \frac{2\ell+1}{2i|\vec{k}|} e^{i\ell\pi} \Rightarrow A_\ell = \frac{2\ell+1}{2i|\vec{k}|} e^{i(\frac{\delta_\ell}{2}+\delta_\ell)} \tag{225}$$

Must hold for each ℓ separately, since the $P_\ell(\cos\theta)$ are linearly independent.

$$(225) \text{ in } (224): \psi_{\vec{k}}(\vec{x}) \xrightarrow{|\vec{x}|\to\infty} \frac{1}{2i|\vec{k}||\vec{x}|}\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\left[e^{i|\vec{k}||\vec{x}|}e^{2i\delta_\ell} - e^{-i|\vec{k}||\vec{x}|}e^{i\ell\pi}\right]$$
$$= e^{i\vec{k}\cdot\vec{x}} + \frac{1}{2i|\vec{k}||\vec{x}|}\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\left[e^{i|\vec{k}||\vec{x}|}e^{2i\delta_\ell} - e^{-i|\vec{k}||\vec{x}|}\right]$$

$$\Rightarrow \psi_{\vec{k}}(\vec{x}) \xrightarrow{|\vec{x}|\to\infty} e^{i\vec{k}\cdot\vec{x}} + \frac{e^{i|\vec{k}||\vec{x}|}}{|\vec{x}|}\underbrace{\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\frac{e^{2i\delta_\ell}-1}{2i|\vec{k}|}}_{f_{\vec{k}}(\theta)} \tag{226}$$

$$\Rightarrow a_\ell(|\vec{k}|) = \frac{e^{2i\delta_\ell(|\vec{k}|)}-1}{2i|\vec{k}|} \tag{227}$$

Establish 1-to-1 correspondence between partial wave amplitude $a_\ell \in \mathbb{C}$ and scattering phase $\delta_\ell \in \mathbb{R}$.
<u>Relation to the Cross Section</u>

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\theta} \equiv 2\pi\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \overset{211}{=} 2\pi|f_{\vec{k}}(\theta)|^2 \tag{228}$$
$$\overset{216}{=} 2\pi\left|\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)a_\ell(|\vec{k}|)\right|^2 \tag{229}$$
$$= 2\pi\sum_{\ell,\ell'=0}^{\infty}(2\ell+1)(2\ell'+1)\underbrace{P_\ell(\cos\theta)P_{\ell'}(\cos\theta)}_{\in\mathbb{R}}a_\ell(|\vec{k}|)a^*_{\ell'}(|\vec{k}|). \tag{230}$$

Different partial waves interfere ($\ell \neq \ell'$ contributes) in the differential cross section:

$$\sigma_{\text{tot}} = \int_{-1}^{1}\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\theta}\mathrm{d}\cos\theta \overset{230}{=} 2\pi\sum_{\ell,\ell'=0}^{\infty}(2\ell+1)(2\ell'+1)a_\ell(|\vec{k}|)a^*_{\ell'}(|\vec{k}|) - \underbrace{\int_{-1}^{1}\mathrm{d}\cos\theta\, P_\ell(\cos\theta)P_{\ell'}(\cos\theta)}_{\frac{2}{2\ell+1}\delta_{\ell\ell'}}$$

$$\Rightarrow \sigma_{\text{tot}} = 4\pi\sum_{\ell=0}^{\infty}(2\ell+1)|a_\ell(|\vec{k}|)|^2 \tag{231}$$

<u>No</u> interference between different partial waves! From (227): $a_\ell(|\vec{k}|) = \frac{e^{2i\delta_\ell}-1}{2i|\vec{k}|} = \frac{e^{i\delta_\ell}}{|\vec{k}|}\frac{e^{i\delta_\ell}-e^{-i\delta_\ell}}{2i}$

$$\Rightarrow a_\ell(|\vec{k}|) = \frac{e^{i\delta_\ell}}{|\vec{k}|}\sin\delta_\ell \tag{232}$$

The total cross-section is given by

$$\sigma_{\text{tot}} = \frac{4\pi}{|\vec{k}|^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell \tag{233}$$

The relation (232) implies the unitarity bound:

$$|a_\ell(|\vec{k}|)| \leq \frac{1}{|\vec{k}|} \tag{234}$$

Remark: The unitarity bound reflects the fact that there cannot be more scattered particles than incoming ones!
Incoming flux cf. (207):

$$(232) \text{ in } (216) f_{\vec{k}}(\theta) = \frac{1}{|\vec{k}|}\sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)e^{i\delta_\ell}\sin\delta_\ell$$

Using $P_\ell(1) = 1$:

$$\operatorname{Im} f_{\vec{k}}(\theta) = \frac{1}{|\vec{k}|}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

Therefore, the total cross-section is given by:

$$\sigma_{\text{tot}}(|\vec{k}|) = \frac{4\pi}{|\vec{k}|} \operatorname{Im} f_{\vec{k}}(\theta), \qquad \text{“optical theorem”} \tag{235}$$

The optical theorem also holds in the presence of inelastic scattering, provided σ_{tot} includes the sum over all channels ($\rightarrow$ Quantum Field Theory, QFT).
Relation to perturbation theory
From equation (232), if $|a_\ell|$ is small, δ_ℓ should also be small, $|\delta_\ell| \ll 1$: Using the approximation:

$$\Rightarrow e^{2i\delta_\ell} \simeq 1 + 2i\delta_\ell \underset{227}{\Rightarrow} a_\ell(|\vec{k}|) \simeq \frac{\delta_\ell}{|\vec{k}|}$$

Note that δ_ℓ can be of either sign.

Bound States and Resonances

Consider a 3-dimensional, spherically symmetric potential well:

$$V(\vec{x}) = V(|\vec{x}|) = \begin{cases} -V_0, & |\vec{x}| \le r_0 \\ 0, & |\vec{x}| > r_0 \end{cases}, \quad V_0 > 0 \tag{236}$$

Spherical symmetry implies $\hat{\vec{L}}^2$ and $\hat{L}_z$ are conserved quantities. Therefore, the eigenstates of the Hamiltonian $\hat{H}$ can be written as:

$$\psi_{|\vec{k}|}(\vec{x}) = Y_{\ell m}(\theta, \varphi) R_\ell(\underbrace{r}_{=|\vec{x}|}) \tag{237}$$

The Schrödinger equation for the radial part becomes:

$$-\frac{\hbar^2}{2M}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell(\ell+1)}{r^2}\right] R_\ell(r) + V(r) R_\ell(r) = E R_\ell(r)$$

Here, $\frac{\ell(\ell+1)}{r^2}$ arises from the $\vec{L}^2$ operator acting on $Y_{\ell m}$.
Since V is piecewise constant, we write:

$$|\vec{k}| = \frac{1}{\hbar}\sqrt{2M(E-V)} \quad \Rightarrow \quad E = \frac{\hbar^2 |\vec{k}|^2}{2M} + V \tag{238}$$

(237) then becomes:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\ell(\ell+1)}{r^2} + |\vec{k}|^2\right] R_\ell(r) = 0 \tag{239}$$

Note: The value of $|\vec{k}|$ is different for $r > r_0$ and $r < r_0$!
Introducing a dimensionless variable:

$$\rho = |\vec{k}| r \quad \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}r} = |\vec{k}|\frac{\mathrm{d}}{\mathrm{d}\rho}; \quad \frac{1}{r} = \frac{|\vec{k}|}{\rho}$$

Substituting into the Schrödinger equation:

$$\left[|\vec{k}|^2 \frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{2|\vec{k}|}{\rho}|\vec{k}|\frac{\mathrm{d}}{\mathrm{d}\rho} - |\vec{k}|^2\frac{\ell(\ell+1)}{\rho^2} + |\vec{k}|^2\right] R_\ell(\rho) = 0$$

Divide through by $|\vec{k}|^2$, and simplify:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{2}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{\ell(\ell+1)}{\rho^2} + 1\right] R_\ell(\rho) = 0 \tag{240}$$

[25.11.2024, Lecture 15]

[27.11.2024, Lecture 16]

Let $\underline{\ell = 0}$, and $f = \rho R_0$. Then:

$$\frac{\mathrm{d}f}{\mathrm{d}\rho} = R_0 + \rho\frac{\mathrm{d}R_0}{\mathrm{d}\rho}$$
$$\frac{\mathrm{d}^2 f}{\mathrm{d}\rho^2} = 2\frac{\mathrm{d}R_0}{\mathrm{d}\rho} + \rho\frac{\mathrm{d}^2 R_0}{\mathrm{d}\rho^2} \overset{240}{=} -\rho R_0 = -f$$
$$\Rightarrow f = A\cos\rho + B\sin\rho$$

Thus, there are two linearly independent solutions for $R_0(\rho)$:

→ **singular solution**:

$$R_0^{(s)} = -\frac{\cos\rho}{\rho} \quad : \text{diverges as } \rho \to 0 \tag{241}$$

→ **Regular solution**:

$$R_0^{(r)} = \frac{\sin\rho}{\rho} \tag{242}$$

For $\underline{\ell > 0}$, we write:

$$R_\ell(\rho) = \rho^\ell f_\ell(\rho)$$
$$\Rightarrow \frac{\mathrm{d}R}{\mathrm{d}\rho} = \ell\rho^{\ell-1} f_\ell + \rho^\ell f_\ell', \frac{\mathrm{d}^2 R_\ell}{\mathrm{d}\rho^2} = \ell(\ell-1)\rho^{\ell-2} f_\ell + 2\ell\rho^{\ell-1} f_\ell' + \rho^\ell f_\ell''$$

Substituting these into (240), we obtain:

$$\rho^\ell f_\ell'' + \cancel{\ell(\ell-1)\rho^{\ell-2}} f_\ell + 2\ell\rho^{\ell-1} f_\ell' + \cancel{\frac{2\ell\rho^{\ell-1} f_\ell}{\rho}} + \frac{2\rho^\ell f_\ell'}{\rho} - \cancel{\ell(\ell+1)\rho^{\ell-2}} f_\ell + \rho^\ell f_\ell = 0$$

Simplify terms:

$$f_\ell'' + \frac{2\ell+1}{\rho} f_\ell' + f_\ell = 0 \tag{243}$$

Using the ansatz:

$$f_\ell = \frac{1}{\rho} f_{\ell-1}' \tag{244}$$

Taking derivatives:

$$f_\ell' = \frac{1}{\rho} f_{\ell-1}'' - \frac{1}{\rho^2} f_{\ell-1}', \qquad f_\ell'' = \frac{1}{\rho} f_{\ell-1}''' - \frac{2}{\rho^2} f_{\ell-1}'' + \frac{2}{\rho^3} f_{\ell-1}'$$

$$\begin{aligned}\Rightarrow f_\ell'' + \frac{2(\ell+1)}{\rho} f_\ell' + f_\ell &= \frac{1}{\rho} f_{\ell-1}''' - \frac{2}{\rho^2} f_{\ell-1}'' + \frac{2}{\rho^3} f_{\ell-1}' + \frac{2(\ell+1)}{\rho}\left(\frac{1}{\rho} f_{\ell-1}'' - \frac{1}{\rho^2} f_{\ell-1}'\right) + \frac{1}{\rho} f_{\ell-1}' \\ &= \frac{1}{\rho}\left[f_{\ell-1}''' + \frac{2\ell}{\rho} f_{\ell-1}'' - \frac{2\ell}{\rho^2} f_{\ell-1}'' + f_{\ell-1}'\right] = \frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\underbrace{\left[f_{\ell-1}'' + \frac{2\ell}{\rho} f_{\ell-1}' + f_{\ell-1}\right]}_{=\,0,\ \text{is } (\ell-1) \text{ of } (244)}\end{aligned}$$

$$f_\ell(\rho) = \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell R_0(\rho) \tag{245}$$

Here, R_0 is one of the solutions from (243)
The regular solution is related to spherical Bessel functions:

$$R_\ell^{(r)}(\rho) = (-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \left(\frac{\sin\rho}{\rho}\right) = j_\ell(\rho) \tag{246}$$

Singular solution: spherical Neumann functions:

$$R_\ell^{(s)}(\rho) = -(-\rho)^\ell \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^\ell \frac{\cos\rho}{\rho} \equiv n_\ell(\rho) \tag{247}$$

Asymptotically:

$$R_\ell^{(s)}(\rho) \xrightarrow{\rho\to 0} -\frac{\cos(\rho - \ell\pi/2)}{\rho}, \quad \text{cf. (220).} \tag{248}$$

The solution can also be expressed in terms of spherical Hankel functions:

$$h_\ell^{(1)}(\rho) = j_\ell(\rho) + i n_\ell(\rho), \quad h_\ell^{(2)}(\rho) = (h_\ell^{(1)}(\rho))^* \tag{249}$$

$$\begin{aligned} j_\ell(\rho) &= \frac{1}{2}\left[h_\ell^{(1)}(\rho) + h_\ell^{(2)}(\rho)\right] = \mathrm{Re}\ h_\ell^{(1)}(\rho) \\ n_\ell(\rho) &= \frac{1}{2i}\left[h_\ell^{(1)}(\rho) - h_\ell^{(2)}(\rho)\right] = \mathrm{Im}\ h_\ell^{(1)}(\rho) \end{aligned}$$

Asymptotically:

$$h_\ell^{(1)}(\rho) \xrightarrow{\rho\to\infty} -\frac{i}{\rho} e^{i(\rho - \ell\frac{\pi}{2})} \tag{250}$$

<u>Bound States</u> Conditions for bound states:
Need $-V_0 \le E \le 0$
For $r > r_0$, $|\vec{K}| \to i\kappa$ is imaginary!
For $r < r_0$, need <u>regular</u> solution only, since $r = 0$ is allowed. The radial wavefunction $R_\ell(r)$ is defined as:

$$R_\ell(r) = \begin{cases} A j_\ell(qr), & r \le r_0 \\ B h_\ell^{(1)}(i\kappa r), & r \ge r_0 \end{cases}$$

where:

$$q = \sqrt{2M(V_0 + E)}/\hbar, \quad \kappa = \sqrt{-2ME}/\hbar$$

For $r \to \infty$, the solution $h_\ell^{(1)} \sim e^{-\rho r}$, solution $\sim h_\ell^{(2)} \sim e^{\rho r}$: not normalizable!
Continuity conditions: 1. Continuity of the wavefunction:

$$A_\ell j_\ell(q r_0) = B_\ell h_\ell^{(1)}(i\kappa r_0) \tag{251}$$

2. Continuity of the derivative:

$$q A_\ell \frac{\mathrm{d}j_\ell(qr)}{\mathrm{d}r}\bigg|_{r=r_0} = i\kappa B_\ell \frac{\mathrm{d}h_\ell^{(1)}(i\kappa r)}{\mathrm{d}r}\bigg|_{r=r_0} \tag{252}$$

Dividing the two equations gives:

$$q\frac{\mathrm{d}\ln j_\ell(\rho)}{\mathrm{d}\rho}\bigg|_{\rho=qr_0} = i\kappa \frac{\mathrm{d}\ln h_\ell^{(1)}(\rho)}{\mathrm{d}\rho}\bigg|_{\rho=i\kappa r_0} \tag{253}$$

(253) fixes E!

[27.11.2024, Lecture 16]

[02.12.2024, Lecture 17]

<u>$\ell = 0$:</u>
Write:

$$u_0(r) = r R_0(r) = \begin{cases} A_0 \sin(qr), & r \le r_0 \\ B_0 e^{-\kappa r}, & r \ge r_0 \end{cases}$$

where the parameters must satisfy the continuity conditions:

$$u_0 \text{ and } u_0' \text{ must be continuous at } r = r_0.$$

$$\left.\begin{aligned} A_0 \sin(qr_0) &= B_0 e^{-\kappa r_0} \\ A_0 q \cos(qr_0) &= -B_0 \kappa e^{-\kappa r_0} \end{aligned}\right\} \Rightarrow q \cot(qr_0) = -\kappa$$

Substituting $\kappa = \sqrt{\frac{2M}{\hbar^2}(V_0 - E)}$:

$$\cot(qr_0) = -\frac{\sqrt{2M|E|}}{\hbar q} = -\sqrt{\frac{2MV_0}{\hbar^2 g^2} - 1} \tag{254}$$

$$\text{using } E = \frac{\hbar^2 q^2}{2M} - V_0 < 0 \tag{255}$$

To have a solution, we need:

$$\cot(qr_0) \le 0 \quad \Rightarrow \quad qr_0 \ge \frac{\pi}{2}$$

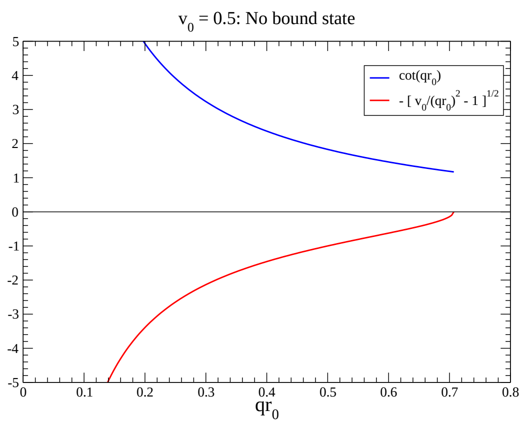
Additionally, if $q^2 < \frac{2MV_0}{\hbar^2}$, we have:

$$\Rightarrow \text{ need } v_0 \equiv \frac{2MV_0}{\hbar^2} r_0^2 \ge \frac{\pi^2}{4} \simeq 2.467\ldots, \qquad qr_0 \le \sqrt{v_0} \tag{256}$$

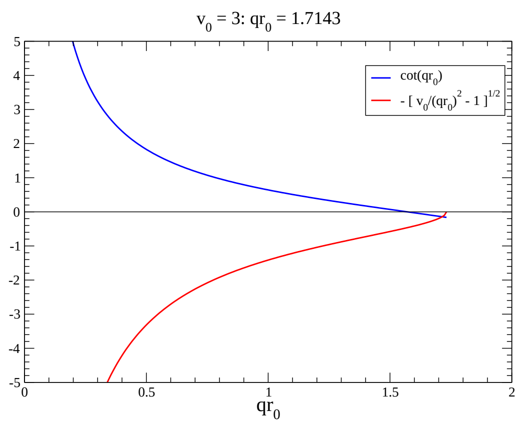
The first bound state appears at $qr_0 = \frac{\pi}{2}$, $\quad V_0 \overset{256}{=} \frac{\pi^2 \hbar^2}{8Mr_0^2}$ which implies $E = 0$. $\Rightarrow \kappa = 0$, i.e.

$$u_0 \xrightarrow[r\to\infty]{} \text{const.}, \qquad R_0 \underset{r>>r_0}{\sim} \frac{1}{r}.$$

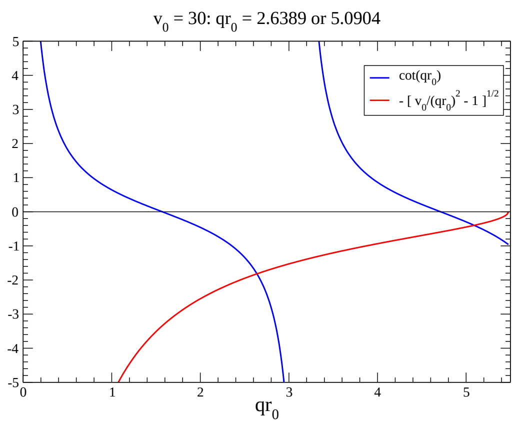
For larger $r_0^2 V_0$, i.e., a "large" well, more bound states can appear. The tightest bound state moves lower in E.



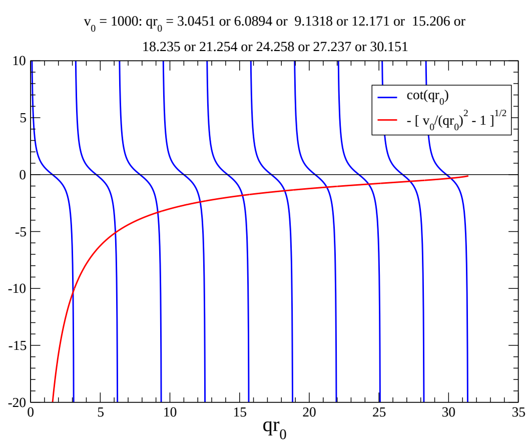
$v_0 = 0.05$



$v_0 = 3$

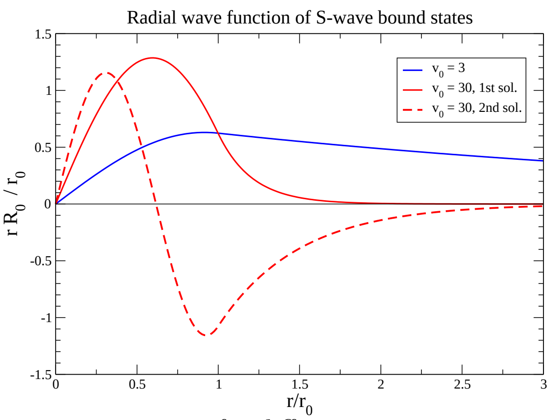


$v_0 = 30$

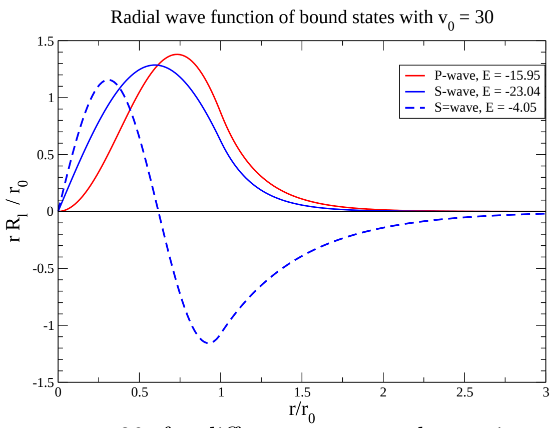


$v_0 = 1000$

1. $v_0 = 0.5$: The potential is too shallow to support a bound state. (Recall: $v_0 = V_0\, 2MV_0^2/\hbar^2$, r_0 being the extension of the well, V_0 its depth, and M the mass of the particle.)
2. $v_0 = 3$:. The potential can now (just) support one bound state.
3. $v_0 = 30$: The potential can now support two bound states.
4. $v_0 = 1000$: The potential can now support ten bound states. The first few solutions occur where the cot function is large and negative, i.e., for qr_0 just below $n\pi$, n being an integer. The last solutions occur near the zeros of the cot function, i.e., for qr_0 near $(n + 1/2)\pi$.



for different v_0



$v_0 = 30$; for different waves and energies

1. for different v_0: The shallow potential only supports a loosely bound state with a very broad wave function. The deeper potential also supports a bound state whose wave function is peaked well within the potential.
   Note that $|rR(r)|^2$ is the probability density to find the particle at distance r from the origin.
2. $v_0 = 30$; for different waves and energies: There are two S-wave states and one P-wave state. The latter is intermediate in energy between the S-wave states. States with larger binding energy (more negative E) fall off faster at large distance.

For $\underline{\ell = 1}$, the radial wavefunction $R_1(r)$ is given by:

$$R_1(r) = \begin{cases} Aj_1(qr) = A\left(\frac{\sin(qr)}{(qr)^2} - \frac{\cos(qr)}{qr}\right), & r \le r_0, \\ Bh_1^{(1)}(i\kappa r) = \frac{iB}{\kappa r} e^{-\kappa r}\left(1 + \frac{1}{\kappa r}\right), & r \ge r_0. \end{cases} \tag{257}$$

quantization condition: (253)

$$\frac{2\cos(qr_0) + \sin(qr_0)\left(qr_0 - \frac{2}{qr_0}\right)}{\sin(qr_0) - qr_0\cos(qr_0)} = -\frac{\kappa}{q}\frac{(\kappa r_0)^2 + 2\kappa r_0 + 2}{(\kappa r_0)^2 + \kappa r_0} \tag{258}$$

The first bound state appears when:

$$v_0 = \frac{2MV_0 r_0^2}{\hbar^2} = \pi^2 \tag{259}$$

For larger ℓ, deeper and/or broader potential wells are required for bound states to exist. This is due to the positive term $\sim \frac{\hbar^2 \ell(\ell+1)}{r^2}$ in the Hamiltonian $\hat{H}$.
For unbound states where $E > 0$, the radial wavefunction is given by:

$$R_\ell(r) = \begin{cases} Aj_\ell(qr), & r \le r_0, \\ Bj_\ell(kr) + Cn_\ell(kr), & r > r_0, \end{cases} \tag{260}$$

where

$$q = \sqrt{\frac{2M(E + V_0)}{\hbar^2}}, \quad k = \sqrt{\frac{2ME}{\hbar^2}}, \tag{261}$$

and $q, k \in \mathbb{R}$, with $q > k$.
Since $k \in \mathbb{R}$, both $B \neq 0$ and $C \neq 0$ are allowed. The solutions are delta-function normalizable (like plane waves).

The continuity equations at $r = r_0$ are given by:

$$Aj_\ell(qr_0) = Bj_\ell(kr_0) + Cn_\ell(kr_0), \tag{262}$$
$$qAj'_\ell(qr_0) = k\left[Bj'_\ell(kr_0) + Cn'_\ell(kr_0)\right] \tag{263}$$

where:

$$j'_\ell(kr_0) \equiv \left.\frac{\mathrm{d}j_\ell(kr)}{\mathrm{d}(kr)}\right|_{r=r_0}.$$

Divide both sides of the second equation:

$$q\frac{qj'_\ell(qr_0)}{j_\ell(qr_0)} = k\frac{j'_\ell(kr_0) + \frac{C}{B}n'_\ell(kr_0)}{j_\ell(kr_0) + \frac{C}{B}n_\ell(kr_0)}, \tag{264}$$

This equation can be solved for $\frac{C}{B}$.
From the continuity equations, the ratio $\frac{C}{B}$ can be expressed as:

$$\frac{C}{B} = \frac{\frac{q}{k}j'_\ell(qr_0)j_\ell(kr_0) - j'_\ell(kr_0)j_\ell(qr_0)}{n'_\ell(kr_0)j_\ell(qr_0) - \frac{q}{k}j'_\ell(qr_0)n_\ell(kr_0)}, \tag{265}$$

Let:

$$\frac{C}{B} = -\tan\tilde{\delta}_\ell(k) = -\frac{\sin\tilde{\delta}_\ell}{\cos\tilde{\delta}_\ell}, \tag{266}$$

Thus, the radial wave function $R_\ell(r)$ can be written as:

$$R_\ell = B\left[j_\ell(kr) + \frac{C}{B}n_\ell(kr)\right].$$

For large r, the asymptotic form $(r \to \infty)$ of $R_\ell(r)$ is:

$$R_\ell \xrightarrow[220,231,266]{r\to\infty} \frac{B}{kr}\left[\sin\left(kr - \frac{\ell\pi}{2}\right) + \frac{\sin\tilde{\delta}_\ell}{\cos\tilde{\delta}_\ell}\cos\left(kr - \frac{\ell\pi}{2}\right)\right].$$

$$R_\ell(r)(r >> r_0) = \frac{B}{kr\cos\tilde{\delta}_\ell}\left[\sin\left(kr - \frac{\ell\pi}{2}\right)\cos\tilde{\delta}_\ell + \cos\left(kr - \frac{\ell\pi}{2}\right)\sin\tilde{\delta}_\ell\right]. \tag{267}$$
$$= \frac{B}{kr\cos\tilde{\delta}_\ell}\sin\left(kr - \frac{\ell\pi}{2} + \tilde{\delta}_\ell(k)\right), \tag{268}$$

compare this with equation (224): $\tilde{\delta}_\ell(k) \equiv$ phase shift $\delta_\ell(k)$.
For $\underline{\ell = 0}$, the spherical Bessel functions (and the spherical Neumann functions) and their derivatives are:

$$j_0(x) = \frac{\sin x}{x}, \quad j'_0(x) = \frac{\cos x}{x} - \frac{\sin x}{x^2},$$
$$n_0(x) = -\frac{\cos x}{x}, \quad n'_0(x) = \frac{\sin x}{x} + \frac{\cos x}{x^2}.$$

From equation (264), we have:

$$\frac{q\left(\frac{\cos(qr_0)}{qr_0} - \frac{\sin(qr_0)}{(qr_0)^2}\right)}{\frac{\sin(qr_0)}{qr_0}} = q\cot(qr_0) - \frac{1}{r_0}.$$
$$\stackrel{!}{=} k\frac{B\left(\frac{\cos(kr_0)}{kr_0} - \frac{\sin(kr_0)}{(kr_0)^2}\right) + C\left(\frac{\sin(kr_0)}{kr_0} + \frac{\cos(kr_0)}{(kr_0)^2}\right)}{B\frac{\sin(kr_0)}{kr_0} - C\frac{\cos(kr_0)}{kr_0}},$$
$$= k\frac{B\cos(kr_0) + C\sin(kr_0)}{B\sin(kr_0) - C\cos(kr_0)} - \frac{1}{r_0}$$
$$\underset{266}{=} k\frac{\cos(\delta_0)\cos(kr_0) - \sin(\delta_0)\sin(kr_0)}{\cos(\delta_0)\sin(kr_0) + \sin(\delta_0)\cos(kr_0)} - \frac{1}{r_0}$$
$$= k\frac{\cos(kr_0 + \delta_0)}{\sin(kr_0 + \delta_0)} - \frac{1}{r_0}.$$

$$\Rightarrow q\cot(qr_0) = k\cot(kr_0+\delta_0) \quad \Rightarrow \quad \tan(kr_0+\delta_0) = \frac{k}{q}\tan(qr_0)$$

which leads to:

$$\delta_0 = \arctan\left[\frac{k}{q}\tan(qr_0)\right] - kr_0. \tag{269}$$

Recall the expressions for q and qr_0 are:

$$q = \sqrt{k^2 + 2MV_0/\hbar^2}, \quad qr_0 = \sqrt{(Kr_0)^2 + v_0}. \tag{270}$$

A resonance occurs when the partial wave saturates the unitarity bound, i.e., for

$$|\sin\delta_0| = 1 \quad \text{or} \quad |\tan\delta_0| \to \infty.$$

From equation (269):

$$\tan\delta_0 = \frac{\frac{k}{q}\tan(qr_0) - \tan(kr_0)}{1 + \frac{k}{q}\tan(qr_0)\tan(kr_0)}. \tag{271}$$

Using the tangent subtraction identity:

$$\tan(\alpha-\beta) = \frac{\tan\alpha - \tan\beta}{1+\tan\alpha\tan\beta}.$$

Three Possibilities for $|\tan\delta_0| \to \infty$
1. $|\tan(qr_0)| \to \infty$:

$$\tan\delta_0 \to \frac{1}{\tan(kr_0)},$$

which also requires $\tan(kr_0) \to 0$.

- To achieve resonance, we require:

$$qr_0 = \left(n+\frac{1}{2}\right)\pi, \quad kr_0 = m\pi,$$

  where $m = n = 0$ represents the lowest case.

- For the lowest case ($m = n = 0$), $qr_0 = \frac{\pi}{2}$, $kr_0 = 0$. Thus:

$$v_0 = \frac{\pi^2}{4}, \tag{272}$$

  which corresponds to the "zero-energy bound state".

2. $|\tan(Kr_0)| \to \infty$:

$$\tan(\delta_0) \to -\frac{q}{k}\frac{1}{\tan(qr_0)}.$$

To satisfy this condition, we need:

-

$$kr_0 = \left(n+\frac{1}{2}\right)\pi, \quad qr_0 = m\pi, \quad \text{where} \quad k < q.$$

- The lowest example ($n = 0, m = 1$) corresponds to:

$$kr_0 = \frac{\pi}{2}, \quad qr_0 = \pi,$$

  which implies:

$$v = \frac{3\pi^2}{4}, \quad \text{(higher than (272))}.$$

3. Generic resonance:

- Generic resonance occurs when:

$$1 + \frac{k}{q}\tan(qr_0)\tan(kr_0) = 0.$$

- Simplifying:

$$\tan(kr_0) = -\frac{q}{k}\cot(qr_0) \underset{270}{=} -\sqrt{1 + \frac{v_0}{(kr_0)^2}}\cot\left(\sqrt{(kr_0)^2 + v_0}\right)$$

- Need

$$qr_0 \geq kr_0 + \frac{\pi}{2} \quad \underset{270}{\Rightarrow} \quad v_0 \geq \frac{\pi^2}{4}.$$

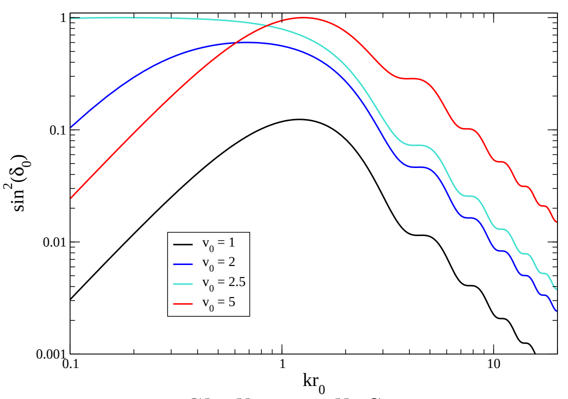
Resonance occurs if a bound state exists.

For $l = 1$, the spherical Bessel functions (and the spherical Neumann functions) and their derivatives are given as follows:

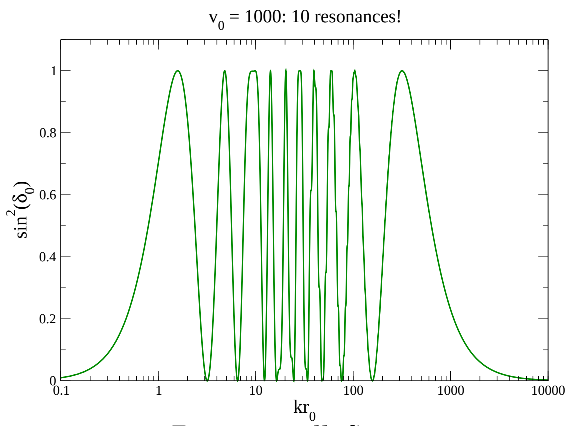
$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \quad j_1'(x) = \frac{2\cos x}{x^2} - \frac{2\sin x}{x^3} + \frac{\sin x}{x}.$$
$$n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \quad n_1'(x) = \frac{2\sin x}{x^2} + \frac{2\cos x}{x^3} - \frac{\cos x}{x}.$$

Phase shift from (265) (266)

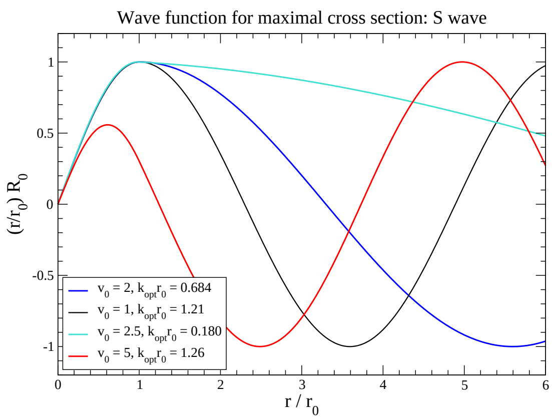
S-wave scattering phase and S-wave unbound wave functions for spherical square well



Shallow well; S-wave



Deeper well; S-wave



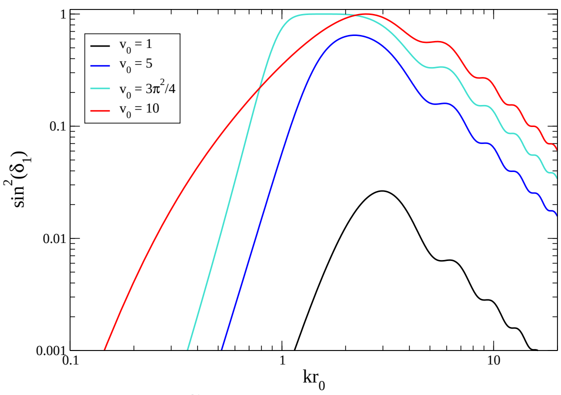
S-wave unbound wave functions

1. **Shallow well**; S-wave: If the potential is so shallow that it does not support a bound state, i.e., for $v_0 < \pi^2/4 = 2.47$, the sine of the scattering phase remains below 1 in magnitude everywhere. Note that the maximum of the scattering cross section moves to *smaller* energies, i.e., smaller k, as v_0 increases in this regime. At the critical value of v_0, the first resonance appears, at $k = 0$. For yet larger v_0, the maximum of the cross section moves to *larger* values of k again, until eventually a second resonance appears at $k = 0$.
Note also that the scattering phase becomes small at small k, except near the critical value of v_0 where a new resonance appears. We saw in class that δ_0 is proportional to k here. Similarly, the scattering phase becomes small again at large k, where $\delta_0 = v_0/(2kr_0) - v_0 \sin(2kr_0)/(2kr_0)^2$.

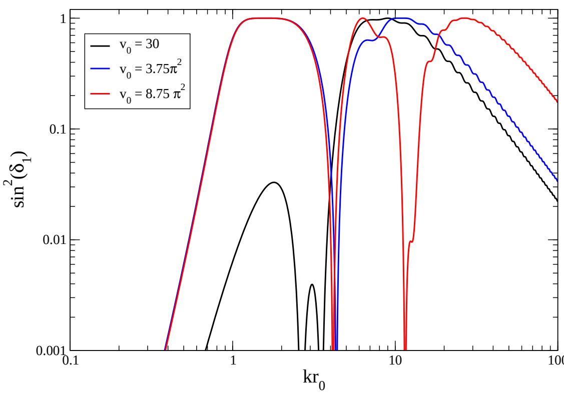
2. **Deeper well**; S-wave: There are now ten resonances. Note that this corresponds exactly to the number of bound states for this value of v_0, see $v_0 = 1000$!

3. **Shallow well**; S-wave unbound wave functions: The values of v_0 are the same as in **Shallow well**; S-wave. k is chosen such that $|\sin(\delta_0)|$ takes its maximal value, i.e., such that the S-wave cross section is maximal. We see that this gives a *universal* result if v_0 is below the critical value, i.e., if no bound state exists, reaching its maximum at $r = r_0$. For larger v_0, the maxima of the wave function outside of the potential, $r > r_0$, are higher than the one inside the potential. Note that the wave functions are normalized such that the maximum of $|rR_0(r)|^2$ is 1.

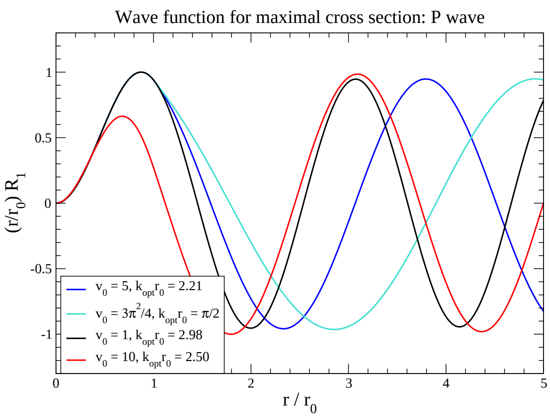
P-wave scattering phase and P-wave unbound wave functions for spherical square well



Shallow well; P-wave



Deeper well; P-wave



P-wave unbound wave functions

1. **Shallow well**; P-wave: For $v_0 < 3\pi^2/4 = 7.4$, the sine of the scattering phase remains below 1 in magnitude everywhere. The maximum of the scattering cross section again moves to *smaller* energies, i.e., smaller k, as v_0 increases in this regime. At the critical value of v_0, the first resonance appears, at $kr_0 = \pi/2$. Note that at this value of v_0, the potential does not yet support a true bound state. However, the presence of a potential barrier in the effective potential already leads to a quasi-bound, resonance, state. For yet larger v_0, the maximum of the cross section moves to *larger* values of k again, until eventually a second resonance appears at $kr_0 = \pi/2$.
Note also that the scattering phase is even more suppressed at small k than the S-wave scattering phase;

we saw in class that δ_1 is proportional to k^3 here. The behavior at large k is very similar as in the case of the S-wave, except that the sign of the modulated term is flipped, $\delta_1 = v_0/(2kr_0) + v_0 \sin(2kr_0)/(2kr_0)^2$.

2. **Deeper well**; P-wave: $v_0 = 30$ is well above the critical value for the first resonance, but still below the value where the second resonance appears. We see that the P-wave cross section has a couple of maxima well below the resonance; however, the cross section at these maxima is still quite small. New resonances appear at $v_0 = (n^2 - 1/4)\pi^2$, whereas new true bound states appear at $v_0 = (n\pi)^2$. We see that at the critical values where the second or third resonance appears, the behavior of the cross section near the first resonance, which always starts at $kr_0 = \pi/2$, is nearly universal.
   Note also that the asymptotic behavior for large k sets in only for $(kr_0)^2 \gg v_0$. Larger values of v_0 also support resonances at quite large values of kr_0.

3. **Shallow well**; P-wave unbound wave functions: The values of v_0 are the same as in **Shallow well**; P-wave. k is chosen such that $|\sin(\delta_1)|$ takes its maximal value, i.e., such that the P-wave cross section is maximal. The behavior of the wave functions is similar to that shown in **Shallow well**; S-wave unbound wave functions for the S-wave, except that the critical value of v_0 a new resonance appears for $kr_0 = \pi/2$, not at $k = 0$ as in the case of the S-wave.

Lessons

- If v_0 is below the value of the first resonance:
  - The wave function that maximizes $\sin^2(\delta_\ell)$ for a given partial wave is *universal* for $r \le r_0$.
  - If resonances exist, the resonant wave function is *large* outside the well.
- For S-**wave:** new resonances appear at the same value of v_0 as new bound states.
- For P-**wave:** resonances appear earlier; related to the existence of quasi-bound states in the effective potential.

[02.12.2024, Lecture 17]

[09.12.2024, Lecture 18]

Second Quantization

Systems of identical particles

Things not larger than molecules can be truly indistinguishable. Physical observables cannot change when identical "particles" are interchanged. Hence: The Hamiltonian describing a system of N such particles must be symmetric:

$$\hat{H}(1,2,\ldots,i,\ldots,k,\ldots,N) \equiv \hat{H}(1,2,\ldots,k,\ldots,i,\ldots,N) \tag{273}$$

The argument "1" stands for all we know about particle 1 (e.g., $\vec{x}_1$, spin $\vec{S}_1$).
The N-particle wave function: $\Psi = \Psi(1,2,\ldots,N)$. The permutation operator $\hat{P}_{ik}$ is defined via:

$$\hat{P}_{ik}\Psi(1,2,\ldots,i,\ldots,k,\ldots,N) = \Psi(1,2,\ldots,k,\ldots,i,\ldots,N) \tag{274}$$

This exchanges arguments i and k of Ψ. Evidently:

$$\hat{P}_{ik}^2 = 1 \quad \Rightarrow \quad \hat{P}_{ik} \text{ has eigenvalues } \pm 1$$

$$(273) \quad \Rightarrow \quad \hat{P}_{ik}\hat{H} = \hat{H}\hat{P}_{ik}, \quad \forall i,k \tag{275}$$

This implies that $\hat{H}$ is symmetric under permutations.
Some Properties of $\hat{P}_{ik}$:

i If $\hat{H}\Psi = E\Psi$, then:

$$\hat{H}(\hat{P}_{ik}\Psi) = E(\hat{P}_{ik}\Psi) \tag{276}$$

This implies that $\hat{P}_{ik}\Psi$ is also an eigenstate of $\hat{H}$.

ii Let φ, ψ be two N-particle wave functions, then:

$$\langle\varphi|\psi\rangle = \langle\hat{P}_{ik}\varphi|\hat{P}_{ik}\psi\rangle \quad \forall i,k \tag{277}$$

by relabelling $\vec{x}_i \leftrightarrow \vec{x}_k$.

iii $\hat{P}_{ik}^\dagger$ is defined as usual:

$$\langle\varphi|\hat{P}_{ik}\psi\rangle = \langle\hat{P}_{ik}^\dagger\varphi|\psi\rangle \tag{278}$$

Since $\hat{P}_{ik}^{-1}$ is also a permutation, in fact $\hat{P}_{ik}^{-1} = \hat{P}_{ik}$:

$$\langle\varphi|\hat{P}_{ik}\psi\rangle \overset{277}{=} \langle\hat{P}_{ik}^{-1}\varphi|\hat{P}_{ik}^{-1}\hat{P}_{ik}\psi\rangle = \langle\hat{P}_{ik}^{-1}\varphi|\psi\rangle$$

but also $\langle\varphi|\hat{P}_{ik}\psi\rangle \overset{278}{=} \langle\hat{P}_{ik}^\dagger\varphi|\psi\rangle$

$$\Rightarrow \quad \hat{P}_{ik}^\dagger = \hat{P}_{ik}^{-1} \quad \Rightarrow \quad \hat{P}_{ik} \text{ is unitary} \tag{279}$$

iv For all symmetrical N-particle operators $\hat{S}(1,2,\dots,N)$, we have:

$$[\hat{P}_{ik}, \hat{S}] = 0, \quad \forall i,k \tag{280}$$

$$\Rightarrow \langle\hat{P}_{ik}\varphi|\hat{S}|\hat{P}_{ik}\Psi\rangle = \langle\varphi|\hat{P}_{ik}^\dagger\hat{S}\hat{P}_{ik}|\Psi\rangle \overset{280}{=} \langle\varphi|\overbrace{\hat{P}_{ik}^\dagger\hat{P}_{ik}}^{=\,1\ (279)}\hat{S}|\Psi\rangle = \langle\varphi|\hat{S}|\Psi\rangle \tag{281}$$

This shows that permutations do not change the matrix elements of a symmetric operator.

v Since the exchange of identical particles must not have observable consequences, all observables must correspond to completely symmetric operators:

$$\hat{O}. \tag{282}$$

Since (282) holds for all physical observables, ψ and $\hat{P}_{ik}\psi$ cannot be distinguished. Through permutations, one can generate $N!$ states from the original $\psi(1,2,\dots,N)$. Eigenstates of all $\hat{P}_{ik}$ play special roles:

* Totally symmetric state:

$$\hat{P}_{ik}\psi_s(1,\dots,N) = \psi_s(1,\dots,N) \quad \forall i,k. \tag{283}$$

* Totally antisymmetric state:

$$\hat{P}_{ik}\psi_a(1,\dots,N) = -\psi_a(1,\dots,N) \quad \forall i,k. \tag{284}$$

Observational Fact: All (known) particles are either bosons, described by ψ_s, or fermions, described by ψ_a.

- Bosons have integer spin, $S_z^{(b)} = n\hbar \quad (n = 0,1,2,\dots)$.
- Fermions have half-integer spin, $S_z^{(f)} = \left(n + \frac{1}{2}\right)\hbar$.

The "spin-statistics theorem" dictates the classification of particles based on their spin.

Note

A general permutation $\hat{P}$ can involve more than 2 particles. However, $\hat{P}$ can always be written as a product of *cyclical permutations*, e.g., $(1\,2\,4)(3\,5)$. For example:

$(1\,2\,4)$ means: particle 1 replaces particle 2, 2 replaces 4, 4 replaces 1.

Each cyclical permutation can be written as a product of 2-particle exchanges:

$$\hat{P}_{124} = \hat{P}_{12}\hat{P}_{24} \quad \text{with} \quad \hat{P}_{24}\hat{P}_{12} = \hat{P}_{12}\hat{P}_{24}.$$

A permutation is **even (odd)** if it can be written in terms of an even (odd) number of 2-particle exchanges.

$$(283) \quad \Rightarrow \quad \hat{P}\psi_s = \psi_s, \quad \forall \text{ permutations} \tag{285}$$

$$(284) \quad \Rightarrow \quad \hat{P}\psi_a = (-1)^P\psi_a \tag{286}$$

where

$$(-1)^P = \begin{cases} +1, & \text{for even permutations,} \\ -1, & \text{for odd permutations.} \end{cases}$$

$\Rightarrow$ states with ≥ 3 particles allow to form higher-dimensional representations of group G_P: "parasymmetric" states, obeying *"parastatistics"*—not realized in Nature, as far as we know.

Constructing completely (anti-) symmetric states

Starting point: single-particle state $|i\rangle \Rightarrow$ the basis of N-particle states is given by product states:

$$|i_1, i_2, \ldots, i_\alpha, \ldots, i_N\rangle = |i_1\rangle_1 |i_2\rangle_2 \cdots |i_\alpha\rangle_\alpha \cdots |i_N\rangle_N \tag{287}$$

where particle 1 is in state $|i_1\rangle$, particle 2 is in state $|i_2\rangle$, particle α is in state $|i_\alpha\rangle$ and so on.
$\hat{H}$ is totally symmetric $\implies$ Lagrangian is symmetric $\overset{98}{\implies}$ propagator is totally symmetric.

$$\begin{aligned}
\psi(t, \vec{x}_i) &= \int \prod_i d^3x_i'\, U(t, \vec{x}_i; \vec{x}_i')\psi(0, \vec{x}_i') \\
\implies \hat{P}\psi(t, \vec{x}_i) &= \int \prod_i d^3x_i'\, \hat{P}U(t, \vec{x}_i; \vec{x}_i')\psi(0, \vec{x}_i') \\
&= \int \prod_i d^3x_i'\, U(t, \vec{x}_i; \vec{x}_i')\hat{P}\psi(0, \vec{x}_i')
\end{aligned}$$

Time evolution does not change symmetry properties of ψ. (**??**): ψ_s, ψ_a form two one-dimensional representations of the permutation group G_P, ψ_s being the "trivial" representation.

- For 2 particles:

$$\psi_s = \frac{1}{\sqrt{2}}\left[\psi(1,2) + \psi(2,1)\right], \quad \psi_a = \frac{1}{\sqrt{2}}\left[\psi(1,2) - \psi(2,1)\right]$$

  Form complete set of states.

- For ≥ 3 particles: not all $\hat{P}_{ik}$ commute. For example:

$$\left.\begin{aligned}
\hat{P}_{ik}\hat{P}_{ij}\psi(1,2,3) = \hat{P}_{ik}\psi(2,1,3) = \psi(3,1,2) \\
\hat{P}_{ij}\hat{P}_{ik}\psi(1,2,3) = \hat{P}_{ij}\psi(1,3,2) = \psi(2,3,1)
\end{aligned}\right\} \implies \hat{P}_{ik}\hat{P}_{ij} \neq \hat{P}_{ij}\hat{P}_{ik},$$

  where i, j, k are not related to the number but the numbers position, so in this case $i = 1^{st}$ position, $j = 2^{nd}$ position, $k = 3^{rd}$ position

$$\begin{aligned}
\hat{P}_{ik}\hat{S}_-|i_1, i_2, \ldots, i_N\rangle &= \frac{1}{\sqrt{N!}}\sum_P (-1)^P \underbrace{\hat{P}_{ik}\hat{P}}_{\hat{P}'}|i_1, i_2, \ldots, i_N\rangle \\
&= \frac{1}{\sqrt{N!}}\sum_{P'} (-1)^P \hat{P}'|i_1, i_2, \ldots, i_N\rangle \underset{(-1)^P = -(-1)^{P'}}{=} -\frac{1}{\sqrt{N!}}\sum_{P'} (-1)^{P'} \hat{P}'|i_1, i_2, \ldots, i_N\rangle \\
&= -\hat{S}_-|i_1, i_2, \ldots, i_N\rangle
\end{aligned}$$

If not all $|i_\alpha\rangle$ are different:

* $\hat{S}_-|i_1, i_2, \ldots, i_N\rangle = 0$ if $\exists\, \alpha, \beta$ such that $|i_\alpha\rangle = |i_\beta\rangle$:

$$\hat{P}_{\alpha\beta}\hat{S}_-|i_1, i_2 \ldots, i_N\rangle = -\hat{S}_-|i_1, i_2, \ldots, i_N\rangle \quad \text{Pauli exclusion principle!}$$
$$\hat{P}_{\alpha\beta}\hat{S}_-|i_1, i_2 \ldots, i_N\rangle = +\hat{S}_+|i_1, i_2, \ldots, i_N\rangle \text{ since the state is symmetric under } \alpha \leftrightarrow \beta$$

* $\hat{S}_+|i_1, i_2, \ldots, i_N\rangle \neq 0$, but is not normalized to unity.
$N = 2:\ \hat{S}_+|i_1, i_2\rangle = \frac{1}{\sqrt{2}}\big(|i_1, i_2\rangle + |i_2, i_1\rangle\big) = \frac{1}{\sqrt{2}}\big[\psi_{i_1}(x_1)\psi_{i_2}(x_2) + \psi_{i_1}(x_2)\psi_{i_2}(x_1)\big]$

$$\begin{aligned}
\implies \|\hat{S}_+|i_1, i_2\rangle\|^2 &= \frac{1}{2}\int dx_1 dx_2 \big[\psi^*_{i_1}(x_1)\psi^*_{i_2}(x_2) + \psi^*_{i_1}(x_2)\psi^*_{i_2}(x_1)\big]\cdot\big[\psi_{i_1}(x_1)\psi_{i_2}(x_2) + \psi_{i_1}(x_2)\psi_{i_2}(x_1)\big] \\
&= \frac{1}{2}\big[1 + 1 + \delta_{i_1 i_2} + \delta_{i_1 i_2}\big] = 1 + \delta_{i_1 i_2} \underset{i_1 = i_2}{=} n_1!
\end{aligned}$$

$n_i!$ = Number of particles in state i_1
If $\{e_k\}$ form a group under multiplication, then $\{e_i e_k\} = \{e_k\}$, for arbitrary e_i.

* $e_i e_k = e_i \in \{e_k\}$ (by definition) $\implies \{e_i e_k\} \subset \{e_k\}$.

* Assume $e_i e_k = e_j,\ e_i e_{k'} = e_j,\ e_i$ has a unique inverse e_i^{-1}
$\implies e_k = e_i^{-1}e_j$ and $e_{k'} = e_i^{-1}e_i$, also $e_k = e_{k'}$
If $\{e_k\}$ are all different, so are all $\{e_i e_k\} \implies$ q.e.d.

$$\hat{P}_{ik}\hat{S}_+|i_1,\ldots,i_N\rangle = \frac{1}{\sqrt{N!}}\sum_P \underbrace{\hat{P}_{ij}\hat{P}}_{\hat{P}'}|i_1,\ldots,i_N\rangle = \frac{1}{\sqrt{N!}}\sum_{P'}\hat{P}'|i_1,\ldots,i_N\rangle = \hat{S}_+|i_1,\ldots,i_N\rangle.$$

If $\{|i\rangle\}$ is a complete orthonormal set of 1-particle states, then (287) form a complete orthonormal set of N-particle states.
The (anti-) symmetrized N-particle basis states are:

$$\hat{S}_\pm|i_1,\ldots,i_\alpha,\ldots,i_N\rangle = \frac{1}{\sqrt{N!}}\sum_P(\pm1)^P\hat{P}|i_1,\ldots,i_\alpha,\ldots,i_N\rangle, \tag{288}$$

where $\pm$ corresponds to symmetry (+) or antisymmetry (−), and there are $N!$ permutations. $\implies$ properly normalized totally symmetric (bosonic) state:

$$\Psi_s(x_1,\ldots,x_N) = \frac{1}{\sqrt{n_1!\,n_2!\cdots n_N!}}\hat{S}_+|i_1,\ldots,i_N\rangle = \frac{1}{\sqrt{N!\,n_1!\,n_2!\cdots n_N!}}\sum_P\hat{P}|i_1,\ldots,i_N\rangle \tag{289}$$

Forms orthonormal basis.

[09.12.2024, Lecture 18]

[11.12.2024, Lecture 19]

Second quantization of Bosons

Normalized symmetric state $\psi_s = \frac{1}{\sqrt{n_1!\cdots n_k!}}\hat{S}_+|i_1,i_2,\ldots,i_N\rangle$ is uniquely defined by the occupation number n_α:

$$|n_1,n_2,\ldots\rangle = \frac{1}{\sqrt{n_1!n_2!\cdots}}\hat{S}_+\underbrace{|i_1,i_2,\ldots,i_N\rangle}_{\text{states with } n_\alpha\geq1} \tag{290}$$

Have to allow $n_\alpha = 0$ on the l.h.s. The set of all states with $N = 0,1,2,\ldots,\infty$ particles define a complete orthonormal basis for states with an arbitrary number of particles.

$$\langle n_1,n_2,\ldots|n_1',n_2',\ldots\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots \tag{291}$$

$$\Rightarrow N \equiv \sum_\alpha n_\alpha = \sum_\alpha n_\alpha' = N'$$

Completeness relation: $\sum_{n_1,n_2,\ldots}|n_1,n_2,\ldots\rangle\langle n_1,n_2,\ldots| = 1$
Corresponding vector space is the direct sum of Hilbert spaces with fixed N: Fock space Usual operators (e.g., $\hat{\vec{x}},\hat{\vec{p}},\hat{\vec{L}},\ldots$) act within the subspace of fixed N. To move between subspaces: introduce creation operator $\hat{a}_i^\dagger$ and annihilation operator $\hat{a}_i$. Definition:

$$\hat{a}_i^\dagger|n_1,\ldots,n_i,\ldots\rangle = \sqrt{n_i+1}|n_1,\ldots,n_i+1,\ldots\rangle \tag{292}$$

One more particle in state i. Important: $n_i = 0$ is also possible.
Take the hermitian conjugate (h.c.) of (292):

$$\langle\ldots,n_i',\ldots,n_1|\hat{a}_i = \sqrt{n_i'+1}|\ldots,n_i'+1,\ldots,n_1\rangle \tag{293}$$

$$\implies \langle\ldots,n_i',\ldots,n_1|\hat{a}_i|n_1,\ldots,n_i,\ldots\rangle \stackrel{293}{=} \sqrt{n_i'+1}\langle\ldots,n_i',\ldots,n_1|n_1,\ldots,n_i,\ldots\rangle = \sqrt{n_i}\,\delta_{n_i,n_i'+1} \tag{294}$$

$\Rightarrow n_i' = n_i - 1$: Reduces the number of particles in state i
$\sqrt{n_i}$ factor:

$$\hat{a}_i|n_1,\ldots,n_i=0,\ldots\rangle = 0 \tag{295}$$

$\Rightarrow \hat{a}_i$ annihilates the state if $n_i = 0$.
From these properties:

$$[\hat{a}_i,\hat{a}_k] = 0 \tag{296}$$
$$[\hat{a}_i^\dagger,\hat{a}_k^\dagger] = 0 \tag{297}$$
$$[\hat{a}_i,\hat{a}_k^\dagger] = \delta_{ik} \tag{298}$$

Proof: (296) is trivial for $i = k$; for $i \neq k$:

$$\begin{aligned}\hat{a}_i\hat{a}_k|n_1,\dots,n_i,\dots,n_k,\dots\rangle &= \hat{a}_i\sqrt{n_k}|n_1,\dots,n_i,\dots,n_k-1,\dots\rangle = \sqrt{n_in_k}|n_1,\dots,n_i,\dots,n_k-1,\dots\rangle \\ &= \hat{a}_k\hat{a}_i|n_1,\dots,n_i,\dots,n_k,\dots\rangle\end{aligned}$$

(297): h.c. of (296)
(298): For $i \neq k$ as for (296). For $i = k$:

$$\left(\hat{a}_i\hat{a}_i^\dagger - \hat{a}_i^\dagger\hat{a}_i\right)|n_1,\dots,n_i,\dots\rangle = \hat{a}_i\sqrt{n_i+1}|n_1,\dots,n_i+1,\dots\rangle - \hat{a}_i^\dagger\sqrt{n_i}|n_1,\dots,n_i-1,\dots\rangle \tag{299}$$

$$= \left(n_i+1-n_i\right)|n_1,\dots,n_i,\dots\rangle. \tag{300}$$

These are as for (dimensionless) ladder operators of harmonic oscillator!
Vacuum ($\equiv$ ground) state $|0\rangle$ is defined by $n_i = 0\ \forall i$:

$$|0\rangle = |0,0,\dots\rangle \tag{301}$$

$$N = 0 \Leftrightarrow \hat{a}_i|0\rangle = 0\ \forall i$$

All N-particle states can be constructed by applying creation operators to $|0\rangle$. N = 1:

$$|0,0,\dots,1,\dots\rangle = \hat{a}_i^\dagger|0\rangle \tag{302}$$

N = 2:

$$|0,\dots,0,2,0,\dots\rangle = \frac{1}{\sqrt{2!}}\left(\hat{a}_i^\dagger\right)^2|0\rangle \tag{303}$$

$$|0,\dots,0,1,0,\dots,0,1,0,\dots,0\rangle = \hat{a}_i^\dagger\hat{a}_k^\dagger|0\rangle \overset{297}{=} \hat{a}_k^\dagger\hat{a}_i^\dagger|0\rangle \tag{304}$$

General N:

$$|n_1,n_2,\dots\rangle = \frac{1}{\sqrt{n_1!\,n_2!\cdots}}\left(\hat{a}_1^\dagger\right)^{n_1}\left(\hat{a}_2^\dagger\right)^{n_2}\cdots|0\rangle \tag{305}$$

Particle or occupation number operators:

$$\hat{n}_i := \hat{a}_i^\dagger\hat{a}_i \tag{306}$$

Product N-particle states are eigenstates of the $\hat{n}_i$:

$$\hat{n}_i|n_1,n_2,\dots,n_i,\dots\rangle = \hat{a}_i^\dagger\hat{a}_i|n_1,n_2,\dots,n_i,\dots\rangle = \sqrt{n_i}\,\hat{a}_i^\dagger|n_1,\dots,n_i-1,\dots\rangle = n_i|n_1,\dots,n_i,\dots\rangle$$

The total particle number operator is defined as:

$$\hat{N} = \sum_i \hat{n}_i \tag{307}$$

with

$$\hat{N}|n_1,n_2,\dots\rangle = \sum_i \hat{n}_i|n_1,n_2,\dots\rangle = \left(\sum_i n_i\right)|n_1,n_2,\dots\rangle = N|n_1,n_2,\dots\rangle \tag{308}$$

[11.12.2024, Lecture 19]

[16.12.2024, Lecture 20]

Consider operators that can be written as a sum of single-particle operators:

$$\hat{T} = \sum_{\alpha=1}^{N}\hat{t}_\alpha, \tag{309}$$

where α labels the particles and not the states.
Acts within subspace with fixed N.

$$\text{Let } t_{ik} = \langle i|\hat{t}|k\rangle \tag{310}$$

$$\text{Then: } \hat{t} = \sum_{i,k} t_{ik}|i\rangle\langle k| \tag{311}$$

Proof:

$$\langle i'|\hat{t}|k'\rangle \overset{311}{=} \sum_{i,k} t_{ik} \underbrace{\langle i'|i\rangle}_{\delta_{ii'}} \underbrace{\langle k'|k\rangle}_{\delta_{kk'}} = t_{i'k'}$$

$$(309)(311): \hat{T} = \sum_{i,k} t_{ik} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle k|_\alpha \tag{312}$$

$$= \sum_{i,k} t_{ik} \hat{a}_i^\dagger \hat{a}_k \tag{313}$$

$$\text{Have used: } \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle k|_\alpha = \hat{a}_i^\dagger \hat{a}_k \tag{314}$$

Prove (314) by application to general N-particle state:

$$\sum_{\alpha=1}^{N} |i\rangle_\alpha \langle k|_\alpha \; |n_1, \dots, n_k, \dots, n_k, \dots, n_i, \dots\rangle \overset{289}{=} \sum_{\alpha} |i\rangle_\alpha \langle k|_\alpha \frac{1}{\sqrt{N! \, n_1! \, n_2! \cdots}} \sum_P \hat{P} |i_1\rangle_1 |i_2\rangle_2 \dots |i_N\rangle_N$$

The terms after summation over α: increases n_i by 1, reduces n_k by 1:

$$= n_k |n_1, \dots, n_k - 1, \dots, n_i + 1, \dots\rangle \cdot \underbrace{\sqrt{\frac{(n_k-1)!}{n_k!}} \cdot \sqrt{\frac{(n_i+1)!}{n_i!}}}_{\text{Restoring normalization}}$$

$$= |n_1, \dots, n_k - 1, \dots, n_i + 1, \dots\rangle \cdot \sqrt{n_k(n_i+1)}$$

$$(\text{with } 296,\ 297,\ 298) = \hat{a}_i^\dagger \hat{a}_k |n_1, \dots, n_k, \dots, n_i, \dots\rangle$$

Special case: N identical bosons that do not interact with each other (e.g., photons):

$$\hat{H} = \sum_{\alpha=1}^{N} H_{(1)}(\vec{x}_\alpha); \text{ let } \langle i|H_{(1)}|k\rangle = \varepsilon_i \delta_{ik} \text{ (choice of basis)} \tag{315}$$

$$\overset{313}{\Longrightarrow} \hat{H} = \sum_{i,k} \varepsilon_i \delta_{ik} \hat{a}_i^\dagger \hat{a}_k = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i \overset{306}{=} \sum_i \varepsilon_i \hat{n}_i \tag{316}$$

Thus:

$$\hat{H}|n_1, n_2, \dots\rangle = \underbrace{\left(\sum_i \varepsilon_i n_i\right)}_{\substack{\text{energy of the} \\ \text{N-particle state}}} |n_1, n_2, \dots\rangle$$

For two-particle operators (e.g., potential energy from two-particle interactions such as Coulomb interactions), the general form is given by:

$$\hat{F} = \frac{1}{2} \sum_{\alpha \neq \beta} f(\vec{x}_\alpha, \vec{x}_\beta) \tag{317}$$

Expanding this in terms of basis states:

$$\hat{F} = \frac{1}{2} \sum_{i,j,k,l} \langle i,j|\hat{f}|k,l\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \tag{318}$$

$$= \frac{1}{2} \sum_{i,j,k,l} \langle i,j|\hat{f}|k,l\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \tag{319}$$

Here:

$$\langle i,j|\hat{f}|k,l\rangle = \int \mathrm{d}^3x \, \mathrm{d}^3y \, \psi_i^*(\vec{x}) \psi_j^*(\vec{y}) \hat{f}(\vec{x}, \vec{y}) \psi_k(\vec{x}) \psi_l(\vec{y})$$

Note: There is no symmetrization applied in the above expressions.
Proof of (319): Consider a single term in the summation:

$$\sum_{\alpha\neq\beta}|i\rangle_\alpha|j\rangle_\beta\langle k|_\alpha\langle l|_\beta = \sum_{\alpha\neq\beta}|i\rangle_\alpha \underbrace{\langle k|_\alpha|j\rangle_\beta}_{\text{can't be contracted for } \alpha\neq\beta} \langle l|_\beta$$

This can be rewritten as:

$$\sum_{\alpha\neq\beta}|i\rangle_\alpha|j\rangle_\beta\langle k|_\alpha\langle l|_\beta = \sum_{\alpha,\beta}|i\rangle_\alpha\langle k|_\alpha|j\rangle_\beta\langle l|_\beta - \sum_{\alpha}|i\rangle_\alpha \underbrace{\langle k|_\alpha|j\rangle_\alpha}_{\delta_{jk}}\langle l|_\alpha$$

$$\overset{314}{=} \hat{a}_i^\dagger\hat{a}_k\hat{a}_j^\dagger\hat{a}_l - \delta_{jk}\hat{a}_j^\dagger\hat{a}_l = \hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l + \cancel{\hat{a}_j^\dagger\delta_{kj}\hat{a}_l} - \cancel{\delta_{jk}\hat{a}_j^\dagger\hat{a}_l}$$

Second quantization of Fermions

Need totally antisymmetric states, which can also be written as a "Slater determinant":

$$\hat{S}_-|i_1,i_2,\dots,i_N\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} |i_1\rangle_1 & |i_2\rangle_1 & \cdots & |i_N\rangle_1 \\ |i_2\rangle_2 & |i_1\rangle_2 & \cdots & |i_N\rangle_2 \\ \vdots & \vdots & \ddots & \vdots \\ |i_N\rangle_N & |i_N\rangle_N & \cdots & |i_N\rangle_N \end{vmatrix} \tag{320}$$

We can define totally antisymmetric states $|n_1,n_2,\dots\rangle$, including the ground state: $|0\rangle = |0,0,\dots,0\rangle$. To generate antisymmetric states from the vacuum, we need anticommuting creation operators $b_i^\dagger$:
The anticommutation relations for the fermionic creation and annihilation operators are:

$$\{\hat{b}_i^\dagger,\hat{b}_k^\dagger\} = \hat{b}_i^\dagger\hat{b}_k^\dagger + \hat{b}_k^\dagger\hat{b}_i^\dagger = 0 \quad\Leftrightarrow\quad \hat{b}_i^\dagger\hat{b}_k^\dagger = -\hat{b}_k^\dagger\hat{b}_i^\dagger \tag{321}$$

The general N-particle state is given by:

$$|n_1,n_2,\dots\rangle = (\hat{b}_1^\dagger)^{n_1}(\hat{b}_2^\dagger)^{n_2}\dots|0\rangle \tag{322}$$

$$(\hat{b}_1^\dagger)^{n_1}(\hat{b}_2^\dagger)^{n_2} = (-1)^{n_1\cdot n_2}(\hat{b}_2^\dagger)^{n_2}(\hat{b}_1^\dagger)^{n_1} \quad \text{for } n_i\in\{0,1\}.$$

The action of the creation operator $\hat{b}_i^\dagger$ should be defined such that (322) produces a totally anti-symmetric state:

$$\hat{b}_i^\dagger|n_1,n_2,\dots\rangle = (1-n_i)(-1)^{\sum_{k<i}n_k}|n_1,\dots,n_{i+1},\dots\rangle \tag{323}$$

Here, each state can have at most one fermion (Pauli exclusion principle).
The action of the annihilation operator $\hat{b}_i$ is given by:

$$\hat{b}_i|n_1,n_2,\dots\rangle = n_i(-1)^{\sum_{k<i}n_k}|n_1,\dots,n_{i-1},\dots\rangle \tag{324}$$

The Hermitian conjugate of Eq. (321) is:

$$\{\hat{b}_i,\hat{b}_k^\dagger\} = 0 \tag{325}$$

$$\{\hat{b}_i,\hat{b}_k^\dagger\} = \delta_{ik} \tag{326}$$

Case: $i = k$

$$\hat{b}_i\hat{b}_i^\dagger|n_1,n_2,\dots,n_i,\dots\rangle \overset{323}{=} (1-n_i)(-1)^{\sum_{k<i}n_k}\hat{b}_i|n_1,\dots,n_i+1,\dots\rangle$$
$$\overset{324}{=} \underbrace{(1-n_i)(n_i+1)}_{1-n_i^2}\left[(-1)^{\sum_{k<i}n_k}\right]^2|n_1,\dots,n_i,\dots\rangle$$

$$\hat{b}_i^\dagger\hat{b}_i|n_1,n_2,\dots,n_i,\dots\rangle \overset{324}{=} n_i(-1)^{\sum_{k<i}n_k}\hat{b}_i^\dagger|n_1,n_2,\dots,n_i-1,\dots\rangle$$
$$\overset{323}{=} = \underbrace{n_i(2-n_i)}_{n_i}\left[(-1)^{\sum_{k<i}n_k}\right]^2|n_1,n_2,\dots,n_i,\dots\rangle$$

$$\{\hat{b}_i, \hat{b}_i^\dagger\} = 1 - n_i^2 + n_i = 1, \quad n_i \in \{0,1\}$$

$$\hat{n}_i^{(f)} = \hat{b}_i^\dagger \hat{b}_i \tag{327}$$

This is the occupation number operator.

$$\hat{T} = \sum_{i,k} \langle i|\hat{f}|k\rangle \hat{b}_i^\dagger \hat{b}_k \quad \text{1-particle operators} \tag{328}$$

For two-particle operators:

$$\hat{F} = \frac{1}{2} \sum_{i,j,k,l} \langle i,j|\hat{f}|k,l\rangle \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_k \hat{b}_l \tag{329}$$

As in (319), there is no antisymmetrization applied.

Field Operators

Consider two complete, orthonormal sets of basis states, $\{|i\rangle\}$ and $\{|\lambda\rangle\}$.

$$|\lambda\rangle = \sum_i |i\rangle\langle i|\lambda\rangle \implies \hat{a}_\lambda^\dagger = \sum_i \langle i|\lambda\rangle \hat{a}_i^\dagger \tag{330}$$

The operator $\hat{a}_\lambda^\dagger$ generates one particle in state $|\lambda\rangle$:

$$\hat{a}_\lambda^\dagger|0\rangle = \sum_i \langle i|\lambda\rangle \underbrace{\hat{a}_i^\dagger|0\rangle}_{|i\rangle} = |\lambda\rangle$$

The Hermitian conjugate of (330) is:

$$\hat{a}_\lambda = \sum_i \langle \lambda|i\rangle \hat{a}_i \tag{331}$$

A special role is played by the eigenstate $|\vec{x}\rangle$ of $\hat{\vec{x}}$, such that:

$$\langle \vec{x}|i\rangle = \varphi_i(\vec{x}) \tag{332}$$

The N-particle wavefunction in coordinate space is used to define the <u>field operator</u>:

$$\hat{\psi}(\vec{x}) = \sum_i \varphi_i(\vec{x})\hat{a}_i \tag{333}$$

$$\implies \hat{\psi}^\dagger(\vec{x}) = \sum_i \varphi_i^*(\vec{x})\hat{a}_i^\dagger \tag{334}$$

Here:
- $\hat{\psi}^\dagger(\vec{x})$ creates one particle at $\vec{x}$.
- $\hat{\psi}(\vec{x})$ annihilates one particle at $\vec{x}$.

The commutation relations for the field operators are given as:

$$[\hat{\psi}(\vec{x}), \hat{\psi}(\vec{x}\,')] = \sum_{i,k} \varphi_i(\vec{x})\varphi_k(\vec{x}\,')[\hat{a}_i, \hat{a}_k] \overset{296}{=} 0 \tag{335}$$

$$[\hat{\psi}^\dagger(\vec{x}), \hat{\psi}^\dagger(\vec{x}\,')] = 0 \tag{336}$$

$$[\hat{\psi}(\vec{x}), \hat{\psi}^\dagger(\vec{x}\,')] = \sum_{i,k} \varphi_i(\vec{x})\varphi_i^*(\vec{x}\,')\left[\hat{a}_i, \hat{a}_k^\dagger\right] \overset{298}{=} \sum_i \varphi_i(\vec{x})\varphi_i^*(\vec{x}\,') = \delta(\vec{x} - \vec{x}\,') \tag{337}$$

Since φ_i form a complete basis:

$$\sum_i \varphi_i(\vec{x})\varphi_i^*(\vec{x}\,') \overset{332}{=} \sum_i \langle \vec{x}|i\rangle\langle i|\vec{x}\rangle = \langle \vec{x}|\vec{x}\rangle = (337)$$

For fermions: $\hat{a}_i \to \hat{b}_i$; commutations in (335, 336, 337) → anticommutations.
Kinetic energy:

$$\hat{T} = \sum_{i,k} \hat{a}_i^\dagger T_{ik}^{(1)} \hat{a}_k \quad , \text{ where } T_{ik}^{(1)} \text{ is the single particle matrix element} \tag{338}$$

$$= \sum_{i,k} \int \mathrm{d}^3x\, \hat{a}_i^\dagger \varphi_i^*(\vec{x}) \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\right) \varphi_k(\vec{x}) \hat{a}_k \overset{\text{partial integration}}{=} \frac{\hbar^2}{2m} \sum_{i,k} \int \mathrm{d}^3x \left[\hat{a}_i^\dagger \vec{\nabla}\varphi_i^*(\vec{x})\right] \cdot \left[\vec{\nabla}\varphi_k(\vec{x})\hat{a}_k\right] \tag{339}$$

$$\overset{333,334}{=} \frac{\hbar^2}{2m} \int \mathrm{d}^3x \left[\vec{\nabla}\hat{\psi}^\dagger(\vec{x})\right]\left[\vec{\nabla}\hat{\psi}(\vec{x})\right] \tag{340}$$

Potential energy (external potential):

$$\hat{U} = \sum_{i,k} \hat{a}_i^\dagger U_{ik} \hat{a}_k \tag{341}$$

$$= \sum_{i,k} \int \mathrm{d}^3x\, \hat{a}_i^\dagger \varphi_i^*(\vec{x}) U(\vec{x}) \phi_k(\vec{x}) \hat{a}_k \overset{333,334}{=} \int \mathrm{d}^3x\, \hat{\psi}^\dagger(\vec{x}) U(\vec{x}) \hat{\psi}(\vec{x}) \tag{342}$$

Two-Particle interaction:

$$\hat{V} = \frac{1}{2} \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{x}') V(\vec{x},\vec{x}') \hat{\psi}(\vec{x}') \hat{\psi}(\vec{x}) \tag{343}$$

The Hamiltonian is given as:

$$\hat{H} = \int \mathrm{d}^3x \left[\frac{\hbar^2}{2m}(\vec{\nabla}\hat{\psi}^\dagger(\vec{x}))(\vec{\nabla}\hat{\psi}(\vec{x})) + \hat{\psi}^\dagger(\vec{x}) U(\vec{x}) \hat{\psi}(\vec{x})\right] + \frac{1}{2} \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{x}') V(\vec{x},\vec{x}') \hat{\psi}(\vec{x}') \hat{\psi}(\vec{x}) \tag{344}$$

The particle density operator (for pointlike particles) is:

$$n(\vec{x}) = \sum_\alpha \delta^{(3)}(\vec{x} - \vec{x}_\alpha)$$

Which can be written as:

$$\hat{n}(\vec{x}) = \sum_{i,k} \hat{a}_i^\dagger \hat{a}_k \int \mathrm{d}^3x'\, \varphi_i^*(\vec{x}') \delta^{(3)}(\vec{x} - \vec{x}') \varphi_k(\vec{x}') = \sum_{i,k} \hat{a}_i^\dagger \hat{a}_k \varphi_i^*(\vec{x}) \varphi_k(\vec{x}) \tag{345}$$

$$\overset{333,334}{=} \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x}) \tag{346}$$

The total particle number operator is:

$$\hat{N} = \int \mathrm{d}^3x\, \hat{n}(\vec{x}) \tag{347}$$

[16.12.2024, Lecture 20]

[18.12.2024, Lecture 21]

Application: Principle of the Laser

Consider a system of atoms or molecules in states $|1\rangle, |2\rangle$, with $E_2 > E_1$, occupations numbers n_1, n_2; and photons with energy $E_\gamma = E_2 - E_1$, i.e. $\omega_\gamma = (E_2 - E_1)/\hbar \implies |\vec{k}_0| = \omega_0/c$ fixed, but direction $\vec{k}_0/|\vec{k}_\gamma|$ is not. $n_{\vec{k}_\gamma}$ number of photons with momentum $\hbar\vec{k}_\gamma$.
Absorption:

$$|1, n_{\vec{k}_\gamma}\rangle \longrightarrow |2, n_{\vec{k}_\gamma} - 1\rangle; \text{ needs matrix element}$$

$$\langle n_{\vec{k}_\gamma} - 1, 2|\hat{H}|n_{\vec{k}_\gamma}, 1\rangle \propto \langle n_{\vec{k}_\gamma} - 1|\hat{a}_{\vec{k}_\gamma}|n_{\vec{k}_\gamma}\rangle \overset{294}{=} \sqrt{n_{\vec{k}_\gamma}} \tag{348}$$

Emission:

$$|2, n_{\vec{k}_\gamma}\rangle \longrightarrow |1, n_{\vec{k}_\gamma} + 1\rangle; \text{ needs matrix element}$$

$$\langle n_{\vec{k}_\gamma}+1,1|\hat{H}|n_{\vec{k}_\gamma},2\rangle \propto \langle n_{\vec{k}_\gamma}+1|\hat{a}^\dagger_{\vec{k}_\gamma}|n_{\vec{k}_\gamma}\rangle \overset{292}{=} \sqrt{n_{\vec{k}_\gamma}+1} \tag{349}$$

Explains the difference betweeen equations (175) and (176). Atomic/ molecular parts of the transition matrix elements arte the same (up to hermitian conjugate) $\implies$ rate of change of $n_{\vec{k}_\gamma}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}n_{\vec{k}_\gamma} = A\cdot\left[n_2(n_{\vec{k}_\gamma}+1)-n_1 n_{\vec{k}_\gamma}\right], \tag{350}$$

where A is a constant from atomic physics, n_2 represents emission and n_1 represents absorption. If $n_{\vec{k}_\gamma}(t=0)=0, n_2>0$, then spontaneous emission produces first photon. Once $n_{\vec{k}_\gamma} >> 1$ (laser), then to further increase $n_{\vec{k}_\gamma}$ requires $\underline{n_2 > n_1}$. That means more atoms/ molecules are needed in a state with higher energy, which is not possible in thermal equilibrium. One cannot achieve $n_2 > n_1$ through optical pumping in 2-state system!

$$\left.\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}n_2 &= A[n_1 n_{\vec{k}_\gamma} - n_2(n_{\vec{k}_\gamma}+1)]\\ \tfrac{\mathrm{d}}{\mathrm{d}t}n_1 &= A[-n_1 n_{\vec{k}_\gamma} + n_2(n_{\vec{k}_\gamma}+1)]\end{aligned}\right\}\implies \frac{\mathrm{d}}{\mathrm{d}t}(n_1+n_2)=0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(n_2-n_1) = 2A(n_1-n_2)n_{\vec{k}_\gamma} - 2An_2$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(n_2-n_1) > 0 \ \underline{\text{only}} \text{ if } n_1>n_2;\ \text{once } n_2=n_1>>1: n_2-n_1\simeq \text{ const.}$$

The parts $n_1 n_{\vec{k}_\gamma}$ correspond to absorption and the parts $n_2(n_{\vec{k}_\gamma}+1)$ and correspond to emission, whereas the part $2An_2$ corresponds to spontaneous emission.
If $n_2 >> n_1$ and const.:

$$n_{\vec{k}_\gamma}(t) = [n_{\vec{k}_\gamma}(0)+1]e^{An_2 t}-1 \tag{351}$$

Exponential growth of photons with fixed $\vec{k}_\gamma$ and hence fixed E_γ.
Possibilitiesto achieve $n_2 > n_1$

* physically seperate states $|2\rangle$ and $|1\rangle$. Example: NH_3 maser (where m stands for microwaves). Excited state $|2\rangle$ couples differently to external $\vec{E}$-fields $\implies$ in presence of $\vec{E}$-fields, molecules in $|2\rangle$ can be locally enhanced relative to those in $|1\rangle$, which allows the existence of masers in space!

* Use 3-level system:

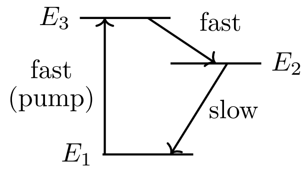


Figure 1: $A_{13}A_{23} >> A_{12}$

Since $|1\rangle \leftrightarrow |2\rangle$ transitions are slow (e.g. due to selection rules), many atoms can be pumped from $|1\rangle$ to $|3\rangle$, which quickly decay to $|2\rangle$, where they stay "a long time", allowing $n_2 >> n_1$. But the disadvantage is, that more than 50% of atomes/ molecules must be excited, which is not very efficient. Example: ruby laser

* Use 4-level scheme:

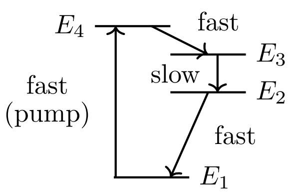


Figure 2: can get $n_3 >> n_2$ even if $n_1 >> n_3$

The pumped atoms accumulate in $|3\rangle$; lasing from $|3\rangle \longrightarrow |2\rangle$ transitions. The pumping does not need to be optical, but thermal excitation does not work.

[18.12.2024, Lecture 21]

[23.12.2024, Lecture 22]

Bell's Inequalitiy

Hold for <u>local</u> alternatives to standard Quantum Mechanics ("hidden variable theories"), are <u>violated</u> by standard Quantum Mechanics as well as by experimental data! The set-up requires the preparation of "entangled states". Simplest example:
2 particles in a spin-singlet state. Here: spin-$\frac{1}{2}$ particles.

$$\psi = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{z,1}|\downarrow\rangle_{z,2} - |\downarrow\rangle_{z,2}|\uparrow\rangle_{z,1}\right) \tag{352}$$

$|\uparrow\rangle_z, |\downarrow\rangle_z$ are one-particle states with $\hat{S}_z = \pm\frac{\hbar}{2}$. This state has the <u>same</u> form when written in eigenstates of another component of $\hat{\vec{S}}$, e.g.,

$$\psi = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{x,1}|\downarrow\rangle_{x,2} - |\downarrow\rangle_{x,2}|\uparrow\rangle_{x,1}\right) \tag{353}$$

$|\uparrow\rangle_x, |\downarrow\rangle_x$ are eigenstates of $\hat{S}_x$ with eigenvalues $\pm\frac{\hbar}{2}$. This leads to the **Einstein-Podolsky-Rosen effect** (<u>not</u> paradox): The result of a measurement on particle 2 depends on what kind of measurement has been performed on particle 1. For example:

* No measurement on particle 1:
A measurement of $\hat{S}_z$ on particle 2 gives $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$ with equal probability of 50%. A measurement of $\hat{S}_x$ on particle 2 also gives $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ with equal probabilities.

* If $\hat{S}_z$ on particle 1 has been measured, a measurement of $\hat{S}_z$ on particle 2 <u>always</u> yields $-S_{z,1}$ with 100% probability, even if the two measurements have space-like separation. (<u>Cannot</u> use this for FTL communication.) A measurement of $\hat{S}_x$ on particle 2 gives $S_x = +\frac{\hbar}{2}$ and $S_x = -\frac{\hbar}{2}$ with equal probability.

* If $\hat{S}_x$ on particle 1 has been measured, a measurement of $\hat{S}_z$ on particle 2 gives $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ with equal probabilities. A measurement of $\hat{S}_x$ on particle 2 <u>always</u> gives $-S_{x,1}$.

Measurement on part. 1	$P(S_{z_2} = +\frac{\hbar}{2})$	$P(S_{z_2} = -\frac{\hbar}{2})$	$P(S_{x_2} = +\frac{\hbar}{2})$	$P(S_{x_2} = -\frac{\hbar}{2})$
none	0.5	0.5	0.5	0.5
$S_{z_1} = +\frac{\hbar}{2}$	0	1	0.5	0.5
$S_{z_1} = -\frac{\hbar}{2}$	1	0	0.5	0.5
$S_{x_1} = +\frac{\hbar}{2}$	0.5	0.5	0	1
$S_{x_1} = -\frac{\hbar}{2}$	0.5	0.5	1	0

More generally, let $\vec{a}, \vec{b}$ be two unit vectors; define measurements A on particle 1, B on particle 2:

$$A(\vec{a}) = \begin{cases} +1, & \text{if } \vec{S}_1 \text{ in } \vec{a}\text{-direction} = +\frac{\hbar}{2} \\ -1, & \text{if } \vec{S}_1 \text{ in } \vec{a}\text{-direction} = -\frac{\hbar}{2} \end{cases} \tag{354}$$

$$B(\vec{b}) = \begin{cases} +1, & \text{if } \vec{S}_2 \text{ in } \vec{b}\text{-direction} = +\frac{\hbar}{2} \\ -1, & \text{if } \vec{S}_2 \text{ in } \vec{b}\text{-direction} = -\frac{\hbar}{2} \end{cases} \tag{355}$$

Bell's inequality concerns <u>correlations</u> between measurements A and B.
For a spin-$\frac{1}{2}$ particle:

$$\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma} \implies P(\vec{a}, \vec{b}) = \langle A(\vec{a})B(\vec{b})\rangle = \langle\psi|\vec{\sigma}(1)\cdot\vec{a}\,\vec{\sigma}(2)\cdot\vec{b}|\psi\rangle \tag{356}$$

$$= \langle\psi| - \vec{\sigma}(1)\cdot\vec{a}\,\vec{\sigma}(1)\cdot\vec{b}|\psi\rangle = -\vec{a}\cdot\vec{b}, \tag{357}$$

where $\vec{\sigma}$ is the vector of Pauli matrices and $\vec{\sigma}(1) = -\vec{\sigma}(2)$ in spin singlet state.
Proof:

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Observation:

$$\sigma_i \sigma_j = \delta_{ij} \mathbb{I} + i \sum_{k=1}^{3} \varepsilon_{ijk} \sigma_k, \tag{358}$$

where ε_{ijk} is the Levi-Civita symbol, and $\varepsilon_{123} = +1$ (totally antisymmetric).
For example:

$$\sigma_1\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \sigma_2\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$\sigma_2\sigma_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\sigma_1 = i\varepsilon_{231}\sigma_1.$$

Hence:

$$P(\vec{a},\vec{b}) = \langle\psi| - \sum_{i,j=1}^{3} \sigma_i(1)\sigma_j(1) a_i b_j |\psi\rangle \overset{358}{=} \langle\psi| - \sum_{i,j=1}^{3} a_i b_j \left(\delta_{ij} + i\sum_{k=1}^{3} \varepsilon_{ijk}\sigma_k(1)\right)|\psi\rangle = -\langle\psi|\sum_{i=1}^{3} a_i b_i |\psi\rangle = -\vec{a}\cdot\vec{b},$$

where for a singlet state $\langle\psi|\sigma_k|\psi\rangle = 0$.
"Hidden-variable theories": measurement on particle 2 must not depend on any possible measurement on particle 1, but both measurements can depend on "hidden variables" λ. As before:

$$A(\vec{a},\lambda) = \pm 1, \quad B(\vec{b},\lambda) = \pm 1 \tag{359}$$

Since the outcome of B is not allowed to depend on $\vec{a}$.

$$P(\vec{a},\vec{b}) = \int \mathrm{d}\lambda\, \rho(\lambda) A(\vec{a},\lambda) B(\vec{b},\lambda) \tag{360}$$

Does not hold in quantum mechanics!

$$\rho(\lambda): \text{ probability distribution, } \int \mathrm{d}\lambda\, \rho(\lambda) = 1 \tag{361}$$

Can engineer $\rho(\lambda)$ such that (e.g.) extreme cases from the table are reproduced:

$$P(\vec{a},\vec{a}) = -P(\vec{a},-\vec{a}) = -1 \tag{362}$$
$$\text{and } P(\vec{a},\vec{b}) = 0 \quad \text{if } \vec{a}\cdot\vec{b} = 0 \tag{363}$$

Simplest solution: Let $\vec{\lambda}$ be a unit vector, $\vec{\lambda} = (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$, with flat distribution in $\cos\theta$ and φ, take:

$$A(\vec{a},\vec{\lambda}) = \mathrm{sign}(\vec{a}\cdot\vec{\lambda}), \tag{364}$$
$$B(\vec{b},\vec{\lambda}) = -\mathrm{sign}(\vec{b}\cdot\vec{\lambda}). \tag{365}$$

$$\rho(\varphi,\cos\theta) = \frac{1}{4\pi} = \text{const.}$$

Let $\vec{a} = (0,0,1)$ (defines frame), and $\vec{b} = (\cos\varphi_b\sin\theta_b, \sin\varphi_b\sin\theta_b, \cos\theta_b)$. Then:

$$P(\vec{a},\vec{b}) = -\frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\varphi\int_{-1}^{1}\mathrm{d}(\cos\theta)\ \mathrm{sign}(\underbrace{\cos\theta}_{\vec{a}\cdot\vec{\lambda}})\mathrm{sign}[\underbrace{(\cos\varphi_b\cos\varphi + \sin\varphi_b\sin\varphi)}_{\cos(\underbrace{\varphi_b-\varphi}_{\tilde{\varphi}})}\sin\theta_b\sin\theta + \cos\theta_b\cos\theta]$$

$$= -\frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\tilde{\varphi}\int_{-1}^{1}\mathrm{d}(\cos\theta)\,\mathrm{sign}(\cos\theta)\mathrm{sign}[\cos\tilde{\varphi}\sin\theta_b\sin\theta + \cos\theta_b\cos\theta]$$

If $\vec{a} = \vec{b}$, then $\cos\theta_b = 1$ and $\sin\theta_b = 0$, so:

$$P(\vec{a},\vec{a}) = -\frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}(\cos\theta)\, \underbrace{[\mathrm{sign}(\cos\theta)]^2}_{1} = -1 \quad \checkmark$$

If $\vec{a}\cdot\vec{b} = 0 \implies \cos\theta_b = 0$, $\sin\theta_b = 1$, then:

$$P(\vec{a},\vec{b}) = -\frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}(\cos\theta)\, \mathrm{sign}(\cos\theta)\mathrm{sign}(\cos\tilde{\varphi}\sin\theta) = 0 \quad \checkmark$$

<u>No</u> local hidden variable theory exists that can reproduce <u>all</u> QM predictions!
<u>Proof:</u> In order to have $P(\vec{a},\vec{a}) = -1$, we need $A(\vec{a},\lambda) = -B(\vec{a},\lambda)\ \forall \vec{a}$ (364,365) follow from (360) and (361).

$$\implies P(\vec{a},\vec{b}) = -\int \mathrm{d}\lambda\, \rho(\lambda) A(\vec{a},\lambda)A(\vec{b},\lambda)$$

Introduce a third unit vector $\vec{c}$:

$$\begin{aligned} P(\vec{a},\vec{b}) - P(\vec{a},\vec{c}) &= -\int \mathrm{d}\lambda\, \rho(\lambda)\left[A(\vec{a},\lambda)A(\vec{b},\lambda) - A(\vec{a},\lambda)A(\vec{c},\lambda)\right] \\ &= \int \mathrm{d}\lambda\, \rho(\lambda) A(\vec{a},\lambda)A(\vec{b},\lambda)\underbrace{\left[-1 + A(\vec{b},\lambda)A(\vec{c},\lambda)\right]}_{\le 0}, \text{ used } \left[A(\vec{b},\lambda)\right]^2 = 1 \end{aligned}$$

Using the linearity of integration and the property $|f(x)| \le \int |f(x)| dx$:

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \le \int \mathrm{d}\lambda\, \rho(\lambda)\, \cancelto{1}{\left|A(\vec{a},\lambda)A(\vec{b},\lambda)\right|}\ \left[1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\right]$$

Since $A(\vec{b},\lambda)A(\vec{c},\lambda) \le 1$:

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \le 1 + P(\vec{b},\vec{c})$$

$$1 + P(\vec{b},\vec{c}) \ge \left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \quad \forall\, \vec{a},\vec{b},\vec{c} \tag{366}$$

Bell's inequality holds for all local hidden variable theories that reproduce $P(\vec{a},\vec{a}) = -1$. However, this does <u>not</u> hold in quantum mechanics!
Let $\vec{a},\vec{b},\vec{c}$ all be in the (x,z) plane. From (357) <u>in QM</u>:

$$P(\vec{a},\vec{b}) = -\cos\theta_{ab}, \tag{367}$$

where θ_{ab} is the angle between $\vec{a}$ and $\vec{b}$.
For example, consider $\theta_{ab} = \theta_{bc} = 45° \implies \theta_{ac} = 90°$. Then: $1 + P(\vec{b},\vec{c}) = 1 - \cos(45°) = 1 - \frac{\sqrt{2}}{2} \approx 0.293$

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| = |-\cos(45°) + \cos(90°)| = \frac{\sqrt{2}}{2} \approx 0.707 > 0.293$$

First convincing measurement showing violation of (366): Aspect, Grangier, Roger (1981), using $\gamma = 0 \longrightarrow \gamma = 1 \longrightarrow \gamma = 0$ 2-photon transition in atomic Ca. Photons must be in spin-singlet state!

[23.12.2024, Lecture 22]

[08.01.2025, Lecture 23]

Relativistic Quantum Mechanics

<u>Problem:</u> Even for a free particle, the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi \tag{368}$$

is not Lorentz covariant: contains only <u>first</u> derivative with respect to time, but <u>second</u> derivative with respect to space; Lorentz transformation mixes space & time.
$\implies$ need different "equation of motion" for the wave function!
<u>Note:</u> The other "axioms" of Quantum Mechanics, see (chapter 1), need not be changed.

Relativistic Kinematics

Very convenient to use notion of 4-vectors. E.g. contravariant space-time 4-vector

$$x^\mu = (ct, \vec{x}) \tag{369}$$

Lorentz-transformation is described by:

$$x^\mu \to x'^\mu = \Lambda^\mu_\nu x^\nu \equiv \sum_{\nu=0}^{3} \Lambda^\mu_\nu x^\nu \tag{370}$$

$$\Lambda^\mu_\nu \text{ is a second-rank tensor. When considered as a matrix: satisfies } \det\Lambda = 1 \tag{371}$$

Example:

* Rotations:

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & & & \\ 0 & & O(3) & \\ 0 & & & \end{pmatrix} \tag{372}$$

$$\text{where } O(3) \text{ is a real, orthogonal } 3\times 3 \text{ matrix: } O(3)O(3)^T = O(3)^T O(3) = \mathbb{I}_{3\times 3} \tag{373}$$

* Boosts: E.g., for boost in x-direction:

$$\Lambda = \begin{pmatrix} \gamma & \beta\gamma & 0 & 0 \\ \beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{374}$$

Here

$$\beta = \frac{v}{c}, \quad v: \text{ relative velocity between 2 inertial frames} \tag{375}$$

$$\text{and } \gamma = \frac{1}{\sqrt{1-\beta^2}} = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \tag{376}$$

Explicitly:

$$ct' = \gamma ct + \beta\gamma x \implies t' = \gamma t + \frac{\beta\gamma x}{c} \xrightarrow{c\to\infty} t \tag{377}$$

$$x' = \beta\gamma ct + \gamma x \underset{375}{=} \gamma(x + vt) \xrightarrow{c\to\infty} x + vt \quad \text{(Galileo transform!)} \tag{378}$$

Usual velocity of a particle:

$$\vec{u} = \frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = c\frac{\mathrm{d}\vec{x}}{\mathrm{d}x^0} \tag{379}$$

In order to construct the velocity 4-vector, use eigentime (proper time) τ, whose differential

$$\mathrm{d}\tau = \frac{1}{\gamma(\vec{u})}\mathrm{d}t = \sqrt{1-\frac{\vec{u}^2}{c^2}}\,\mathrm{d}t \tag{380}$$

τ is Lorentz-invariant: time as measured in the particle's rest frame.
Define velocity 4-vector:

$$u^\mu = \gamma(\vec{u})(c, \vec{u}) \tag{381}$$

Multiply this with rest mass m to get 4-momentum:

$$p^\mu = m u^\mu = m\gamma(\vec{u})(c, \vec{u}) \tag{382}$$

Massless particle with finite momentum (e.g., photon): $m\gamma \xrightarrow{m\to 0} \text{const.} \implies \frac{m}{\sqrt{1-\frac{\vec{u}^2}{c^2}}} \xrightarrow{m\to 0} \text{const.} \implies |\vec{u}| \to c$:
massless particles travel with the speed of light in vacuum.
The zeroth component of p^μ is relativistic energy divided by c:

$$p^0 = \frac{E}{c} \overset{382}{=} m\gamma(\vec{u})c \implies E(\vec{u}) \qquad = mc^2\gamma(\vec{u}) \tag{383}$$

Lorentz-invariant quantities can be obtained by saturating all Lorentz indices. To that end, introduce the covariant 4-vector with lower indices; raising/lowering indices with the help of the Minkowski metric:

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{384}$$

$$a_\nu = g_{\nu\mu} a^\mu \tag{385}$$

If $a^\mu = (a^0, \vec{a})$, then $a_\mu = (a^0, -\vec{a})$.

$$a^2 \equiv a_\mu a^\mu = a^\mu g_{\mu\nu} a^\nu = (a^0)^2 - \vec{a}^2 \tag{386}$$

is Lorentz-invariant, as are all products:

$$a \cdot b \equiv a_\mu b^\mu = a^\mu b_\nu = a^\mu b^\nu g_{\mu\nu} \tag{387}$$

Check:

$$\begin{aligned} x^\mu x_\mu &\overset{386}{=} c^2 t^2 - \vec{x}^2 \to c^2 t'^2 - \vec{x}'^2 \\ &= c^2 \left(\gamma t + \beta\gamma \frac{x}{c} \right)^2 - \gamma^2 (x + \beta c t)^2 - y^2 - z^2, \quad \text{used 377 and 378} \\ &= c^2\gamma^2 t^2 + \beta^2\gamma^2 x^2 + \cancel{2\beta\gamma^2 ctx} - \gamma^2 x^2 - \beta^2\gamma^2 c^2 t^2 - \cancel{2\beta\gamma^2 ctx} - y^2 - z^2 \\ &= c^2 t^2 \underbrace{(\gamma^2 - \beta^2\gamma^2)}_{\gamma^2(1-\beta^2)=1} - x^2(\gamma^2 - \beta^2\gamma^2) - y^2 - z^2 \\ &= c^2 t^2 - x^2 - y^2 - z^2 = c^2 t^2 - \vec{x}^2 \end{aligned}$$

[8.01.2025, Lecture 23]

[13.01.2025, Lecture 24]

$$p^2 \equiv p_\mu p^\mu \overset{382}{=} m^2 \gamma^2(\vec{u})(c^2 - \vec{u}^2) \overset{376}{=} \frac{m^2}{1 - \frac{\vec{u}^2}{c^2}} (c^2 - \vec{u}^2) = m^2 c^2 \tag{388}$$

Since $p^\mu = (\frac{E}{c}, \vec{p})$, where $\vec{p} = \gamma(\vec{u}) m \vec{u}$

$$\Rightarrow p^2 = \frac{E^2}{c^2} - \vec{p}^2 \overset{388}{=} m^2 c^2 \quad \Rightarrow \quad E^2 = m^2 c^4 + \vec{p}^2 c^2 \tag{389}$$

Low-energy expansion:

$$E = \sqrt{m^2 c^4 + \vec{p}^2 c^2} = mc^2 \sqrt{1 + \frac{\vec{p}^2}{m^2 c^2}} \simeq mc^2 (1 + \frac{\vec{p}^2}{2m^2 c^2}) = mc^2 + \frac{\vec{p}^2}{2m},$$

where mc^2 is a irrelevant constant and $\frac{\vec{p}^2}{2m}$ is the non-relativistic kinetic Energy E_{kin}.
High-energy expansion: $E \simeq |\vec{p}|c$; agrees with $\omega = |\vec{k}| \cdot c$ for photons.

The Klein-Gordon Equation

Expression for $E(\vec{p})$ is related to free-particle wave equation via $0 \to \hat{0}$.

$$E \to \hat{E} = i\hbar \frac{\partial}{\partial t}, \quad \vec{p} \to \hat{\vec{p}} = -i\hbar \vec{\nabla} \tag{390}$$

In non-relativistic case: $E = \vec{p}^2/2m$ gives

$$i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} = -\frac{\hbar^2 \vec{\nabla}^2}{2m} \psi(\vec{x}, t): \text{ free Schrödinger equation} \tag{391}$$

In relativistic case: $E^2 = \vec{p}^2c^2 + m^2c^4 \Rightarrow E = \sqrt{\vec{p}^2c^2 + m^2c^4}$: would give

$$i\hbar\frac{\partial\phi(\vec{x},t)}{\partial t} \underset{\text{no!}}{\overset{?}{=}} \sqrt{m^2c^4 - \hbar^2c^2\vec{\nabla}^2}\phi(\vec{x},t) \tag{392}$$

Obvious difficulty: interpretation of $\sqrt{\ }$: if written as power series would involve arbitrary high derivatives. Instead: use (389) directly (Schrödinger 1926; Gordon 1926; Klein 1927)

$$\begin{aligned}
-\hbar^2\frac{\partial^2\phi(\vec{x},t)}{\partial t^2} &= (-\hbar^2c^2\vec{\nabla}^2 + m^2c^4)\phi(\vec{x},t), \quad t = \frac{x^0}{c}\\
\Rightarrow -\hbar^2c^2\frac{\partial^2\phi(x^\mu)}{\partial x^{0^2}} &= \hbar^2c^2\sum_i\frac{\partial^2\phi(x^\mu)}{\partial x^i} + m^2c^4\phi(x^\mu)\\
\Rightarrow (\frac{\partial^2}{\partial x^{0^2}} - \sum_i\frac{\partial^2}{\partial x^{i^2}})\phi(x^\mu) &+ \frac{m^2c^2}{\hbar^2}\phi(x^\mu) = 0
\end{aligned}$$

$$\partial_\mu\partial^\mu\phi(x^\mu) + \frac{m^2c^2}{\hbar^2}\phi(x^\mu) = 0 \tag{393}$$

This is the Klein-Gordon equation, where $\partial_\mu\partial^\mu$ is manifestly Lorentz-invariant; used

$$\partial_\mu \equiv \frac{\partial}{\partial x^\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}) \tag{394}$$

$$\Rightarrow \partial^\mu = (\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}) \tag{395}$$

$\frac{m^2c^2}{\hbar^2} = \frac{1}{\lambda_c^2}; \lambda_c = \frac{\hbar}{mc}$: Compton wavelength

Probabilistic interpretation of wave function $\psi(\vec{x},t)$ is motivated by continuity equation:

$$\psi^*(391) - \psi(391)^* = \psi^*\underbrace{\left(i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2\vec{\nabla}^2\psi}{2m}\right)}_{=0} - \psi\underbrace{\left(-i\hbar\frac{\partial\psi^*}{\partial t} + \frac{\hbar^2\vec{\nabla}^2\psi^*}{2m}\right)}_{=0} = 0$$

$$\begin{aligned}
\Longrightarrow i\hbar\frac{\partial}{\partial t}\left(\psi^*\psi + \psi\frac{\partial\psi^*}{\partial t}\right) + \frac{\hbar^2}{2m}\left(\psi^*\vec{\nabla}^2\psi - \psi\vec{\nabla}^2\psi^*\right) &= 0\\
\Longrightarrow i\hbar\frac{\partial}{\partial t}(\psi^*\psi) + \frac{\hbar^2}{2m}\vec{\nabla}\cdot\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) &= 0\\
\Longrightarrow \frac{\partial}{\partial t}(\psi^*\psi) + \frac{\hbar}{2im}\vec{\nabla}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) &= 0
\end{aligned}$$

$$\Longrightarrow \frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0 \tag{396}$$

with:

$$\rho = |\psi(t)|^2, \quad \vec{j} = \frac{i\hbar}{2m}\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\varphi\right) \tag{397}$$

Analogously:

$$\begin{aligned}
\phi^*\cdot(393) - \phi\cdot(393)^* &= \phi^*\left(\partial_\mu\partial^\mu + \cancel{\frac{m^2c^2}{\hbar^2}}\right)\phi - \phi\left(\partial_\mu\partial^\mu + \cancel{\frac{m^2c^2}{\hbar^2}}\right)\phi^*\\
&= \frac{1}{c^2}\phi^*\frac{\partial^2\phi}{\partial t^2} - \phi^*\vec{\nabla}^2\phi - \frac{1}{c^2}\phi\frac{\partial^2\phi^*}{\partial t^2} + \phi\vec{\nabla}^2\phi^*\\
&= \frac{1}{c^2}\frac{\partial}{\partial t}\left(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t}\right) + \vec{\nabla}\cdot\left(\phi\vec{\nabla}\phi^* - \phi^*\vec{\nabla}\phi\right) \qquad \Big|\cdot\frac{i\hbar}{2m}
\end{aligned}$$

$$\Longrightarrow \frac{\partial}{\partial t}\left[\frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t}\right)\right] + \vec{\nabla}\cdot\underbrace{\left[\frac{i\hbar}{2m}\left(\phi\vec{\nabla}\phi^* - \phi^*\vec{\nabla}\phi\right)\right]}_{\text{non-relativistic 3-current}} = 0 \tag{398}$$

$$\implies \rho = \frac{i\hbar}{2mc^2}\left(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t}\right) \tag{399}$$

Problem: While the non-relativistic density (397) is manifestly non-negative, and can hence be a probability density, the expression in (399) may be negative!
The Klein-Gordon equation is 2nd order in time derivative $\implies$ can choose $\phi(\vec{x},0)$ and $\frac{\partial\phi}{\partial t}(\vec{x},0)$ freely as initial conditions.
Possible way out: interpret (399) as "charge density" of some charge; charge can have either sign! Solutions of the Klein-Gordon equation can be expanded in plane waves:

$$\phi(x^\mu) = Ne^{-ip\cdot x/\hbar} = Ne^{-i(p^0x^0-\vec{p}\cdot\vec{x})/\hbar} = Ne^{-i(Et-\vec{p}\cdot\vec{x})/\hbar} \tag{400}$$

Check:

$$\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = -\frac{E^2}{\hbar^2c^2}\phi, \quad \vec{\nabla}^2\varphi = -\frac{\vec{p}^2}{\hbar^2}\phi$$
$$\implies \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \vec{\nabla}^2 + \frac{m^2c^2}{\hbar^2}\right)\phi = \left(-\frac{E^2}{\hbar^2c^2} + \frac{\vec{p}^2}{\hbar^2} + \frac{m^2c^2}{\hbar^2}\right)\phi = -\frac{1}{\hbar^2c^2}\left(E^2 - \vec{p}^2c^2 - m^2c^4\right)\phi \stackrel{!}{=} 0$$
$$\implies E^2 = \vec{p}^2c^2 + m^2c^4$$

Problem: (400) solves (393) with given $\vec{p}$ for either sign of E:

$$E = \pm\sqrt{\vec{p}^2c^2 + m^2c^4} \tag{401}$$

Insert (400) in (399):

$$\rho_{PW} = \frac{i\hbar}{2mc^2}|N|^2(-iE\cdot 2) = \frac{E\hbar|N|^2}{mc^2} \tag{402}$$

Solution of $E < 0$ problem:

* Ignore: not an option $\implies$ need all linearly independent solutions of K-G equation to solve general problems $\implies$ K-G equation was abandoned for a while.

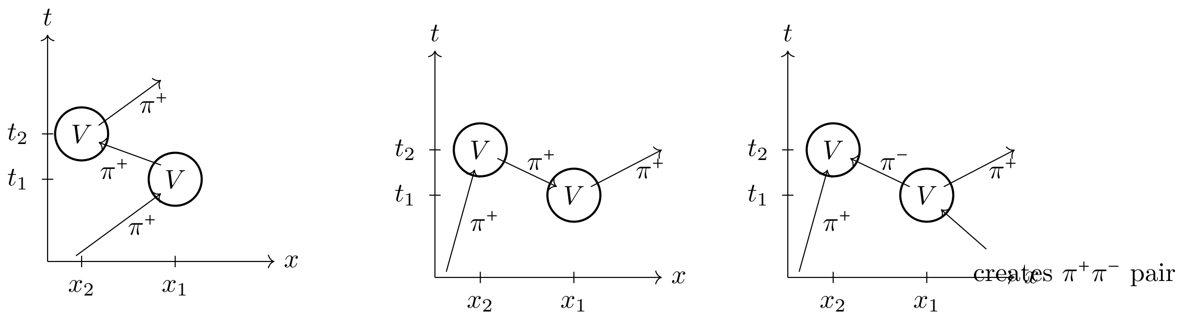
* (402) indicates a connection to antiparticles: have the same mass as usual particles, and the same spin, but opposite charge (s). Example for spin-0 particle charged pion π^+: $q_{\pi^+} = +e, \alpha$-particle (in ground state), ...; corresponding antiparticles are π^- ($q_{\pi^-} = -e$), $\bar{\alpha}$, ... This allows consistent treatment of $E < 0$ solutions! Heuristically (Feynman 1962):

  Negative-energy particle solution traveling "backward in time" $\equiv$ positive-energy antiparticle solution traveling forw (403)

  plane-wave $\sim e^{-i(p^0x^0-\vec{p}\cdot\vec{x})/\hbar}$ is supposed to travel in the $+\vec{p}$ direction: $-i\vec{\nabla}\phi_{PW} = +\vec{p}\phi_{PW}$. But: step $\vec{x} \to \vec{x} + \mathrm{d}\vec{x}$, with $\mathrm{d}\vec{x} \uparrow\uparrow \vec{p}$, leaves phase constant if $p^0\mathrm{d}t > 0 \implies$ need $\mathrm{d}t < 0$ if $p^0 < 0$!

Illustration of (403):

* Second-order scattering of π^+ on external potential: two paths are possible!



π^+ always travels forward in time: no problem

$E < 0$ travels backward in time

$E > 0$ travels forward in time

- More generally: emitting a π^- with $E_{\pi^-} > 0$, $\vec{p}_{\pi^-}$ is physically equivalent to <u>absorbing</u> a π^+ with $E_{\pi^+} < 0$, $\vec{p}_{\pi^+}$, i.e. $p^\mu_{\pi^+} = -p^\mu_{\pi^-}$
  - charge: $Ze \to Z'e$, emit $\pi^- : Z' = Z + 1 = Z'$ absorb π^+
  - 4-momentum: $p^\mu \to p'^\mu$: emit $\pi^- : p^\mu = p'^\mu + p^\mu_{\pi^-} \implies p'^\mu = p^\mu - p^\mu_{\pi^-} = p^\mu + p^\mu_{\pi^+} = p'^\mu$: absorb π^+
- Electromagnetic current of π^- from (390, 400):

$$j_{\pi^-}(p_{\pi^-}) = |N|^2 \cdot \underbrace{(-e)}_{q_{\pi^-}} \cdot \left(\frac{E_{\pi^-}\hbar}{m_{\pi^-}c^2}, \frac{\hbar}{m_{\pi^-}}\vec{p}_{\pi^-}\right) = |N|^2 \cdot \underbrace{e}_{q_{\pi^+}} \cdot \left(-\frac{E_{\pi^-}\hbar}{m_{\pi^-}c^2}, \frac{\hbar}{\underbrace{m_{\pi^-}}_{=\, m_{\pi^+}}}(-\vec{p}_{\pi^-})\right) = j_{\pi^+}(p_{\pi^+} = -p_{\pi^-})$$

<u>Rigorous Treatment:</u> Use (Heisenberg-picture) field operator: satisfy Klein-Gordon equation. In terms of momentum eigenstates:

$$\hat{\phi}_{\pi^+}(x^\mu) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{1}{\sqrt{2E_{\vec{p}}}} \left(\hat{a}_{\vec{p}} e^{-ip\cdot x} + \hat{b}^\dagger_{\vec{p}} e^{ip\cdot x}\right) \tag{404}$$

where the Integral is over 3-momentum only and $E_{\vec{p}} = +\sqrt{\vec{p}^2c^2 + m^2_{\pi^+}c^4}$.

$$\left.\begin{aligned} &\hat{a}_{\vec{p}} : \text{destroys } \pi^+ \\ &\hat{b}^\dagger_{\vec{p}} : \text{creates } \pi^- \end{aligned}\right\} \implies \hat{\phi}_{\pi^+} \text{ can destroy a } \pi^+ \text{ \underline{or} create a } \pi^-.$$

Similarly,

$$\hat{\phi}_{\pi^-}(x^\mu) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{1}{\sqrt{2E_{\vec{p}}}} \left(\hat{a}^\dagger_{\vec{p}} e^{ip\cdot x} + \hat{b}_{\vec{p}} e^{-ip\cdot x}\right) \tag{405}$$

can create a $\pi^+(\hat{a}^\dagger_{\vec{p}})$ or destroy a $\pi^-(\hat{b}_{\vec{p}}) \implies \hat{\phi}_{\pi^+} \equiv \hat{\phi}_{\pi^-}$.
Normalization used here (Peskin & Schroeder):

$$\langle \vec{p} | \vec{q} \rangle = 2E_\pi (2\pi)^3 \delta^3(\vec{p} - \vec{q}) \tag{406}$$

is Lorentz-invariant, as is:

$$\frac{\mathrm{d}^3 p}{\sqrt{2E_{\vec{p}}}}; \quad |\vec{p}\rangle = \sqrt{2E_{\vec{p}}}\hat{a}^\dagger_{\vec{p}}|0\rangle \tag{407}$$

$$\hat{a}_{\vec{p}}|0\rangle = \hat{b}_{\vec{p}}|0\rangle = 0.$$

[13.01.2025, Lecture 24]

[15.01.2025, Lecture 25]

The Dirac Equation

Idea: to avoid negative density, write an equation that is first order in derivatives.

$$\text{Ansatz (Dirac 1928):} \quad i\hbar \frac{\partial \psi(x^\mu)}{\partial t} = -i\hbar c \sum_{k=1}^{3} \alpha_k \frac{\partial}{\partial x^k} \psi(x^\mu) + \beta mc^2 \psi(x^\mu) \tag{408}$$

Would violate rotational invariance if coefficients α_k were different $\mathbb{C}$-numbers $\implies \alpha_k, \beta$ must be <u>matrices</u> acting on N-component object ψ, which transforms nontrivially under rotations.

$$\text{R.h.s. of (408)} = \hat{H}\psi, \text{ with } \hat{H} \overset{!}{=} \hat{H}^\dagger \implies \alpha_k = \alpha_k^\dagger,\ \beta = \beta^\dagger \text{ hermitian} \tag{409}$$

Since the L.h.s. has N components $\implies \alpha_k, \beta$ must be $N \times N$ matrices. Coefficients α_k, β must be chosen such that the following conditions are satisfied:

(i) Components of ψ must satisfy the Klein-Gordon equation, since <u>all</u> relativistic particles satisfy $E^2 = \vec{p}^2c^2 + m^2c^4$.

(ii) $\exists$ a conserved 4-current j^μ, such that $j^0 = \rho c \geq 0$ manifestly.

(iii) (408) should be Lorentz-covariant, i.e. should have the same form in all inertial frames.

Start with (i). Take $i\hbar\partial_t$ (408):

$$
\begin{aligned}
(i\hbar)^2\frac{\partial^2\psi}{\partial t^2} &= -i\hbar c\sum_k \alpha_k \frac{\partial}{\partial x^k} i\hbar\frac{\partial\psi}{\partial t} + \beta mc^2 i\hbar\frac{\partial\psi}{\partial t} \\
&\overset{408}{=} -i\hbar c\sum_k \alpha_k\frac{\partial}{\partial x^k}\left[-i\hbar c\sum_j \alpha_j\frac{\partial\psi}{\partial x^j} + \beta mc^2\psi\right] + \beta mc^2\left[-i\hbar c\sum_k\alpha_k\frac{\partial\psi}{\partial x^k} + \beta mc^2\psi\right] \\
\implies -\hbar^2\frac{\partial^2\psi}{\partial t^2} &= -\hbar^2c^2\sum_{k,j}\alpha_k\alpha_j \underbrace{\frac{\partial^2\psi}{\partial x^k\partial x^i}}_{\text{sym. under } j\leftrightarrow k} - i\hbar mc^3\sum_k(\alpha_k\beta+\beta\alpha_k)\frac{\partial\psi}{\partial x^k} + m^2c^4\beta^2\psi \\
&= -\hbar^2c^2\sum_{j,k}\frac{1}{2}(\alpha_k\alpha_j + \alpha_j\alpha_k)\frac{\partial^2\psi}{\partial x^k\partial x^j} - i\hbar mc^3\sum_k(\alpha_k\beta+\beta\alpha_k)\frac{\partial\psi}{\partial x^k} + m^2c^4\beta^2\psi \\
&\underset{\text{K.-G.}}{\overset{!}{=}} -\hbar^2c^2\sum_l\frac{\partial^2\psi}{\partial x^{l2}} + m^2c^4\psi
\end{aligned}
$$

$$\implies \frac{1}{2}\{\alpha_k,\alpha_j\} = \delta_{kj}\mathbb{I} \implies \{\alpha_k,\alpha_j\} = 2\delta_{kj}\mathbb{I} \implies \alpha_k^2 = \mathbb{I} \quad \forall k \tag{410}$$

$$\{\alpha_k,\beta\} = 0 \quad \forall k \tag{411}$$

$$\beta^2 = \mathbb{I} \tag{412}$$

From (411):

$$\alpha_k\beta + \beta\alpha_k = 0 \implies \beta\alpha_k\beta + \beta^2\alpha_k = \beta\alpha_k\beta + \alpha_k = 0 \implies \alpha_k = -\beta\alpha_k\beta,$$

Take the trace on both sides $\left(\text{tr } M = \sum_{k=1}^N M_{kk}\right)$:

$$\implies \text{tr }\alpha_k = -\text{tr }(\underbrace{\beta}_{A}\underbrace{\alpha_k\beta}_{B}) \underset{\text{tr}(AB)\,=\text{tr}(BA)}{=} -\text{tr }(\alpha_k\underbrace{\beta^2}_{\mathbb{I}}) = -\text{tr }\alpha_k \implies \text{tr }\alpha_k = 0 \quad \forall k \tag{413}$$

$$\text{Similarly, from } \alpha_k \text{ and (411)} : \text{tr }(\beta) = 0 \tag{414}$$

Since $\alpha_k^2 = \beta^2 = \mathbb{I}$, the eigenvalues of α_k and β are ± 1. This and (414) $\implies$ N must be even (equal number of $+1$ and -1 eigenvalues)
For $N = 2$: All hermitian 2×2 matrices are linear combinations of $\mathbb{I}_{2\times 2}$ and the three Pauli matrices. This contains only 3 anti-commuting matrices, but we need $N = 4$. $\implies$ smallest possibility: $N = 4$
One set of matrices satisfying eqs. (410,411,412): ("Dirac representation")

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0\end{pmatrix}; \quad \beta = \begin{pmatrix}\mathbb{I}_{2\times 2} & 0 \\ 0 & -\mathbb{I}_{2\times 2}\end{pmatrix} \tag{415}$$

$$\alpha_k^2 = \begin{pmatrix}\sigma_k^2 & 0 \\ 0 & \sigma_k^2\end{pmatrix} = \mathbb{I}_{4\times 4}$$

The Dirac representation is <u>not</u> the only choice! If $\alpha_k \to U\alpha_k U^{-1}$, $\quad \beta \to U\beta U^{-1} \quad$ (same U)

$$
\begin{aligned}
\{\alpha_k,\alpha_\ell\} = \alpha_k\alpha_\ell + \alpha_\ell\alpha_k &\to U\alpha_k \cancelto{\mathbb{I}}{U^{-1}U}\alpha_\ell U^{-1} + U\alpha_\ell\cancelto{\mathbb{I}}{U^{-1}U}\alpha_k U^{-1} \\
&= U\{\alpha_k,\alpha_\ell\}U^{-1}
\end{aligned}
$$

$$\underset{410}{=} U\cdot 2\delta_{k\ell}\mathbb{I}_{4\times 4}\cdot U^{-1} = 2\delta_{k\ell}\mathbb{I}_{4\times 4}.$$

This transformation works for any non-singular 4×4 matrix U.

[15.01.2025, Lecture 25]

[20.01.2025, Lecture 26]

continuity equation

In (408) ψ is N-component column vector in Dirac space (called "spinor"). Define hermitian conjugate for $1 \times N$ matrix:

$$\psi^\dagger = \psi^{*^\dagger} = (\psi_1^*, \psi_2^*, \dots, \psi_N^*) \tag{416}$$

is row vector.

$$\psi^\dagger (408) : i\hbar \underbrace{\psi^\dagger \frac{\partial \psi}{\psi t}}_{\in \mathbb{C}} + i\hbar c \sum_{k=1}^{3} \psi^\dagger \alpha_k \frac{\partial \psi}{\partial x^k} - mc^2 \psi^\dagger \beta \psi = 0 \tag{417}$$

Take complex conjugate ≡ hermitian conjugate of this:

$$-i\hbar \frac{\partial \psi^\dagger}{\psi t} \psi - i\hbar c \sum_{k=1}^{3} \frac{\partial \psi^\dagger}{\partial x^k} \underbrace{\alpha_k^\dagger}_{\alpha_k} \psi - mc^2 \psi^\dagger \underbrace{\beta^\dagger}_{\beta} \psi \tag{418}$$

(417) - (418):

$$i\hbar \left(\psi^\dagger \frac{\partial \psi}{\partial t} + \frac{\partial \psi^\dagger}{\partial t} \psi \right) + i\hbar c \sum_{k=1}^{3} \left(\psi^\dagger \alpha_k \frac{\partial \psi}{\partial x^k} + \frac{\partial \psi^\dagger}{\partial x^k} \alpha_k \psi \right) = 0$$
$$\Leftrightarrow \cancel{i\hbar} \frac{\partial}{\partial t} (\psi^\dagger \psi) + \cancel{i\hbar} c \sum_{k=1}^{3} \frac{\partial}{\partial x^k} (\psi^\dagger \alpha_k \psi) = 0$$

Has form of a continuity equation, with

$$\rho = \psi^\dagger \psi = \sum_{a=1}^{4} |\psi_a|^2 \tag{419}$$
$$j^k = c \psi^\dagger \alpha_k \psi \tag{420}$$

$\rho \geq 0$ manifestly! Introduce 4-current $j^\mu = (j^0, \vec{\jmath}) = (c\rho, \vec{\jmath})$, such that $\partial_\mu j^\mu = \frac{1}{c} \frac{\partial j^0}{\partial t} + \sum_{k=1}^{3} \frac{\partial j^k}{\partial x^k} = 0$ In order to write the Dirac equation in covariant form, define new Dirac (4×4) matrices:

$$\gamma^0 = \beta, \tag{421}$$
$$\gamma^k = \beta \alpha_k \tag{422}$$

$$\beta = \beta^\dagger \implies \gamma^0 = \gamma^{0\dagger} \text{ is hermitian} \tag{423}$$

$$\alpha_k = \alpha_k^\dagger \implies \gamma^{k\dagger} = (\beta \alpha_k)^\dagger = \alpha_k^\dagger \beta^\dagger = \alpha_k \beta \overset{411}{=} -\beta \alpha_k = -\gamma^k \text{ anti-hermitian}$$

$$\gamma^{0^2} = \beta^2 = \mathbb{I} \tag{424}$$
$$\gamma^{k^2} = \beta \alpha_k \beta \alpha_k \overset{411}{=} -\beta^2 \alpha_k^2 \overset{410,412}{=} -\mathbb{I} \tag{425}$$

Non-diagonal anti-commutation relation:

$$\{\gamma^0, \gamma^k\} = \{\beta, \beta \alpha_k\} = \beta^2 \alpha_k + \beta \alpha_k \beta \overset{411}{=} \alpha_k - \beta^2 \alpha_k = 0 \tag{426}$$
$$\{\gamma^i, \gamma^k\} = \{\beta \alpha_i, \beta \alpha_k\} = -\{\alpha_i, \alpha_k\} = -2\delta_{ik} \mathbb{I} \tag{427}$$

(424,425,426,427) can be combined to:

$$\{\gamma^\mu, \gamma^\nu\} = 2 g^{\mu\nu} \mathbb{I}_{4\times 4} \tag{428}$$

where $g^{\mu\nu}$ is the Minkowski metric.

$$\beta \cdot (408) : -i\hbar \underbrace{\beta}_{\gamma^0} \underbrace{\frac{\partial \psi}{\partial t}}_{c \cdot \frac{\partial \psi}{\partial x^0}} - i\hbar c \sum_k \underbrace{\beta \alpha_k}_{\gamma^k} \frac{\partial \psi}{\partial x^k} + \beta^2 mc^2 \psi = 0$$

$$\Rightarrow (-i\gamma^\mu\partial_\mu + \underbrace{\frac{mc}{\hbar}}_{1/\lambda_C})\psi = 0 \tag{429}$$

Introduce "Dirac slash": for any 4-vector a_μ,

$$\not{a} \equiv \gamma^\mu a_\mu = \gamma_\mu a^\mu \tag{430}$$

$$\gamma_\mu = g_{\mu\nu}\gamma^\nu \tag{431}$$

where a_μ is a 4-vector in space-time, and γ^μ are constant. 4×4 matrices acting on spinors. In this notation:

$$\text{Free Dirac equation:} \left(-i\not{\partial} + \frac{mc}{\hbar}\right)\psi = 0 \tag{432}$$

Dirac representation of γ matrices:

$$(416), (421) \implies \gamma^0 = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \quad \gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix} \tag{433}$$

(429) looks "relativistic". In the case of the Klein-Gordon equation: ϕ is invariant. Here, ψ is <u>not</u> invariant, but the form of (429) should be the same in all inertial frames.
Had: $x' = \Lambda x$ (370). Since the Dirac equation is linear in $\psi \implies \psi$ must transform accordingly.

$$\psi'(x') = S(\Lambda)\psi(x) = S(\Lambda)\psi(\Lambda^{-1}x') \tag{434}$$

$S(\Lambda)$ must be a 4×4 matrix acting on spinor indices.
$\psi'(x')$ should satisfy the Dirac equation:

$$-i\gamma^\mu \frac{\partial}{\partial x'^\mu}\psi'(x') + \frac{mc}{\hbar}\psi'(x') = 0$$

Using (429):

$$\begin{aligned}
&-i\gamma^\mu \frac{\partial}{\partial x^\mu}\psi(x) + \frac{mc}{\hbar}\psi(x) = 0 \\
&\frac{\partial}{\partial x^\mu} = \frac{\partial}{\partial x'^\nu}\frac{\partial x'^\nu}{\partial x^\mu} \overset{370}{=} \Lambda^\nu{}_\mu \frac{\partial}{\partial x'^\nu}; \quad \psi(x) \overset{434}{=} S^{-1}(\Lambda)\psi'(x')
\end{aligned}$$

$$\begin{aligned}
&\implies \left(-i\gamma^\mu\Lambda^\nu{}_\mu \frac{\partial}{\partial x'^\nu} + \frac{mc}{\hbar}\right)S^{-1}(\Lambda)\psi'(x') = 0 \qquad \Big| S\cdot \quad \text{(from left)} \\
&\implies -i\underbrace{S(\Lambda)\Lambda^\nu{}_\mu\gamma^\mu S^{-1}(\Lambda)}_{\overset{!}{=}\gamma^\nu}\frac{\partial}{\partial x'^\nu}\psi'(x') + \frac{mc}{\hbar}\psi'(x') = 0
\end{aligned}$$

The Dirac equation is form-invariant, if $S(\Lambda)\Lambda^\nu{}_\mu\gamma^\mu S^{-1}(\Lambda) = \gamma^\nu$

$$\Rightarrow S^{-1}(\Lambda)\gamma^\nu S(\Lambda) \overset{!}{=} \Lambda^\nu{}_\mu\gamma^\mu \tag{435}$$

Let's construct $S(\Lambda)$ for infinitesimal Lorentz transformations:

$$\Lambda^\nu{}_\mu = g^\nu{}_\mu + \Delta\omega^\nu{}_\mu \tag{436}$$

with

$$\omega^{\nu\mu} = -\omega^{\mu\nu} \quad \text{note: two upper indices} \tag{437}$$

For example, in a boost: off-diagonal entries ($\beta\gamma$) are $\mathcal{O}(\beta)$; diagonal entries (γ) are $1 + \mathcal{O}(\beta^2)$.
For a rotation: off-diagonal elements are $\mathcal{O}(\theta)$ ($\pm\sin\theta$); diagonal elements ($\cos\theta$) are $1 + \mathcal{O}(\theta^2)$.
(437) $\Rightarrow$ only 6 independent $\Delta\omega^{\mu\nu}$ (small boost along or small rotation around, the three axes).
Check:

$$\begin{aligned}
\Lambda^\mu{}_\alpha g^{\alpha\beta}\underbrace{\Lambda^\nu{}_\beta}_{(\Lambda^T)_\beta{}^\nu} &= (g^\mu{}_\alpha + \Delta\omega^\mu{}_\alpha)g^{\alpha\beta}(g^\nu{}_\beta + \Delta\omega^\nu{}_\beta) \\
&= (g^{\mu\beta} + \Delta\omega^{\mu\beta})g^\nu{}_\beta + g^\mu{}_\alpha\Delta\omega^{\nu\alpha} + \mathcal{O}(\Delta\omega^2) \\
&= g^{\mu\nu} + \cancel{\Delta\omega^{\mu\nu}} + \cancel{\Delta\omega^{\nu\mu}} = g^{\mu\nu} \quad \checkmark
\end{aligned}$$

(Leads to $S(\Lambda) \to \mathbb{I}$ as $\Delta\omega \to 0$)
Ansatz:

$$S = \mathbb{I} + \tau, \quad S^{-1} = \mathbb{I} - \tau, \tag{438}$$

where τ is an infinitesimal (4×4) Dirac matrix.
From (429), (436) in (435):

$$(\mathbb{I} - \tau)\gamma^\nu(\mathbb{I} + \tau) = \cancel{\gamma^\nu} - \tau\gamma^\nu + \gamma^\nu\tau + \mathcal{O}(\tau^2) \overset{!}{=} (g^\nu{}_\mu + \Delta\omega^\nu{}_\mu)\gamma^\mu = \cancel{\gamma^\nu} + \Delta\omega^\nu{}_\mu\gamma^\mu \tag{439}$$

In addition, we require:

$$\det S = 1 \tag{440}$$

$$\implies \det(\mathbb{I} + \tau) = \underbrace{\det(\mathbb{I})}_{=1} + \underbrace{\mathrm{tr}(\tau)}_{\sum_{a=1}^4 \tau_{aa}} + \mathcal{O}(\tau^2) \overset{!}{=} 1 \implies \mathrm{tr}(\tau) = 0 \tag{441}$$

<u>Solution:</u>

$$\tau = -\frac{i}{4}\Delta\omega^{\mu\nu}\sigma_{\mu\nu}, \quad \text{with} \quad \sigma_{\mu\nu} = \frac{i}{2}\underbrace{[\gamma_\mu, \gamma_\nu]}_{\text{commutator}} \tag{442}$$

General transformation: make many small transformations:

$$S(\Lambda) = e^{-\frac{i}{4}\omega^{\mu\nu}\sigma_{\mu\nu}}, \quad \text{where } \Lambda^\alpha{}_\beta = g^\alpha{}_\beta + \omega^\alpha{}_\beta \tag{443}$$

<u>Solving the Dirac equation</u>
Let's first consider a particle in its rest frame: $\vec{p} = 0 \Rightarrow \frac{\partial\psi}{\partial x^k} = 0$

$$\overset{408}{\implies} i\frac{\partial\psi}{\partial t} = \frac{mc^2}{\hbar}\beta\psi \overset{416}{=} \frac{mc^2}{\hbar}\begin{pmatrix} \mathbb{I}_{2\times2} & 0 \\ 0 & -\mathbb{I}_{2\times2} \end{pmatrix}\psi$$

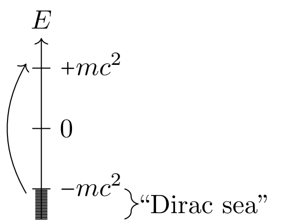
Obviously, this equation has four independent solutions, which can be written in terms of two-component spinors:

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{444}$$

$$\psi_r^{(+)}(t) = u_r(m, \vec{p} = 0)e^{-imc^2t/\hbar} = \begin{pmatrix} \chi_r \\ 0 \end{pmatrix} e^{-imc^2t/\hbar} \tag{445}$$

$$\psi_r^{(-)}(t) = v_r(m, \vec{p} = 0)e^{imc^2t/\hbar} = \begin{pmatrix} 0 \\ \chi_r \end{pmatrix} e^{imc^2t/\hbar} \tag{446}$$

ψ^- has negative energy: $E(\psi^-)\psi^- = i\hbar\frac{\partial\psi^-}{\partial t} = -mc^2\psi^-$!
Thus, we have two solutions with $E > 0$ (particle states) and two solutions with $E < 0$ (anti-particle states).
For $r = 1, 2$, in the rest frame, this describes <u>spin-$\frac{1}{2}$ fermions</u>.
Existence of $E < 0$ solutions arises from negative entries in β: necessary for $\{\alpha_k, \beta\} = 0$
Relativistic quantum mechanics <u>requires</u> the existence of antiparticles! Dirac's interpretation of $E < 0$ states: they are all *filled* in the ground state!



need $\Delta E > +2mc^2$ to lift a particle from sea:
leaves a "hole": acts like antiparticle

lifting corresponds to e^+e^- pair production.

[20.01.2025, Lecture 26]

[22.01.2025, Lecture 27]

[22.01.2025, Lecture 27]

[27.01.2025, Lecture 28]

[27.01.2025, Lecture 28]

[29.01.2025, Lecture 29]

Appendix A

The Fourier Transform

Let $f(t)$ be continuous with at most finitely many discontinuities of the first kind (i.e., $f(t+0)$ and $f(t-0)$ exist) and

$$\int_{-\infty}^{+\infty} \mathrm{d}t\, |f(t)| < \infty.$$

Then the Fourier transform

$$\tilde{f}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{i\omega t} f(t)$$

exists, and the inverse transform gives

$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \tilde{f}(\omega) = \begin{cases} f(t) & \text{at continuous points,} \\ \frac{1}{2}\left(f(t+0) + f(t-0)\right) & \text{at the discontinuities.} \end{cases}$$

The Delta Function and Distributions

This section is intended to give a heuristic understanding of the δ-function and other related distributions as well as a feeling for the essential elements of the underlying mathematical theory.
Definition of a "test function" $F(x), G(x), \ldots$: All derivatives exist and vanish at infinity faster than any power of $1/|x|$, e.g., $\exp\{-x^2\}$. In order to introduce the δ-function heuristically, we start with (for arbitrary $F(x)$)

$$F(x) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega x} \int_{-\infty}^{+\infty} \mathrm{d}x' e^{i\omega x'} F(x'),$$

and exchange – without investigating the admissibility of these operations – the order of the integrations:

$$F(x) = \int_{-\infty}^{+\infty} \mathrm{d}x' F(x') \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} e^{i\omega(x'-x)} = \int_{-\infty}^{+\infty} \mathrm{d}x' F(x') \delta(x'-x).$$

From this, we read off

$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} e^{i\omega(x'-x)} = \delta(x'-x) = \begin{cases} 0 & \text{for } x' \neq x, \\ \infty & \text{for } x' = x. \end{cases} \tag{447}$$

This "function" of x' thus has the property of vanishing for all $x' \neq x$ and taking the value infinity for $x' = x$. It is thus the analogue for integrals of the Kronecker-δ for sums,

$$\sum_{n'} K_{n'} \delta_{n,n'} = K_n.$$

The Dirac δ-function is not a function in the usual sense. In order to give it a precise meaning, we consider in place of the above integral (447) one that exists. We can either allow the limits of integration to extend only to some finite value or else introduce a weighting function falling off at infinity. Accordingly, we define the following sequence of functions parameterized by n,

$$\delta_n(x) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} \exp\left(i\omega x - \frac{1}{n}|\omega|\right) = \frac{1}{\pi} \frac{1/n}{x^2 + (1/n)^2} \tag{A.4a}$$

with the following properties:

$$\text{I. } \lim_{n\to\infty} \delta_n(x) = \begin{cases} \infty & \text{for } x = 0, \\ 0 & \text{for } x \neq 0, \end{cases}$$

$$\text{II. } \lim_{n\to\infty} \int_{-a}^{b} \mathrm{d}x\, \delta_n(x) G(x) = G(0).$$

Proof of II:

$$\lim_{n\to\infty} \int_{-an}^{bn} \frac{\mathrm{d}y}{\pi} \frac{1}{y^2+1} G\left(\frac{y}{n}\right) = G(0) \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\pi} \frac{1}{y^2+1} = G(0).$$

We thus define the δ-function (distribution) by

$$\int_{-a}^{b} \mathrm{d}x\, \delta(x) G(x) = \lim_{n\to\infty} \int_{-a}^{b} \mathrm{d}x\, \delta_n(x) G(x).$$

This definition suggests the following generalization.
Let a sequence of functions $d_n(x)$ be given whose limit as $n \to \infty$ does not necessarily yield a function in the usual sense. Let

$$\lim_{n\to\infty} \int \mathrm{d}x\, d_n(x) G(x)$$

exist for each G. One then defines the distribution $d(x)$ via

$$\int \mathrm{d}x\, d(x) G(x) = \lim_{n\to\infty} \int \mathrm{d}x\, d_n(x) G(x).$$

This generalization allows one to introduce additional definitions of importance for distributions.

(i) Definition of the equality of two distributions: Two distributions are equal,

$$a(x) = b(x),$$

if $\int \mathrm{d}x\, a(x) G(x) = \int \mathrm{d}x\, b(x) G(x)$ for every $G(x)$.

(ii) Definition of the sum of two distributions:

$$c(x) = a(x) + b(x);$$

$c(x)$ is defined by $c_n(x) = a_n(x) + b_n(x)$.

(iii) Definition of the multiplication of a distribution by a function $F(x)$:

$$d(x)F(x) \text{ is defined by } d_n(x)F(x).$$

(iv) Definition of an affine transformation:

$$d(\alpha x + \beta) \text{ is defined by } d_n(\alpha x + \beta).$$

(v) Definition of the derivative of a distribution:

$$d'(x) \text{ is defined by } d_n'(x).$$

From these definitions, one has that the same linear operations can be performed for distributions as for ordinary functions. It is not possible to define the product of two arbitrary distributions in a natural way.

Properties of the δ-function:

$$\begin{aligned}
&\int_{-\infty}^{+\infty} \mathrm{d}x\, \delta(x - x_0) F(x) = F(x_0), \\
&\int_{-\infty}^{+\infty} \mathrm{d}x\, \delta'(x) F(x) = -F'(0), \\
&\delta(x)F(x) = \delta(x)F(0), \\
&\delta(\alpha x) = \frac{1}{|\alpha|}\delta(x).
\end{aligned}$$

Remark:

$$\begin{aligned}
\int_{-\infty}^{+\infty} \mathrm{d}x\, \delta(\alpha x) F(x) &= \lim_{n\to\infty} \int_{-\infty}^{+\infty} \mathrm{d}x\, \delta_n(\alpha x) F(x) = \lim_{n\to\infty} \int_{-\infty}^{+\infty} \mathrm{d}x\, \delta_n(x|\alpha|) F(x), \\
&= \lim_{n\to\infty} \frac{1}{|\alpha|} \int_{-\infty}^{+\infty} \mathrm{d}y\, \delta_n(y) F\left(\frac{y}{|\alpha|}\right) = \frac{1}{|\alpha|} F(0).
\end{aligned}$$

$$\delta(f(x)) = \sum_i \frac{1}{|f'(x_i)|}\delta(x - x_i), \quad x_i \text{ simple zeros of } f.$$

It follows that

$$x\delta(x) = x^2\delta(x) = \ldots = 0,$$
$$\delta(-x) = \delta(x).$$

Fourier transform of the δ-function:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-i\omega x}\delta(x) = 1.$$

Three-dimensional δ-function:

$$\delta^{(3)}(\mathbf{x} - \mathbf{x}') = \delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3').$$

In spherical coordinates:

$$\delta^{(3)}(\mathbf{x} - \mathbf{x}') = \frac{1}{r^2}\delta(r - r')\delta(\cos\vartheta - \cos\vartheta')\delta(\varphi - \varphi').$$

Step function:

$$\Theta_n(x) = \frac{1}{2} + \frac{1}{\pi}\arctan nx,$$
$$\Theta_n'(x) = \delta_n(x),$$
$$\to \Theta'(x) = \delta(x).$$

Other sequences which also represent the δ-function:

$$\delta_n(x) = \frac{1}{\pi x}\sin nx = \int_{-n}^{n} \frac{\mathrm{d}k}{2\pi} e^{ikx},$$
$$\delta_n(x) = \sqrt{\frac{2}{\pi}} e^{-n^2x^2}.$$

If a sequence $d_n(x)$ defines a distribution $d(x)$, one then writes symbolically

$$d(x) = \lim_{n\to\infty} d_n(x).$$

Integral representations

We conclude this section by giving a few integral representations for $\delta(x)$ and related distributions:

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, e^{ikx},$$
$$\Theta(x) = \lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{-\infty}^{+\infty} \mathrm{d}k\,\frac{e^{ikx}}{k - i\epsilon}.$$

We also define the distributions

$$\delta_+(x) = \frac{1}{2\pi}\int_0^{\infty} \mathrm{d}k\, e^{ikx},$$
$$\delta_-(x) = \frac{1}{2\pi}\int_{-\infty}^{0} \mathrm{d}k\, e^{ikx}.$$

These can also be represented in the form

$$\delta_\pm(x) = \pm\frac{1}{2\pi i}\lim_{\varepsilon\to 0}\frac{1}{x \pm i\varepsilon}.$$

Further one has

$$\lim_{\varepsilon\to 0}\frac{1}{x \pm i\varepsilon} = P\frac{1}{x} \mp i\pi\delta(x),$$

where P designates the Cauchy principal value,

$$P\int \frac{\mathrm{d}x}{x}G(x) = \lim_{\varepsilon\to 0}\left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{+\infty}\right)\mathrm{d}x\,\frac{1}{x}G(x).$$

The distributions $\delta_\pm$ have the properties

$$\begin{aligned}
\delta_\pm(-x) &= \delta_\mp(x), \\
x\delta_\pm(x) &= \mp\frac{1}{2\pi i}, \\
\delta_+(x) + \delta_-(x) &= \delta(x), \\
\delta_+(x) - \delta_-(x) &= \frac{i}{\pi} P\frac{1}{x}.
\end{aligned}$$

Green's Functions

Starting from a linear differential operator D and a function $f(x)$, we study the linear inhomogeneous differential equation

$$D\psi(x) = f(x) \tag{448}$$

for $\psi(x)$.
Replacing the inhomogeneity by a δ-distribution located at x', one finds

$$DG(x, x') = \delta(x - x').$$

The quantity $G(x, x')$ is called the Green's function of the differential operator D. For translationally invariant D, $G(x, x') = G(x - x')$.
Using the Green's function, one finds for the general solution of (448)

$$\psi(x) = \psi_0(x) + \int \mathrm{d}x' G(x, x') f(x'), \tag{449}$$

where $\psi_0(x)$ is the general solution of the homogeneous differential equation

$$D\psi_0(x) = 0.$$

Equation (449) contains a particular solution of the inhomogeneous differential equation (448), given by the second term, which is not restricted to any special form of the inhomogeneity $f(x)$. A great advantage of the Green's function is that, once it has been determined, it enables one to compute a particular solution for arbitrary inhomogeneities.
In scattering theory, we require the Green's function for the wave equation

$$(\nabla^2 + k^2) G(\mathbf{x} - \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \tag{450}$$

The Fourier transform of $G(\mathbf{x} - \mathbf{x}')$

$$\tilde{G}(\mathbf{q}) = \int \mathrm{d}^3 y\, e^{-i\mathbf{q}\cdot\mathbf{y}} G(\mathbf{y})$$

becomes, with (450),

$$(-q^2 + k^2)\tilde{G}(\mathbf{q}) = 1.$$

Inverting the last two functions, one first obtains for the Green's function

$$G(\mathbf{y}) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{y}} \frac{1}{-q^2 + k^2}. \tag{451}$$

However, because of the poles at $\pm k$, the integral in (451) does not exist ($k > 0$). In order to obtain a well-defined integral, we must displace the poles by an infinitesimal amount from the real axis:

$$G_\pm(\mathbf{x}) = -\lim_{\varepsilon\to 0} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{q^2 - k^2 \mp i\varepsilon}. \tag{452}$$

In the integrand of G_+, the poles are at the locations $q = \pm(k + i\varepsilon/2k)$, and in the integrand of G_-, they are at $q = \pm(k - i\varepsilon/2k)$. From this one sees that the shift of the poles of G_+ in the limit $\varepsilon \to 0$ is equivalent to deforming the path of integration along the real axis. After carrying out the angular integration, one finds

$$G_\pm(\mathbf{x}) = -\frac{1}{4\pi 2ir} \int_{-\infty}^{+\infty} \frac{\mathrm{d}q\, q e^{iqr}}{q^2 - k^2 \mp i\varepsilon}.$$

Since $r = |\mathbf{x}| > 0$, the path of integration can be closed by an infinite semicircle in the upper half-plane, so that the residue theorem then yields

$$G_\pm(\mathbf{x}) = -\frac{e^{\pm ikr}}{4\pi r}.$$

The quantity G_+ is called the *retarded Green's function*. The solution (449) is composed of a free solution of the wave equation and an outgoing spherical wave.
The quantity G_- is called the *advanced Green's function*. The solution (449) then consists of a free solution of the wave equation and an incoming spherical wave.

Baker-Campbell-Hausdorff Formula and Magnus Expansion

The standard Baker-Campbell-Hausdorff formula reads

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{C}},$$

where

$$\hat{C} = \hat{B} + \int_0^1 \mathrm{d}t\, g(e^{\mathrm{ad}\,\hat{A}\,t}e^{\mathrm{ad}\,\hat{B}})[\hat{A}], \tag{453}$$

and $g(z)$ is the function

$$g(z) \equiv \frac{\log z}{z-1} = \sum_{n=0}^{\infty} \frac{(1-z)^n}{n+1}, \tag{454}$$

and $\mathrm{ad}B$ is the operator associated with $\hat{B}$ in the so-called *adjoint representation*, which is defined by

$$\mathrm{ad}B[\hat{A}] \equiv [\hat{B}, \hat{A}]. \tag{455}$$

One also defines the trivial adjoint operator $(\mathrm{ad}B)^0[\hat{A}] = 1[\hat{A}] \equiv \hat{A}$. By expanding the exponentials in Eq. (453) and using the power series (454), one finds the explicit formula

$$\hat{C} = \hat{B} + \hat{A} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n+1} \sum_{p_i,q_i;p_i+q_i\geq 1} \frac{1}{1+\sum_{i=1}^n p_i} \frac{(\mathrm{ad}A)^{p_1}}{p_1!}\frac{(\mathrm{ad}B)^{q_1}}{q_1!}\cdots\frac{(\mathrm{ad}A)^{p_n}}{p_n!}\frac{(\mathrm{ad}B)^{q_n}}{q_n!}[\hat{A}]. \tag{456}$$

The lowest expansion terms are

$$\begin{aligned}\hat{C} = \hat{B} + \hat{A} &- \frac{1}{2}\left[\frac{1}{2}\mathrm{ad}A + \mathrm{ad}B + \frac{1}{6}(\mathrm{ad}A)^2 + \frac{1}{2}\mathrm{ad}A\mathrm{ad}B + \frac{1}{2}(\mathrm{ad}B)^2 + \ldots\right][\hat{A}]\\ &+ \frac{1}{3}\left[\frac{1}{3}(\mathrm{ad}A)^2 + \frac{1}{2}\mathrm{ad}A\mathrm{ad}B + \frac{1}{2}\mathrm{ad}B\mathrm{ad}A + (\mathrm{ad}B)^2 + \ldots\right][\hat{A}]\end{aligned}$$

$$\Rightarrow \hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{12}([\hat{A},[\hat{A},\hat{B}]] + [\hat{B},[\hat{B},\hat{A}]]) + \frac{1}{24}[\hat{A},[[\hat{A},\hat{B}],\hat{B}]]\ldots \tag{457}$$

The result can be rearranged to the closely related *Zassenhaus formula*

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{\hat{Z}_2}e^{\hat{Z}_3}e^{\hat{Z}_4}\ldots, \tag{458}$$

where

$$\begin{aligned}\hat{Z}_2 &= \frac{1}{2}[\hat{B},\hat{A}],\\ \hat{Z}_3 &= -\frac{1}{3}[\hat{B},[\hat{B},\hat{A}]] - \frac{1}{6}[\hat{A},[\hat{B},\hat{A}]],\\ \hat{Z}_4 &= \frac{1}{8}\left([[[\hat{B},\hat{A}],\hat{B}],\hat{B}] + [[[\hat{B},\hat{A}],\hat{A}],\hat{B}]\right) + \frac{1}{24}[[[\hat{B},\hat{A}],\hat{A}],\hat{A}]\\ &\vdots\end{aligned}$$

To prove formula (453) and thus the expansion (457), we proceed by deriving and solving a differential equation for the operator function

$$\hat{C}(t) = \log(e^{\hat{A}t}e^{\hat{B}}). \tag{459}$$

Its value at $t = 1$ will supply us with the desired result $\hat{C}$ in (456). The starting point is the observation that for any operator $\hat{M}$,

$$e^{\hat{C}(t)}\hat{M}e^{-\hat{C}(t)} = e^{\mathrm{ad}C(t)}[\hat{M}], \tag{460}$$

by definition of ad$C$. Inserting (459), the left-hand side can also be rewritten as $e^{\hat{A}t}e^{\hat{B}}\hat{M}e^{-\hat{B}}e^{-\hat{A}t}$, which in turn is equal to $e^{\mathrm{ad}At}e^{\mathrm{ad}B}[\hat{M}]$, by definition (455). Hence we have

$$e^{\mathrm{ad}C(t)} = e^{\mathrm{ad}At}e^{\mathrm{ad}B}. \tag{461}$$

Differentiation of (459) yields

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -\hat{A}. \tag{462}$$

The left-hand side, on the other hand, can be rewritten in general as

$$e^{\hat{C}(t)}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{463}$$

where

$$f(z) \equiv \frac{e^z - 1}{z}. \tag{464}$$

It implies that

$$f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)] = \hat{A}. \tag{465}$$

We now define the function $g(z)$ as in (454) and see that it satisfies

$$g(e^z)f(z) \equiv 1. \tag{466}$$

We therefore have the trivial identity

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)]. \tag{467}$$

Using (465) and (461), this turns into the differential equation

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})[\hat{A}] = e^{\mathrm{ad}At}e^{\mathrm{ad}B}[\hat{A}], \tag{468}$$

from which we find directly the result (453).
To complete the proof we must verify (463). The expression is not simply equal to $-e^{\hat{C}(t)}\dot{\hat{C}}(t)\hat{M}e^{-\hat{C}(t)}$ since $\dot{\hat{C}}(t)$ does not, in general, commute with $\hat{C}(t)$. To account for this consider the operator

$$\hat{O}(s,t) \equiv e^{\hat{C}(t)s}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)s}. \tag{469}$$

Differentiating this with respect to s gives

$$\begin{aligned}
\partial_s\hat{O}(s,t) &= e^{\hat{C}(t)s}\hat{C}(t)\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-\hat{C}(t)s}\right) - e^{\hat{C}(t)s}\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{C}(t)e^{-\hat{C}(t)s}\right), &(470)\\
&= -e^{\hat{C}(t)s}\dot{\hat{C}}(t)e^{-\hat{C}(t)s} &(471)\\
&= -e^{\mathrm{ad}C(t)s}[\dot{\hat{C}}(t)]. &(472)
\end{aligned}$$

Hence

$$\hat{O}(s,t) - \hat{O}(0,t) = \int_0^s \mathrm{d}s'\partial'_s\hat{O}(s',t) = -\sum_{n=0}^{\infty}\frac{s^{n+1}}{(n+1)!}(\mathrm{ad}C(t))^n[\dot{\hat{C}}(t)], \tag{473}$$

from which we obtain

$$\hat{O}(1,t) = e^{\hat{C}(t)}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{474}$$

which is what we wanted to prove.
Note that the final form of the series for $\hat{C}$ in (457) can be rearranged in many different ways, using the Jacobi identity for the commutators. It is a nontrivial task to find a form involving the smallest number of terms.[1]
The same mathematical technique can be used to derive a useful modification of the Neumann-Liouville expansion or Dyson series. This is the so-called Magnus expansion[2], in which one writes $\hat{U}(t_b, t_a) = e^{\hat{E}}$, and expands the exponent $\hat{E}$ as

$$\hat{E} = \frac{1}{i\hbar}\int_{t_a}^{t_b} \mathrm{d}t_1 \hat{H}(t_1) + \frac{1}{2}\left(\frac{1}{i\hbar}\right)^2 \int_{t_a}^{t_b} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 [\hat{H}(t_2), \hat{H}(t_1)] \tag{475}$$

$$+ \frac{1}{4}\left(\frac{1}{i\hbar}\right)^3 \left\{ \int_{t_a}^{t_b} \mathrm{d}t_3 \int_{t_a}^{t_3} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 \left[\hat{H}(t_3), \left[\hat{H}(t_2), \hat{H}(t_1)\right]\right] \right. \tag{476}$$

$$\left. + \frac{1}{3}\int_{t_a}^{t_b} \mathrm{d}t_3 \int_{t_a}^{t_3} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 \left[\left[\hat{H}(t_3), \hat{H}(t_2)\right], \hat{H}(t_1)\right] \right\} + \ldots, \tag{477}$$

which converges faster than the Neumann-Liouville expansion.

Hermite, Legendre and Laguerre polynomials

Hermite polynomials

Hermite polynomials were defined by Pierre-Simon Laplace in 1810, though in scarcely recognizable form, and studied in detail by Pafnuty Chebyshev in 1859. They were consequently not new, although Hermite was the first to define the multidimensional polynomials in his later 1865 publications.

The differential equation of the form

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + 2ny = 0 \tag{478}$$

is called Hermite equation. The solution of (478) is known as Hermite's polynomial.
Suppose its series solution is

$$y = a_0 x^m + a_1 x^{m+1} + a_2 x^{m+2} + a_3 x^{m+3} + \cdots + a_k x^{m+k} \quad \text{or } y = \sum_{k=0}^{\infty} a_k x^{m+k} \tag{479}$$

$$\Longrightarrow \frac{\mathrm{d}y}{\mathrm{d}x} = \sum_{k=0}^{\infty} a_k (m+k) x^{m+k-1} \quad \wedge \quad \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = \sum_{k=0}^{\infty} a_k (m+k)(m+k-1) x^{m+k-2}$$

Inserting this in (478), we get

$$\sum_k a_k (m+k)(m+k-1) x^{m+k-2} - 2x \sum_k a_k (m+k) x^{m+k-1} + 2n \sum_{k=0} a_k x^{m+k} = 0 \tag{480}$$

$$\Longrightarrow \sum_k a_k (m+k)(m+k-1) x^{m+k-2} - 2x \sum_k a_k [(m+k) - n] x^{m+k} = 0 \tag{481}$$

This equation holds for $k = 0$ and all positive integer. By our assumption k cannot be negative. To get the lowest degree term x^{m-2}, we put $k = 0$ in the first summation of (481) and we cannot have x^{m-2} from the second summation (since $k \neq -2$). The coefficient of x^{m-2} is

$$a_0 m(m-1) = 0 \Longrightarrow m = 0, m = 1, \text{ since } a_0 \neq 0 \tag{482}$$

This is the indicial equation. Now equating the coefficient of next lowest degree term x^{m-1}, we get by $k = 1$ in the first summation and again we cannot have x^{m-1} from the second summation since $K \neq -1$.

$$a_1 m(m+1) = 0 \Longrightarrow \begin{cases} a_1 \text{ may or may not be zero when } m = 0 \\ a_1 = 0, \text{ when } m = 1 \end{cases}$$

Again equating the coefficient of the general term x^{m-k} to zero, we get

$$a_{k+2}(m+k+2)(m+k+1) - 2a_k(m+k-n) = 0 \quad \longrightarrow \quad a_{k+2} = \frac{2(m+k-n)}{(m+k+2)(m+k+1)} a_k \tag{483}$$

[1] For a discussion see J.A. Oteo, J. Math. Phys. *32*, 419 (1991)
[2] See A. Iserles, A. Marthinsen, and S.P. Norsett, *On the implementation of the method of Magnus series for linear differential equations*, BIT **39**, 281 (1999) (http://www.damtp.cam.ac.uk/user/ai/Publications).

$$\text{If } m = 0, \text{ then} \quad a_{k+2} = \frac{2(k-n)}{(k+2)(k+1)} a_k \tag{484}$$

$$\text{If } m = 0, \text{ then} \quad a_{k+2} = \frac{2(k+1-n)}{(k+3)(k+2)} a_k \tag{485}$$

When $m = 0, a_{k+2} = \frac{2(k-n)}{(k+2)(k+1)} a_k$:

$$\begin{aligned}
&\text{If } k = 0, \text{ then} \quad a_2 = \frac{-2n}{2} a_0 = -n a_0 \\
&\text{If } k = 1, \text{ then} \quad a_3 = \frac{2(1-n)}{6} a_1 = -2\frac{(n-1)}{3!} a_1 \\
&\text{If } k = 2, \text{ then} \quad a_4 = \frac{2(2-n)}{12} a_2 = 2\frac{(2-n)}{12}(-n a_0) = (2)^2 \frac{n(n-2)}{4!} a_0 \\
&\text{If } k = 3, \text{ then} \quad a_5 = \frac{2(3-n)}{20} a_3 = 2\frac{2(3-n)}{20}\left(-\frac{2(n-1)}{3!} a_1\right) = (2)^2 \frac{(n-1)(n-3)}{5!} a_1 \\
&\implies a_{2r} = \frac{(-2)^r n(n-2)(n-4)\cdots(n-2r+2)}{(2r)!} a_0 \\
&\implies a_{2r+1} = \frac{(-2)^r (n-1)(n-3)\cdots(n-2r+1)}{(2r+1)!} a_0
\end{aligned}$$

When $m = 0$, then there are two possibilities:

$$1^{\text{st}}: \quad a_1 = 0 \Rightarrow a_3 = a_5 = a_{2r+1} = 0$$

$$2^{\text{nd}}: \quad a_1 \neq 0 \Rightarrow y = \sum_{k=0}^{\infty} a_k x^k$$

$$\text{i.e. } y = a_0 + a_1 x + a_2 x^2 + \cdots = a_0 + a_2 x^2 + a_4 x^4 + \cdots + a_1 x + a_3 x^3 + a_5 x^5 + \cdot \tag{486}$$

Inserting the values of a_0, a_1, a_2, a_3, a_4 and a_5 in (486), we get

$$= a_0 \left[1 - \frac{2n}{2!} x^2 + \frac{2^2 n(n-2)}{4!} x^4 - \cdots + (-1)^r \frac{2^r}{(2r)!} n(n-2)\cdots(n-2r+2) x^{2r} + \cdots\right] \tag{487}$$

$$+ a_1 x \left[1 - \frac{2(n-1)}{3!} x^2 + \frac{2^2(n-1)(n-3)}{5!} x^4 - \cdots + (-1)^r \frac{2^r}{(2r+1)!}(n-1)(n-3)\cdots(n-2r+1) x^{2r} + \cdots\right] \tag{488}$$

$$= a_0 \left[1 + \sum_{r=1}^{\infty} \frac{(-1)^r 2^r}{(2r)!} n(n-2)\cdots(n-2r+2) x^{2r}\right] + a_1 x \left[1 + \sum_{r=1}^{\infty} \frac{(-1)^r 2^r}{(2r+1)!}(n-1)(n-3)\cdots(n-2r+1) x^{2r}\right] \tag{489}$$

When $m = 1$, then $a_1 = 0$ and so by putting $k = 0, 1, 2, 3, \ldots$ in (485), we get

$$\begin{aligned}
&a_{k+2} = \frac{2(k+1-n)}{(k+3)(k+2)} \\
&\implies a_2 = -\frac{2(n-1)}{3!} a_0, a_4 = \frac{2^2(n-1)(n-3)}{5!} a_0, \ldots, a_{2r}(-1)^r = \frac{2^r(n-1)(n-3)\cdots(n-2r+1)}{(2r+1)!} a_0
\end{aligned}$$

Hence, the solution is

$$= a_0 x \left[1 - \frac{2(n-1)}{3!} x^2 + \frac{2^2(n-1)(n-3)}{5!} x^4 + \cdots + \frac{(-1)^r 2^r (n-1)(n-3)\cdots(n-2r+1)}{(2r+1)!} x^{2r} + \cdots\right] \tag{490}$$

It is clear that the solution (490) is included in the second part of (488) except that a_0 is replaced by a_1 and hence in order that the Hermite equation may have two independent solutions, a_1 must be zero, even if $m = 0$ and then (488) reduces to

$$= a_0 x \left[1 - \frac{2(n-1)}{3!} x^2 + \frac{2^2(n-1)(n-3)}{5!} x^4 + \cdots + \frac{(-1)^r 2^r (n-1)(n-3)\cdots(n-2r+1)}{(2r+1)!} x^{2r} + \cdots\right] \tag{491}$$

The complete integral of (478) is then given by

$$y = A\left[1 - \frac{2n}{2!} x^2 + \frac{2^2 n(n-2)}{4!} - \cdots\right] + B\left[1 - \frac{2(n-1)}{3!} x^2 + \frac{2^2(n-1)(n-3)}{5!} x^4 + \cdots\right] \tag{492}$$

where A and B are arbitrary constants.

Hermite polynomials (Rodrigues formula)

There are several theorems concerning Hermite polynomials, which show up in the solution of the Schrödinger equation for the harmonic oscillator. First, we'll look at the Rodrigues formula (which is a different formula from the Rodrigues formula for Legendre polynomials).
Suppose we start with $u = e^{-x^2}$ and take its derivative. We have

$$u' = -2xe^{-x^2} \tag{493}$$
$$u' + 2xu = 0 \tag{494}$$

We can now take the derivative of the second equation $n+1$ times and use Leibniz's formula for the n-th derivative of a product, which is

$$(fg)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(k)} g^{(n-k)} \tag{495}$$

We get

$$(xu)^{(n+1)} = \sum_{k=0}^{n+1} \binom{n+1}{k} x^{(k)} u^{(n+1-k)} \tag{496}$$

Since any derivative of x higher than the first gives zero, we have

$$(xu)^{(n+1)} = xu^{(n+1)} + (n+1)u^{(n)} \tag{497}$$

Applying this to the original equation, we get

$$u^{(n+2)} + 2xu^{(n+1)} + 2(n+1)u^{(n)} = 0 \tag{498}$$

Defining yet another variable $v \equiv (-1)^n u^{(n)}$ (we get the factor of $(-1)^n$ inserted to make things come out right at the other end):

$$v'' + 2xv' + 2(n+1)v = 0 \tag{499}$$

Finally, defining $y \equiv e^{x^2} v$, we have

$$v = e^{-x^2} y \tag{500}$$
$$v' = e^{-x^2}\left[y' - 2xy\right] \tag{501}$$
$$v'' = -2xe^{-x^2}\left[y' - 2xy\right] + e^{-x^2}\left[y'' - 2y - 2xy'\right] \tag{502}$$
$$= e^{-x^2}\left[y'' - 4xy' + (4x^2 - 2)y\right] \tag{503}$$

Substituting this into (499), we get, after dividing out the common factor of e^{-x^2}:

$$y'' - 4xy' + (4x^2 - 2)y + 2x\big(y' - 2xy\big) + 2(n+1)y = 0 \tag{504}$$
$$y'' - 2xy + 2ny = 0 \tag{505}$$

This last equation is the same as that obtained from the Schrödinger equation (with different variable names):

$$\frac{d^2 f}{d\xi^2} - 2\xi \frac{df}{d\xi} + (\epsilon - 1) f = 0 \tag{506}$$
$$\epsilon = \frac{2E}{\hbar\omega} \tag{507}$$
$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \tag{508}$$

We can see by comparing the two forms of the equation that a solution to the latter is

$$f = y \tag{509}$$
$$= e^{\xi^2} v \tag{510}$$
$$= (-1)^n e^{\xi^2} u^{(n)} \tag{511}$$
$$= (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \tag{512}$$

Since this is a solution it must be a multiple of the Hermite polynomial. To see that it is actually the Hermite polynomial itself, consider the derivative term. Each derivative of $e^{-\xi^2}$ will have a term multiplying the previous derivative by -2ξ, so the term with the highest power of ξ in the n-th derivative will be

$$(-2\xi)^n = (-1)^n 2^n \xi^n e^{-\xi^2}.$$

We now see why the factor of $(-1)^n$ was introduced earlier: by the usual convention, the coefficient of the highest power of a Hermite polynomial is 2^n, which is what we obtain from the formula above. Thus the Rodrigues formula for Hermite polynomials is

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{513}$$

We can apply this formula directly to get the first few polynomials. We get

$$\begin{aligned}
H_0 &= 1 && (514)\\
H_1 &= 2x && (515)\\
H_2 &= e^{x^2} \frac{d}{dx}\big(-2xe^{-x^2}\big) && (516)\\
&= 4x^2 - 2 && (517)\\
H_3 &= -e^{x^2} \frac{d}{dx}\big(-2e^{-x^2} + 4x^2 e^{-x^2}\big) && (518)\\
&= 8x^3 - 12x && (519)\\
H_4 &= e^{x^2} \frac{d}{dx}\big(4xe^{-x^2} + 8xe^{-x^2} - 8x^3 e^{-x^2}\big) && (520)\\
&= e^{x^2} \frac{d}{dx}\big(12xe^{-x^2} - 8x^3 e^{-x^2}\big) && (521)\\
&= 16x^4 - 48x^2 + 12 && (522)
\end{aligned}$$

Hermite polynomials - recursion relations

Hermite polynomials can be obtained from a *generating function*. The derivation of generating functions is something of a black art, as it requires the use of complex variable theory (in particular, Cauchy's integral formula), but we'll just accept it without proof for now. The result is

$$e^{-z^2+2zx} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x) \tag{523}$$

Here z is a dummy variable which is used to generate the Taylor series of the exponential on the left. Since the k-th derivative with respect to z of the series eliminates all powers with $n < k$, retains z^{n-k} terms for $n > k$, and reduces the term in z^k to $(k!/k!)H_k(x) = H_k(x)$, if we take the k-th derivative and then set $z = 0$, we're left, magically, with $H_k(x)$. Taking high-order derivatives of the exponential isn't exactly pretty, of course, but it's quite marvellous that such a result exists at all.

As an example, we'll use the generating function to derive the first three polynomials. We get

$$\begin{aligned}
H_0(x) &= e^0 && (524)\\
&= 1 && (525)\\
H_1(x) &= \frac{d}{dz} e^{-z^2+2zx}\bigg|_{z=0} && (526)\\
&= (-2z + 2x)e^{-z^2+2zx}\bigg|_{z=0} && (527)\\
&= 2x && (528)\\
H_2(x) &= \frac{d^2}{dz^2} e^{-z^2+2zx}\bigg|_{z=0} && (529)\\
&= \big[-2 + (-2z+2x)^2\big] e^{-z^2+2zx}\bigg|_{z=0} && (530)\\
&= 4x^2 - 2 && (531)
\end{aligned}$$

Starting from the generating function, we can derive two recursion relations for the polynomials. If we take the derivative of (523) with respect to z, we get

$$(-2z+2x)e^{-z^2+2zx}=\sum_{n=1}^{\infty}\frac{z^{n-1}}{(n-1)!}H_n(x) \tag{532}$$

If we replace the exponential on the left by its series expansion, we get

$$-2\sum_{n=0}^{\infty}\frac{z^{n+1}}{n!}H_n(x)+2x\sum_{n=0}^{\infty}\frac{z^n}{n!}H_n(x)=\sum_{n=1}^{\infty}\frac{z^{n-1}}{(n-1)!}H_n(x) \tag{533}$$

We now pull the usual trick of relabelling the summation index on the first and last sum in order to make the power of z the same in all sums. For the first sum, we get

$$\begin{aligned}-2\sum_{n=0}^{\infty}\frac{z^{n+1}}{n!}H_n(x)&=-2\sum_{n=1}^{\infty}\frac{z^n}{(n-1)!}H_{n-1}(x) &(534)\\ &=-2\sum_{n=1}^{\infty}\frac{z^n}{n!}nH_{n-1}(x) &(535)\end{aligned}$$

For the sum on the right, we get

$$\sum_{n=1}^{\infty}\frac{z^{n-1}}{(n-1)!}H_n(x)=\sum_{n=0}^{\infty}\frac{z^n}{n!}H_{n+1}(x) \tag{536}$$

Combining these results we get

$$-2\sum_{n=1}^{\infty}\frac{z^n}{n!}nH_{n-1}(x)+2x\sum_{n=0}^{\infty}\frac{z^n}{n!}H_n(x)=\sum_{n=0}^{\infty}\frac{z^n}{n!}H_{n+1}(x) \tag{537}$$

For $n>0$, we can equate the coefficients of z^n to get

$$H_{n+1}(x)=2xH_n(x)-2nH_{n-1}(x) \tag{538}$$

For the special case of $n=0$, the first sum on the left makes no contribution and the other two terms give us

$$2xH_0(x)=H_1(x) \tag{539}$$

which, since $H_0=1$, gives us $H_1=2x$, which is correct. We saw when discussing the *Rodrigues formula* that

$$\begin{aligned}H_3(x)&=8x^3-12x &(540)\\ H_4(x)&=16x^4-48x^2+12 &(541)\end{aligned}$$

so we can use the recursion relation to get the next couple of polynomials:

$$\begin{aligned}H_5(x)&=2xH_4(x)-8H_3(x) &(542)\\ &=32x^5-96x^3+24x-64x^3+96x &(543)\\ &=32x^5-160x^3+120x &(544)\\ H_6(x)&=2xH_5(x)-10H_4(x) &(545)\\ &=64x^6-320x^4+240x^2-160x^4+480x^2-120 &(546)\\ &=64x^6-480x^4+720x^2-120 &(547)\end{aligned}$$

A second recursion relation can be found by differentiating (523) with respect to x rather than z. We get

$$2ze^{-z^2+2zx}=\sum_{n=0}^{\infty}H_n'(x)\frac{z^n}{n!} \tag{548}$$

Again, we replace the exponential by the series to get

$$2\sum_{n=0}^{\infty}H_n(x)\frac{z^{n+1}}{n!}=\sum_{n=0}^{\infty}H_n'(x)\frac{z^n}{n!} \tag{549}$$

Relabelling the summation index on the left, we get

$$2\sum_{n=1}^{\infty} H_{n-1}(x)\frac{z^n}{(n-1)!} = \sum_{n=0}^{\infty} H_n'(x)\frac{z^n}{n!} \tag{550}$$

Equating coefficients of z^n, we get

$$H_n'(x) = 2nH_{n-1}(x) \tag{551}$$

For example:

$$H_6'(x) = 384x^5 - 1920x^3 + 1440x \tag{552}$$
$$= 12\big(32x^5 - 160x^3 + 120x\big) \tag{553}$$
$$= 2 \times 6H_5 \tag{554}$$
$$H_5'(x) = 160x^4 - 480x^2 + 120 \tag{555}$$
$$= 10\big(16x^4 - 48x^2 + 12\big) \tag{556}$$
$$= 2 \times 5H_4 \tag{557}$$

Examples

Find the value of

$$\int_{-\infty}^{\infty} e^{-x^2} H_2(x)H_3(x)\mathrm{d}x \tag{558}$$
$$\int_{-\infty}^{\infty} e^{-x^2} H_2(x)H_2(x)\mathrm{d}x \tag{559}$$
$$\tag{560}$$

Solutions

(558) : Using the orthogonality of Hermite polynomials:

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x)H_m(x)\,\mathrm{d}x = \begin{cases} 0, & n \neq m, \\ 2^n n!\sqrt{\pi}, & n = m. \end{cases}$$

Since $n = 2 \neq 3 = m$, the integral evaluates to 0.

(559) : Here $n = m = 2$. Using the orthogonality property:

$$\int_{-\infty}^{\infty} e^{-x^2} H_2(x)H_2(x)\,\mathrm{d}x = 2^2 2!\sqrt{\pi} = 8\sqrt{\pi}.$$

Legendre polynomials

A differential equation that occurs frequently in physics (as part of the solution of Laplace's equation, which occurs in such areas as electrodynamics and quantum mechanics, among others) is *Legendre's equation*.
The equation occurs while solving Laplace's equation in spherical coordinates. Although the origins of the equation are important in the physical applications, for our purposes here we need concern ourselves only with the equation itself, which is usually first encountered in the following form:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]P = 0 \tag{561}$$

where l and m are constants and the angle θ is the spherical coordinate that gives the angle from the z-axis, and which can range over the interval $[0, \pi]$. The problem is to determine the function $P(\theta)$.
The first step in solving the equation is usually to transform the variable to $x \equiv \cos\theta$. Under this transformation:

$$dx = -\sin\theta d\theta \tag{562}$$
$$\frac{dP}{d\theta} = -\sin\theta\frac{dP}{dx} \tag{563}$$
$$\sin^2\theta = 1 - x^2 \tag{564}$$

so the equation becomes

$$\frac{1}{\sin\theta}\left(-\sin\theta\frac{d}{dx}\left(-\sin^2\theta\frac{dP}{dx}\right)\right)+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]P=0 \tag{565}$$

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P=0 \tag{566}$$

The solutions $P(x)=P(\cos\theta)$ of this equation are called *associated Legendre functions*. Before we dive in and try to find these general solutions, however, it is a bit easier if we look at the simpler case where $m=0$:

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)+l(l+1)P=0 \tag{567}$$

Since the coefficients of P and its derivatives are all polynomials in x, a standard solution technique is to try proposing P as a power series. That is, we try a solution of the form

$$P(x)=\sum_{j=0}^{\infty}a_jx^j \tag{568}$$

where the a_j are coefficients to be determined. To substitute this into (567), we need to work out the various terms and derivatives:

$$\frac{dP}{dx}=\sum_{j=0}^{\infty}ja_jx^{j-1} \tag{569}$$

$$(1-x^2)\frac{dP}{dx}=\sum_{j=0}^{\infty}ja_jx^{j-1}-\sum_{j=0}^{\infty}ja_jx^{j+1} \tag{570}$$

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)=\sum_{j=0}^{\infty}j(j-1)a_jx^{j-2}-\sum_{j=0}^{\infty}j(j+1)a_jx^j \tag{571}$$

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)+l(l+1)P=\sum_{j=0}^{\infty}j(j-1)a_jx^{j-2}-\sum_{j=0}^{\infty}\left[j(j+1)a_j+l(l+1)a_j\right]x^j \tag{572}$$

$$=\sum_{j=0}^{\infty}\left[(j+2)(j+1)a_{j+2}-j(j+1)a_j+l(l+1)a_j\right]x^j=0 \tag{573}$$

where in the penultimate line we rearranged the first term so that both terms were summing over the same power of x.
If a series such as this is to be zero everywhere, then every term in the series must be zero (this is a theorem from infinite series theory), which provides a condition on the coefficients:

$$a_{j+2}=\frac{j(j+1)-l(l+1)}{(j+1)(j+2)}a_j \tag{574}$$

Since this recursion formula relates each coefficient to one *two* steps before it, we see we need to specify two of the coefficients to get the formula started. This is what we would expect, since a second order differential equation should have two constants that need specifying. So to start things off, we need to specify a_0 and a_1.
Now in order for this to be a sensible solution, the series needs to converge for all possible values of x. Remember that $x=\cos\theta$, so the range of possible values of x is $x\in[-1,1]$. If the series is infinite, then for large j we can take the limit $j\to\infty$ in (574) and we get that the recursion formula is approximately

$$a_{j+2}\approx a_j \tag{575}$$

so the series behaves like the geometric series $a\sum_{j=0}^{\infty}x^j$. Most mathematics textbooks deal with the geometric series and show that if the series is finite, it can be written in closed form as

$$\sum_{j=0}^{n}x^j=\frac{1-x^{n+1}}{1-x} \tag{576}$$

In the limit of $n\to\infty$, this formula converges to

$$\sum_{j=0}^{\infty}x^j=\frac{1}{1-x} \tag{577}$$

provided $|x| < 1$. In our case, however, we need the series to converge for $x \pm 1$ as well.
The way out of this dilemma is to require the series to terminate, so that $a_j = 0 \forall j > j_{\max}$, where $j_{\max}$ is some finite value. From the recursion formula (574), we see this can be arranged if $j_{\max}(j_{\max}+1) = l(l+1)$, so $j_{\max} = l$ or $-l-1$. Since $j_{\max}$ must be a non-negative integer, only one of these solutions is acceptable, so we might as well concentrate on values of l that are non-negative integers (if $l < 0$, the constatnt $l(l+1)$ is still non-negative anyway, and that constant is all that appears in the original equation so we don't lose anything by restricting to $l \geq 0$). It then follows that if l is even, the highest value of j for which $a_j \neq 0$ must also be even, which in turn requires that all a_j for odd j must be zero. Conversely, if l is odd, then the even sub-series must be zero. That is depending on the value of l, we must choose eiter $a_0 = 0$ or $a_1 = 0$.
Thus the solutions to (567) turn out to be polynomials in x, the forms of which are determined by the constant l, which must be a non-negative integer in order for the solutions to converge over the entire range of x. The first few such polynomials, called *Legendre polynomials*, are (taking $a_0 = 1$ or $a_1 = 1$ to get the series started; the subscript l on P_l is the value of l in each case).

$$P_0 = 1 \tag{578}$$
$$P_1 = x \tag{579}$$
$$P_2 = 1 - 3x^2 \tag{580}$$
$$P_3 = x - \frac{5}{3}x^3 \tag{581}$$

Since the differential equation is linear in P, each polynomial above can be multiplied by any constant and still be a solution, and the actual constant chosen depends on the normalization desired. This is equivalent to choosing a different value for a_0 or a_1 which, since these coefficients are arbitrary, is permissible. One convention is to normalize the polynomials so that $p_l(1) = 1 \forall l$, and in that case, the polynomials start off as follows:

$$P_0 = 1 \tag{582}$$
$$P_1 = x \tag{583}$$
$$P_2 = \frac{1}{2}(3x^2 - 1) \tag{584}$$
$$P_3 = \frac{1}{2}(5x^3 - 3x) \tag{585}$$

Legendre polynomials - geometric origin

We've seen how *Legendre polynomials* arise from a simplified version of Legendre's differential equation. Here we have a look at how the polynomials can be generated from a simple geometric situation.
We start with an ordinary triangle with sides of lengths a, b, and c, and define the angle θ between sides a and b. Then the cosine rule (a generalization of Pythagoras's theorem) says:

$$c = \sqrt{a^2 + b^2 - 2ab\cos\theta} \tag{586}$$

If the triangle is right-angled, then $\theta = \pi/2$ and we get back Pythagoras's theorem.
Now if we consider the reciprocal of c (encountered in physics in any situation where some phenomenon depends on the inverse of the distance, as in the electrostatic or gravitational potential functions), we get:

$$\frac{1}{c} = \left(a^2 + b^2 - 2ab\cos\theta\right)^{-1/2} \tag{587}$$
$$= \frac{1}{b}\left(1 + (a/b)^2 - 2(a/b)\cos\theta\right)^{-1/2} \tag{588}$$

Now suppose we consider triangles where $b > a$. We can expand the term in brackets in a Taylor series in the quantity (a/b). To make the notation easier, we define $x \equiv \cos\theta$ and $t \equiv a/b$. Then the Taylor series will have the general form:

$$(1 + t^2 - 2tx)^{-1/2} = \sum_{n=0}^{\infty} P_n(x)t^n \tag{589}$$

This formula can be used as the starting point for a study of the Legendre polynomials if we *define* the quantities $P_n(x)$ to be the Legendre polynomials. Obviously, if we do this, we need to demonstrate that they are the same polynomials that turn up as the solutions to Legendre's differential equation, but we'll leave that to another part. What we'll do here is use this definition to derive an explicit formula for calculating

$P_n(x)$.

First, we'll have a look at the Taylor series for the function $f(u) = (1-u)^{-1/2}$. Remember that the Taylor series about the reference point $u = 0$ has the form:

$$f(u) = \sum_{n=0}^{\infty} \frac{u^n}{n!} f^{(n)}(0) \tag{590}$$

where $f^{(n)}(0)$ is the n-th derivative of $f(u)$ evaluated at $u = 0$. Calculating the first few derivatives of $f(u) = (1-u)^{-1/2}$, we get:

$$f(u) = (1-u)^{-1/2} \tag{591}$$
$$f^{(1)}(u) = \frac{1}{2}(1-u)^{-3/2} \tag{592}$$
$$f^{(2)}(u) = \frac{3}{2} \cdot \frac{1}{2}(1-u)^{-5/2} \tag{593}$$
$$f^{(3)}(u) = \frac{5}{2} \cdot \frac{3}{2} \cdot \frac{1}{2}(1-u)^{-7/2} \tag{594}$$

It's fairly obvious that a pattern is forming, and the general formula for the n-th derivative is:

$$f^{(n)}(u) = \frac{(2n-1)!!}{2^n}(1-u)^{-(2n+1)/2} \tag{595}$$

where the notation $(2n-1)!!$ is a *double factorial*, which means the product of every second number from $2n-1$ down to 1. That is:

$$(2n-1)!! = (2n-1)(2n-3)(2n-5)\ldots(3)(1) \tag{596}$$

Thus the derivatives evaluated at $u = 0$ are:

$$f^{(n)}(0) = \frac{(2n-1)!!}{2^n} \tag{597}$$

and the Taylor series is:

$$f(u) = 1 + \sum_{n=1}^{\infty} \frac{(2n-1)!!}{2^n n!} u^n \tag{598}$$

We've separated out the first term (586) in order to avoid a negative factorial from the $(2n-1)!!$ term.
We can get rid of the double factorial by noting that

$$(2n-1)!! = \frac{(2n)!}{(2n)!!} \tag{599}$$
$$= \frac{(2n)!}{2^n n!} \tag{600}$$

The first line follows since the numerator is the product of all integers up to $2n$ and the denominator cancles off all the even integers, leaving the product of all the odd ones. The last line follows since

$$(2n)!! = (2n)(2n-2)(2n-4)\cdots(2) \tag{601}$$
$$= (2n)(2(n-1))(2(n-2))\cdots(2(1)) \tag{602}$$
$$= 2^n n! \tag{603}$$

Thus we can write the Taylor series as

$$f(u) = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} u^n \tag{604}$$

Using this in (589), we get

$$(1-2xt+t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2}(2xt-t^2)^n \tag{605}$$

Although it is possible to use this formula to pick out individual Legendre polynomials, it isn't very convenient, since we need to finde all terms in a particular power of t to get the corresponding polynomial. However, the factor $(2xt - t^2)^n$ is an ordinary binomial, so we can use the binomial theorem to expand it.
The binomial theorem states

$$(a+b)^n = \sum_{k=0}^{n} \binom{n}{k} a^n b^{n-k} \tag{606}$$

$$= \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k \tag{607}$$

where:

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \tag{608}$$

The second line (607) in the theorem above points out that the expansion is symmetric in a and b.
With $a = 2xt$ and $b = -t^2$, we have we get:

$$(2xt - t^2)^n = \sum_{k=0}^{n} \binom{n}{k} (2x)^{n-k} (-t^2)^k \tag{609}$$

$$= \sum_{k=0}^{n} \binom{n}{k} (-1)^k (2x)^{n-k} t^{n+k} \tag{610}$$

$$= \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} (-1)^k (2x)^{n-k} t^{n+k} \tag{611}$$

Substituting this back into (605), we get:

$$(1 - 2xt + t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} (-1)^k (2x)^{n-k} t^{n+k} \tag{612}$$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{(2n)!}{2^{2n} n! k! (n-k)!} (-1)^k (2x)^{n-k} t^{n+k} \tag{613}$$

We might still appear to be no further ahead, since we still need to pick out several seperate terms to find all those terms where t has a particular exponent. However, there is a summation trick we can use to simplify things.
If we think of the term being summed as one entry in a matrix, we can write it using the notation

$$a_{nk} \equiv \frac{(2n)!}{2^{2n} n! k! (n-k)!} (-1)^k (2x)^{n-k} t^{n+k} \tag{614}$$

If the index n represents the row in the matrix and k the column, the summation in (613) extends over the lower triangular section of the matrix (that is, from the diagonal down to the lower left corner). The summation as written sums each row in turn from the first column out to the diagonal.
What we would like to do is to group the terms in the sum so that all terms with the same exponent for t are grouped together. That is, we are looking for those terms in the sum where $n + k = r$ for some particular value of r. Since we are considering the lower triangle of the matrix, these groups consist of:

$$a_{00} \quad r = 0 \tag{615}$$

$$a_{10} \quad r = 1 \tag{616}$$

$$a_{20}, a_{11} \quad r = 2 \tag{617}$$

$$a_{30}, a_{21} \quad r = 3 \tag{618}$$

$$a_{40}, a_{31}, a_{22} \quad r = 4 \tag{619}$$

$$\ldots \quad r = \ldots \tag{620}$$

Thus for a given value of r, the matrix elements we want to select are of the form $a_{r-s,s}$ where $s = 0, 1, \ldots, \lfloor r/2 \rfloor$ where the notation $\lfloor r/2 \rfloor$ means 'greatest integer less than or equal to $r/2$'.
We can therefore rearrange the sum by making the summation index substitutions $k = s, n = r - s$, and alter the summation ranges so that r runs from 0 to ∞ and s from 0 to $\lfloor r/2 \rfloor$. We then get:

$$(1 - (2xt - t^2))^{-1/2} = \sum_{r=0}^{\infty} \sum_{s=0}^{\lfloor r/2 \rfloor} \frac{(2r-2s)!}{2^{2r-2s}(r-s)! s! (r-2s)!} (-1)^s (2x)^{r-2s} t^r \tag{621}$$

We can now relabel the summation indexes back to k and n (since they are dummy indexes, we can call them whatever we like), and get:

$$(1-(2xt-t^2))^{-1/2} = \sum_{n=0}^{\infty}\sum_{k=0}^{\lfloor n/2\rfloor}\frac{(2n-2k)!}{2^{2n-2k}(n-k)!k!(n-2k)!}(-1)^k(2x)^{n-2k}t^n \tag{622}$$

$$= \sum_{n=0}^{\infty} P_n(x)t^n \tag{623}$$

where the last line is by comparison with (589).
By the uniqueness of power series, the coefficients of each power of t must be equal on either side of the equation, so we get our explicit formula for the Legendre polynomials:

$$P_n(x) = \sum_{k=0}^{\lfloor n/2\rfloor}\frac{(2n-2k)!}{2^{2n-2k}(n-k)!k!(n-2k)!}(-1)^k(2x)^{n-2k} \tag{624}$$

$$= \sum_{k=0}^{\lfloor n/2\rfloor}\frac{(2n-2k)!}{2^{n}(n-k)!k!(n-2k)!}(-1)^k x^{n-2k} \tag{625}$$

Legendre polynomials - Rodrigues formula and orthogonality

In the part before, we found that the Legendre polynomials could be written as an explicit sum (625).
This can be written as a derivative if we observe that if $k \le \lfloor n/2\rfloor$,

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}x^{2n-2k} = \frac{(2n-2k)!}{(n-2k)!}x^{n-2k} \tag{626}$$

Note that if $k > \lfloor n/2\rfloor$, the n-th derivative of x^{2n-2k} is zero, since after $\lfloor n/2\rfloor$ derivatives, the term x^{2n-2k} is reduced to a constant. We can use this fact to rewrite the sum above as:

$$P_n(x) = \sum_{k=0}^{\lfloor n/2\rfloor}\frac{(-1)^k}{2^n(n-k)!k!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}x^{2n-2k} \tag{627}$$

$$= \sum_{k=0}^{n}\frac{(-1)^k}{2^n(n-k)!k!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}x^{2n-2k} \tag{628}$$

$$= \frac{1}{2^n n!}\sum_{k=0}^{n}\frac{(-1)^k n!}{(n-k)!k!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}x^{2n-2k} \tag{629}$$

$$= \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\sum_{k=0}^{n}\frac{(-1)^k n!}{(n-k)!k!}x^{2n-2k} \tag{630}$$

The sum in the last line is the binomial expansion of $(x^2-1)^n$ (since the factorials within the sum form the binomial coefficient $\binom{n}{k}$), so we can write this as:

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n \tag{631}$$

This is known as the *Rodrigues formula* for Legendre polynomials. Although it's not all that convenient for calculating the polynomials themselves, it can be used to prove various properties about them. One of the most important theorems is that the polynomials are orthogonal. This means that if $n \neq m$, we have:

$$\int_{-1}^{1} P_m(x)P_n(x)\mathrm{d}x = 0 \tag{632}$$

This property turns out to be of vital importance in quantum mechanics, where the polynomials form the basis of the associated Legendre functions, which in turn form part of the solution of the three-dimensional Schrödinger equation. We'll run through the proof here.
Using the Rodrigues formula, we have:

$$\int_{-1}^{1} P_m(x)P_n(x)\mathrm{d}x = \frac{1}{2^{m+n}n!m!}\int_{-1}^{1}\frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^2-1)^m\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\mathrm{d}x \tag{633}$$

Before doing the integration, we note that all derivatives of the function $(x^2-1)^m$ up to the $(m-1)$-th derivative have x^2-1 as a factor (we can see this by applying the chain rule), and are therefore zero at $x=\pm1$. Now assume that $m<n$ for the purposes of being definite (it won't matter if $m>n$ since we can just swap

the two indexes throughout the argument).
If we integrate (633) by parts, we get:

$$\int_{-1}^{1}\frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^2-1)^m\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n\mathrm{d}x=\left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}}(x^2-1)^n\frac{\mathrm{d}^m}{\mathrm{d}x^m}(x^2-1)^m\right]_{-1}^{1}-\tag{634}$$

$$\int_{-1}^{1}\frac{\mathrm{d}^{m+1}}{\mathrm{d}x^{m+1}}(x^2-1)^m\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}}(x^2-1)^n\mathrm{d}x\tag{635}$$

Because of the condition just stated, the boundary term at the start is zero, so we can continue by integrating the remaining integral by parts, throwing away the boundary term until we have done n integrations. At this point, we will have:

$$\int_{-1}^{1}P_m(x)P_n(x)\mathrm{d}x=\frac{1}{2^{m+n}m!n!}(-1)^n\int_{-1}^{1}(x^2-1)^n\frac{\mathrm{d}^{m+n}}{\mathrm{d}x^{m+n}}(x^2-1)^m\mathrm{d}x\tag{636}$$

Since $m<n$, the derivative inside the integral is zero, since the largest power of x in $(x^2-1)^m$ is x^{2m} and $2m<m+n$. Therefore, the overall integral is zero, and we have shown that the Legendre polynomials are orthogonal (that is, (632) is true).
What if $n=m$? In that case, the integration by parts technique won't work, since we can't count on the final integral being zero. However, after n integrations by parts, we get to the formula:

$$\int_{-1}^{1}P_n(x)P_n(x)\mathrm{d}x=\frac{(-1)^n}{(n!)^2 2^{2n}}\int_{-1}^{1}(x^2-1)^n\frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}(x^2-1)^n\mathrm{d}x\tag{637}$$

The derivative inside the integral will kill off all terms within $(x^2-1)^n$ except for the highest power of x^{2n} and the derivative of that is:

$$\frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}(x^2-1)^n=\frac{\mathrm{d}^{2n}}{\mathrm{d}x^{2n}}x^{2n}\tag{638}$$

$$=(2n)!\tag{639}$$

We can therefore write:

$$\int_{-1}^{1}P_n(x)P_n(x)\mathrm{d}x=\frac{(-1)^n(2n)!}{(n!)^2 2^{2n}}\int_{-1}^{1}(x^2-1)^n\mathrm{d}x\tag{640}$$

The final integral can be done by using a trigonometric substitution (e.g. $x=\sin\theta$ so $x^2-1=-\cos\theta$ and $\mathrm{d}x=\cos\theta\mathrm{d}\theta$). This still requires the integration of a high power of $\cos\theta$ so we can take the easy way out and use mathematical software such as Maple or Mathematica to do the integral directly. In that case we find:

$$\int_{-1}^{1}(x^2-1)^n\mathrm{d}x=\frac{(-1)^n\Gamma(n+1)\sqrt{\pi}}{\Gamma(n+3/2)}\tag{641}$$

The gamma function $\Gamma(x)$ is a generalization of the factorial function and has a number of convenient properties we can use to simplify this. In particular, we have:

$$\Gamma(n+1)=n!\tag{642}$$

$$\Gamma(z)\Gamma(z+1/2)=2^{1-2z}\sqrt{\pi}\Gamma(2z)\tag{643}$$

The second of these formulas (known as the duplication formula) can be used to show that:

$$\Gamma(n+3/2)=\Gamma((n+1)+1/2)=\frac{\sqrt{\pi}(2n+1)!}{2^{1+2n}n!}\tag{644}$$

So plugging this into (641), we find that

$$\int_{-1}^{1}(x^2-1)^n\mathrm{d}x=\frac{(-1)^n(n!)2^{1+2n}}{(2n+1)!}\tag{645}$$

so plugging this back into (640), we finally get

$$\int_{-1}^{1}P_n(x)P_n(x)\mathrm{d}x=\frac{1}{(n!)^2 2^{2n}}(2n)!(-1)^n\frac{(n!)2^{1+2n}}{(2n+1)!}\tag{646}$$

$$=\frac{2}{2n+1}\tag{647}$$

We can combine the results on integration of the Legendre polynomials to get the overall orthogonality condition:

$$\int_{-1}^{1}P_n(x)P_m(x)\mathrm{d}x=\frac{2}{2n+1}\delta_{nm}\tag{648}$$

Associated Legendre functions

One of the differential equations that turns up in the solution in the three-dimensional Schrödinger equation is *Legendre's equation*:

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P=0 \tag{649}$$

We saw before that if we take $m=0$, the solutions are the Legendre polynomials $P_l(x)$. That is, they are the solutions of:

$$\frac{d}{dx}\left((1-x^2)\frac{dP_l}{dx}\right)+l(l+1)P_l=0 \tag{650}$$

$$(1-x^2)P_l''-2xP_l'+l(l+1)P_l=0 \tag{651}$$

To find the solution to the general Legendre equation (649), we can, oddly enough, start with the simpler equation. We can use Leibniz's formula to differentiate the $m=0$ equation m times. For each term in the above equation, we get:

$$\left[(1-x^2)P_l'\right]^{(m)}=(1-x^2)P_l^{(m+2)}-2mxP_l^{(m+1)}-m(m-1)P_l^{(m)} \tag{652}$$

$$\left[-2xP_l'\right]^{(m)}=-2xP_l^{(m+1)}-2mP_l^{(m)} \tag{653}$$

$$\left[l(l+1)P_l\right]^{(m)}=l(l+1)P_l^{(m)} \tag{654}$$

Adding up these three terms, we get:

$$(1-x^2)P_l^{(m+2)}-2x(m+1)P_l^{(m+1)}+\left[l(l+1)-m^2-m\right]P_l^{(m)}=0 \tag{655}$$

We can simplify the notation a bit by defining $u(x)\equiv P_l^{(m)}$:

$$(1-x^2)u''-2x(m+1)u'+\left[l(l+1)-m^2-m\right]u=0 \tag{656}$$

This still doesn't look much like Legendre's general equation, so next we use the substitution (I know, I know - how would you think of this?).

$$u=v(1-x^2)^{-m/2} \tag{657}$$

$$u'=v'(1-x^2)^{-m/2}+mxv(1-x^2)^{-(m+2)/2} \tag{658}$$

$$=\left(v'+\frac{mxv}{1-x^2}\right)(1-x^2)^{-m/2} \tag{659}$$

$$u''=\left(v''+\frac{mxv'}{1-x^2}+\frac{mv}{1-x^2}+\frac{2mx^2v}{(1-x^2)^2}\right)(1-x^2)^{-m/2}+\left(v'+\frac{mxv}{1-x^2}\right)xm(1-x^2)^{-(m+2)/2} \tag{660}$$

$$=\left(v''+\frac{2mxv'}{1-x^2}+\frac{mv}{1-x^2}+\frac{m(m+2)x^2v}{(1-x^2)^2}\right)(1-x^2)^{-m/2} \tag{661}$$

We can substitute these terms into (656) and collect terms to finally get Legendre's equation back again:

$$(1-x^2)v''-2xv'+mv+\frac{v}{1-x^2}(m(m+2)x^2-2m(m+1)x^2)+[l(l+1)-m^2-m]v=0 \tag{662}$$

$$(1-x^2)v''-2xv'+mv-\frac{m^2x^2v}{1-x^2}+l(l+1)v-m^2\frac{1-x^2}{1-x^2}v-mv=0 \tag{663}$$

$$(1-x^2)v''-2xv'+l(l+1)v-\frac{m^2}{1-x^2}v=0 \tag{664}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left((1-x^2)v'\right)+l(l+1)v-\frac{m^2}{1-x^2}v=0 \tag{665}$$

Thus, the function $v(x)$ is a solution to the general Legendre equation with an arbitrary value of m. These solutions are called associated Legendre functions, and from the definitions above, we get:

$$v(x)=u(x)(1-x^2)^{m/2} \tag{666}$$

$$=(1-x^2)^{m/2}\frac{\mathrm{d}^mP_l(x)}{\mathrm{d}x^m} \tag{667}$$

$$\equiv P_l^m(x) \tag{668}$$

where the term $P_l^m(x)$ is the symbol typically reserved for the associated Legendre function with indexes l and m.
Although the derivation is fairly straightforward once it is laid in front of you, it is still a bit of magic when you see the substitution that needs to be made to end up with Legendre's general equation.
From this formula, we can use the *explicit sum version* of the Legendre polynomials to get an explicit formula for the associated Legendre functions:

$$P_l(x) = \sum_{k=0}^{\lfloor l/2 \rfloor} \frac{(2l-2k)!}{2^l(l-k)!k!(l-2k)!}(-1)^k x^{l-2k} \tag{669}$$

Since the highest power of x in $P_l(x)$ is x^l, we see that if $m > l$, $\frac{\mathrm{d}^m P_l}{\mathrm{d}x^m} = 0$, so we must have $m \le l$. Further, since the m-th derivative of x^{l-2k} is $x^{l-2k-m}(l-2k)!/(l-2k-m)!$, the highest non-zero value of k in the sum is $\lfloor (l-m)/2 \rfloor$, and we have (up to a normalization factor):

$$P_l^m(x) = (1-x^2)^{m/2} \frac{\mathrm{d}^m P_l(x)}{\mathrm{d}x^m} \tag{670}$$

$$= (1-x^2)^{m/2} \sum_{k=0}^{\lfloor (l-m)/2 \rfloor} \frac{(2l-2k)!}{2^l(l-k)!k!(l-2k-m)!}(-1)^k x^{l-m-2k} \tag{671}$$

Associated Legendre functions - orthogonality

In terms of the Legendre polynomials, the associated Legendre functions can be written as in (670).
Although we can continue from this point and write the functions as explicit sums, here, we want to prove something else: that the associated Legendre functions are a set of orthogonal functions. This property is of importance in quantum mechanics, among other places in physics, so we need to establish this foundation of the theory.
To proceed, we can use the *Rodrigues formula* for the Legendre polynomials (exchanging n with l in (631)). Inserting this into (670), we get:

$$P_l^m(x) = \frac{1}{2^l l!}(1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} \left(x^2-1\right)^l \tag{672}$$

We can make the notation a bit simpler by defining:

$$X(x) \equiv (x^2-1) \tag{673}$$

We can then rewrite (672) as:

$$P_l^m(x) = \frac{1}{2^l l!}(-X)^{m/2} \frac{d^{l+m} X^l}{dx^{l+m}} \tag{674}$$

At this point, we can pause to notice that this definition allows us to let m range over negative values as well as positive, so we can use this as a definition of the associated Legendre functions for $-l \le m \le l$.
Now to the orthogonality condition. Since the functions are defined over the range $-1 \le x \le 1$, we need to evaluate the integral $\int_{-1}^{1} P_p^m P_q^m \, dx$ for some values p and q. Note that we are restricting m to be the same in both functions. First, we'll consider the case $p < q$, which covers all cases where the lower indices are unequal. Using (674), we can write:

$$\int_{-1}^{1} P_p^m P_q^m \,\mathrm{d}x = \frac{(-1)^m}{2^p p! q!} \int_{-1}^{1} X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}} X^p \frac{\mathrm{d}^{q+m}}{\mathrm{d}x^{q+m}} X^q \,\mathrm{d}x \tag{675}$$

Now we can use integration by parts to write:

$$\int_{-1}^{1} P_p^m P_q^m \,\mathrm{d}x = \frac{(-1)^m}{2^{p+q} p! q!} \left[\frac{\mathrm{d}^{q+m-1}}{\mathrm{d}x^{q+m-1}} X^q X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}} X^p \right]_{-1}^{1} - \int_{-1}^{1} \frac{\mathrm{d}^{q+m-1}}{\mathrm{d}x^{q+m-1}} X^q \frac{\mathrm{d}}{\mathrm{d}x} \left(X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}} X^p \right) \mathrm{d}x \tag{676}$$

The integrated term will be zero, since $X = 0$ at both endpoints. Thus:

$$\int_{-1}^{1} P_p^m P_q^m \,\mathrm{d}x = \frac{(-1)^m(-1)}{2^{p+q} p! q!} \int_{-1}^{1} \frac{\mathrm{d}^{q+m-1}}{\mathrm{d}x^{q+m-1}} X^q \frac{\mathrm{d}}{\mathrm{d}x} \left(X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}} X^p \right) \mathrm{d}x \tag{677}$$

If we repeat the integration by parts, the integrated term is:

$$\frac{\mathrm{d}^{q+m-2}}{\mathrm{d}x^{q+m-2}} X^q \frac{\mathrm{d}}{\mathrm{d}x} \left(X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}} X^p \right) \tag{678}$$

The derivative in large parentheses in this term contains the factor X^{m-1}, so (if $m > 1$) will again be zero at the endpoints. By the same reasoning, since the degree of the derivative of this term in parentheses increases by 1 on each integration, the j-th integration by parts will contain a factor of X^{m-j+1} provided $j < m$, and will therefore be zero.
If we integrate by parts beyond this point, the second derivative factor will no longer be zero at the endpoints. However, now the *first* derivative factor becomes $\frac{d^{q+m-j}}{dx^{q+m-j}}X^q$. Since $j > m$ at this stage, this derivative will now contain a factor of $X^{q-(q+m-j)} = X^{j-m}$ and will now be zero. (Actually, due to the product rule being applied successively as we calculate higher and higher derivatives, there will be a sum of terms, but the *lowest* power of X in any of these terms will be X^{j-m}, so every term in the product rule sum will go to zero at the endpoints.)
That is, if we integrate by parts $q+m$ times, the integrated term will be zero at every stage, and we get for the final result:

$$\int_{-1}^{1} P_p^m P_q^m \,\mathrm{d}x = \frac{(-1)^m(-1)^{q+m}}{2^{p+q}p!q!}\int_{-1}^{1} X^q \frac{\mathrm{d}^{q+m}}{\mathrm{d}x^{q+m}}\left(X^m \frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}X^p\right)\mathrm{d}x \tag{679}$$

This might not look much better, but we can examine the integrand a bit more closely. The highest power of x in X^p is x^{2p}, so the highest power of x in $\frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}X^p$ is $x^{2p-p-m} = x^{p-m}$. Multiplying this by X^m, which has a highest power of x^{2m}, gives an overall leading term of $x^{p-m+2m} = x^{p+m}$. Now since we assumed $q > p$, taking the $(q+m)$-th derivative of x^{p+m} (or any lower power) will always give zero, so we've shown that the integrand is always zero if $q \neq p$ (since p and q appeared symmetrically in the original integral, the argument is exactly the same if we assume $q < p$). Thus the associated Legendre functions are orthogonal.
What if $p = q$? In that case, the derivative part of the integrand in (679) will be a constant, as we'll now see. We can work out $\frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}(x^{2p})$ first. Since each derivative brings down the exponent and then reduces the exponent by 1, we get:

$$\frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}x^{2p} = \frac{(2p)!}{(2p-(p+m))!}x^{2p-(p+m)} + \dots \tag{680}$$

$$= \frac{(2p)!}{(p-m)!}x^{p-m} + \dots \tag{681}$$

Similarly, we get:

$$\frac{(2p)!}{(p-m)!}\frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}\left(X^m x^{p-m}\right) = \frac{(2p)!}{(p-m)!}\frac{\mathrm{d}^{p+m}}{\mathrm{d}x^{p+m}}\left(x^{2m}x^{p-m} + \dots\right) \tag{682}$$

$$= \frac{(2p)!}{(p-m)!}\frac{d^{p+m}}{dx^{p+m}}\left(x^{p+m} + \dots\right) \tag{683}$$

$$= \frac{(2p)!}{(p-m)!}(p+m)! \tag{684}$$

Note that the final derivative kills off all lower powers of x so we need consider only the leading term. Substituting all this back into (679) with $p = q$, we get:

$$\int_{-1}^{1}\left(P_p^m\right)^2\mathrm{d}x = \frac{(-1)^{p+2m}}{2^{2p}(p!)^2}\frac{(2p)!}{(p-m)!}(p+m)!\int_{-1}^{1}X^p\mathrm{d}x \tag{685}$$

$$= \frac{(-1)^{p+2m}}{2^{2p}(p!)^2}\frac{(2p)!}{(p-m)!}(p+m)!\int_{-1}^{1}(x^2-1)^p\mathrm{d}x \tag{686}$$

The integral is the same one we ran into when calculating the orthogonality of the Legendre polynomials, so we can just quote the result here:

$$\int_{-1}^{1}(x^2-1)^p\mathrm{d}x = \frac{(-1)^p(p!)^2 2^{1+2p}}{(2p+1)!} \tag{687}$$

The final result is then

$$\int_{-1}^{1}\left(P_p^m\right)^2\mathrm{d}x = \frac{2}{2p+1}\frac{(p+m)!}{(p-m)!} \tag{688}$$

or, combining the orthogonality results:

$$\int_{-1}^{1}P_p^m P_q^m\mathrm{d}x = \frac{2}{2p+1}\frac{(p+m)!}{(p-m)!}\delta_{pq} \tag{689}$$

Exercises

Using Rodrigue's formula for $P_n(x)$, prove the following:

1. $$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1), \quad P_3(x) = \frac{1}{2}(5x^3 - 3x) \quad \text{and } P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3).$$

2. Show that $P_n(1) = 1$.

3. (i) Show that $P_n(-x) = (-1)^n P_n(x)$. Hence, deduce that $P_n(-1) = (-1)^n$.
   (ii) Prove that $P_n(x)$ is an even or odd function of x according as n is even or odd respectively.

4. Prove that $P_n'(x) - P_{n-2}'(x) = (2n-1)P_{n-1}(x)$.

5. Prove that $xP_9'(x) = P_8'(x) + 9P_9(x)$.

6. Show that $11(x^2 - 1)P_5'(x) = 30[P_6(x) - P_4(x)]$.

7. Prove that $\frac{(1+z)}{z(1-2xz+z^2)^{1/2}} - \frac{1}{z} = \sum_{n=0}^{\infty}[P_n(x) + P_{n+1}(x)]z^n$.

8. Show that $\frac{(1-z^2)}{(1-2xz+z^2)^{3/2}} = \sum_{n=0}^{\infty}(2n+1)P_n(x)z^n$.

9. Prove that
$$(i) \int P_n(x)\mathrm{d}x = \frac{P_{n+1}(x) - P_{n-1}(x)}{2n+1} + C \quad \text{and} \quad (ii) \int_x P_n(x)\mathrm{d}x = \frac{P_{n-1}(x) - P_{n+1}(x)}{2n+1}.$$

10. Show that $\int_{-1}^{+1} xP_n(x)P_{n-1}(x)\mathrm{d}x = \frac{2n}{4n^2-1}$.

11. Prove that $\int_{-1}^{+1}(1-x^2)\left[P_n'(x)\right]^2 \mathrm{d}x = \frac{2n(n+1)}{2n+1}$.

12. Prove that $(i) \int_{-1}^{+1} P_n(x)\mathrm{d}x = 0, \quad n \neq 0$ and $(ii) \int_{-1}^{+1} P_0(x)\mathrm{d}x = 2$.

13. Evaluate $(i) \int_{-1}^{+1} x^3 P_4(x)\mathrm{d}x, (ii) \int_{-1}^{+1} x^{99} P_{100}(x)\mathrm{d}x$ and $(iii) \int_{-1}^{+1} x^2 P_2(x)\mathrm{d}x$.

14. If $P_n(x)$ is defined by the relation $(1 - 2xh + h^2)^{-1/2} = \sum_{n=0}^{\infty} h^n P_n(x)$, then, show that $(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0$.

15. Prove that $\int_{-1}^{+1}\left[P_n'(x)\right]^2 \mathrm{d}x = n(n+1)$.

16. Express x^8 as a series in Legendre's polynomials of various degrees.

17. Express the following in terms of Legendre's polynomials:
    $(i)x^2 - 5x^2 + 6x + 1$ and $(ii)5x^3 + x$.

18. Prove that
    $(i)x^2 + \frac{1}{2}P_0(x) + \frac{2}{3}P_2(x), \quad (ii)x^3 = \frac{3}{5}P_1(x) + \frac{2}{5}P_3(x)$.

19. If: $f(x) = \begin{cases} 0, & -1 < x < 0, \\ x, & 0 < x < 1, \end{cases}$ then show that
    $f(x) = \frac{1}{4}P_0(x) + \frac{1}{2}P_1(x) + \frac{5}{16}P_2(x) - \frac{3}{32}P_4(x) + \cdots$

20. Prove that $x^4 = \frac{1}{35}\left[8P_4(x) + 20P_2(x) + 7P_0(x)\right]$.

21. Solve the Legendre's differential equation $(1-x^2)y'' - 2xy' + n(n+1)y = 0$ about its ordinary point $x = 0$ by assuming a solution of the form $y = \sum_{m=0}^{\infty} c_m x^m$ and show that the general solution of it is given by $y = au + bv$, where:
$$u = 1 - \frac{n(n+1)}{2!}x^2 + \frac{n(n-2)(n+1)(n+3)}{4!}x^4 - \ldots$$
$$\text{and } v = x - \frac{(n-1)(n+2)}{3!}x^3 + \frac{(n-1)(n-3)(n+2)(n+4)}{5!}x^5 - \ldots$$

22. Prove that:

(i) $(2n+1)xP_n(x) = (n+1)P_{n+1}(x) + nP_{n-1}(x)$.
(ii) $nP_n(x) = xP_n'(x) - P_{n-1}'(x)$.
(iii) $(2n+1)P_n(x) = P_{n+1}'(x) - P_{n-1}'(x)$.
(iv) $(n+1)P_n(x) = P_{n+1}'(x) - xP_n'(x)$.

23. Prove that:

(i) $(1-x^2)P_n'(x) = n[P_{n-1}(x) - xP_n(x)]$.
(ii) $(1-x^2)P_n'(x) = (n+1)[xP_n(x) - P_{n+1}(x)]$.

24. Prove that $(2n+1)(x^2-1)P_n'(x) = n(n+1)[P_{n+1}(x) - P_{n-1}(x)]$.

Laplace's equation in spherical coordinates

In spherical coordinates, Laplace's equation is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 V}{\partial\phi^2} = 0 \tag{690}$$

We can cancel off the factor of r^2. If we further assume that V is independent of ϕ, as is true for many problems, the last term disappears (we'll hopefully get around to considering the general case eventually), and we are left with

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right) = 0 \tag{691}$$

We can try the usual technique of separation of variables, and assume that

$$V(r,\theta) = R(r)\Theta(\theta) \tag{692}$$

Plugging this into the equation and dividing through by V, we get

$$\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \frac{1}{\Theta\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) = 0 \tag{693}$$

The argument that we use in the rectangular coordinate case applies here too: since each term on the left depends on only one of the two independent variables (r and θ), each term must be a constant. After solving the equation, in hindsight it turns out that the best way to write this constant is:

$$\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) = l(l+1) \tag{694}$$

$$\frac{1}{\Theta\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) = -l(l+1) \tag{695}$$

The general solution of the radial equation is

$$R(r) = Ar^l + \frac{B}{r^{l+1}} \tag{696}$$

as may be verified by direct substitution. Note that here, the constant l can be any real number; it's not restricted to being an integer.
The angular equation is more complex, but we've already considered it. As we saw there, the solutions are the Legendre polynomials. Moreover, as we worked through the solution of this equation to get the Legendre polynomials, we found that the only physically acceptable solutions (that is, ones that don't become infinite at some point) are those for which l is a positive integer. So we get

$$\Theta(\theta) = P_l(\cos\theta) \tag{697}$$

where P_l is the Legendre polynomial corresponding to a particular integer l. It turns out that P_l is a polynomial of degree l in its argument.
The polynomials can be generated by using the Rodrigues formula, as we saw earlier. The Rodrigues formula also allowed us to derive an orthogonality property of the Legendre polynomials (648).
Thus, for a particular value of l, the solution to Laplace's equation is

$$V_l(r,\theta) = \left(A_l r^l + \frac{B_l}{r^{l+1}}\right)P_l(\cos\theta) \tag{698}$$

where A_l and B_l are constants to be determined by the boundary conditions of the particular problem.
As before, since Laplace's equation is linear, we can form a general solution by summing up the particular solutions for all the values of l.

$$V(r,\theta) = \sum_{l=0}^{\infty}\left(A_l r^l + \frac{B_l}{r^{l+1}}\right)P_l(\cos\theta) \tag{699}$$

Example 1. The standard problem for illustrating how this general formula can be used is that of a hollow sphere of radius R, on which a potential $V_R(\theta)$ that depends only on θ is specified. The problem is to find the potential inside and outside the sphere, assuming no other charge is present.
For the inside problem, we must have $B_l = 0$ for all l, to prevent an infinity at the origin. On the boundary (that is, the sphere), we know the potential to be $V_R(\theta)$, so we have a boundary condition:

$$V(R,\theta) = \sum_{l=0}^{\infty} A_l R^l P_l(\cos\theta) = V_R(\theta) \tag{700}$$

We can now use the orthogonality condition (697) to find an expression for the coefficients A_l. If we multiply this equation through by $P_m(\cos\theta)\sin\theta$ and integrate from 0 to π, we get

$$\begin{aligned}
\sum_{l=0}^{\infty} A_l R^l \int_0^{\pi} P_l(\cos\theta)P_m(\cos\theta)\sin\theta \mathrm{d}\theta &= \int_0^{\pi} V_R(\theta)P_m(\cos\theta)\sin\theta d\theta &(701)\\
A_m R^m \frac{2}{2m+1} &= \int_0^{\pi} V_R(\theta)P_m(\cos\theta)\sin\theta \mathrm{d}\theta &(702)\\
A_m &= \frac{2m+1}{2R^m}\int_0^{\pi} V_R(\theta)P_m(\cos\theta)\sin\theta \mathrm{d}\theta &(703)
\end{aligned}$$

In the second line, we are able to eliminate all terms from the sum where $l \neq m$ by using the orthogonality condition. To proceed any further, we would need to know the function $V_R(\theta)$.
For the outside problem, we set $A_l = 0$ to prevent V from becoming infinite for large r. This time the general solution is:

$$V(r,\theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos\theta) \tag{704}$$

At the boundary, we get:

$$\sum_{l=0}^{\infty} \frac{B_l}{R^{l+1}} P_l(\cos\theta) = V_R(\theta) \tag{705}$$

We can use exactly the same procedure to find the coefficients B_l. Multiplying through by $P_m(\cos\theta)\sin\theta$ and integrating from 0 to π, we obtain:

$$\begin{aligned}
\frac{B_m}{R^{m+1}}\frac{2}{2m+1} &= \int_0^{\pi} V_R(\theta)P_m(\cos\theta)\sin\theta \mathrm{d}\theta &(706)\\
B_m &= \frac{(2m+1)R^{m+1}}{2}\int_0^{\pi} V_R(\theta)P_m(\cos\theta)\sin\theta \mathrm{d}\theta &(707)
\end{aligned}$$

where again we need an explicit form for $V_R(\theta)$ to proceed.

Laplace's equation in spherical coordinates - examples

Example 2. We saw that the coefficients A_l and B_l can be found by working out integrals, but in some special cases, it is easier to match up terms in the series on both sides of the equation. This happens if we can express V as a series of cosines (admittedly, this doesn't happen very often, but they are popular student exercises). For example, suppose we have a spherical shell of radius R on which the potential is $V(\theta) = k\cos 3\theta$. Using some trig identities, we can convert the cosine term:

$$\begin{aligned}
\cos 3\theta &= \cos(2\theta + \theta) &(708)\\
&= \cos 2\theta\cos\theta - \sin 2\theta \sin\theta &(709)\\
&= (2\cos^2\theta - 1)\cos\theta - 2\sin^2\theta\cos\theta &(710)\\
&= 2\cos^3\theta - \cos\theta - 2(1-\cos^2\theta)\cos\theta &(711)\\
&= 4\cos^3\theta - 3\cos\theta &(712)
\end{aligned}$$

We can now apply this to the general solution. Inside the sphere, the B_l terms are all zero to prevent an infinity at the origin, so we get at the boundary:

$$V(R,\theta) = \sum_{l=0}^{\infty} A_l R^l P_l(\cos\theta) \tag{713}$$

$$k\left(4\cos^3\theta - 3\cos\theta\right) = \sum_{l=0}^{\infty} A_l R^l P_l(\cos\theta) \tag{714}$$

Since the only terms appearing in the potential are of degree 1 and 3, only P_1 and P_3 appear in the series on the right. From tables of Legendre polynomials, we have:

$$P_1(\cos\theta) = \cos\theta \tag{715}$$

$$P_3(\cos\theta) = \frac{5}{2}\cos^3\theta - \frac{3}{2}\cos\theta \tag{716}$$

Matching up terms for the 3rd degree term, we get:

$$4k = \frac{5}{2}A_3R^3 \tag{717}$$

$$A_3 = \frac{8k}{5R^3} \tag{718}$$

With this value of A_3, the $l = 3$ term in the series contributes a term $-\frac{12}{5}k\cos\theta$, so combining this with the $l = 1$ term and equating this to the degree 1 term on the LHS, we get

$$-3k = A_1R - \frac{12}{5}k \tag{719}$$

$$A_1 = -\frac{3k}{5R} \tag{720}$$

The potential inside the sphere is thus:

$$V_{\text{in}}(r,\theta) = \frac{k}{5}\left(-\frac{3r}{R}P_1(\cos\theta) + \frac{8r^3}{R^3}P_3(\cos\theta)\right) \tag{721}$$

Outside the sphere, we can use the technique, except this time it is the A_l terms that are all set to zero to avoid an infinite potential for large r. We get, at the boundary:

$$V(R,\theta) = \sum_{l=0}^{\infty} B_l R^{-(l+1)} P_l(\cos\theta) \tag{722}$$

$$k\left(4\cos^3\theta - 3\cos\theta\right) = \sum_{l=0}^{\infty} B_l R^{-(l+1)} P_l(\cos\theta) \tag{723}$$

For the 3rd degree term:

$$4k = \frac{5}{2}B_3R^{-4} \tag{724}$$

$$B_3 = \frac{8kR^4}{5} \tag{725}$$

The $l = 3$ term contributes a term of $-\frac{12}{5}k\cos\theta$ as before, so combining this with the $l = 1$ term, we get

$$-3k = \frac{B_1}{R^2} - \frac{12}{5}k \tag{726}$$

$$B_1 = -\frac{3kR^2}{5} \tag{727}$$

The outside potential is

$$V_{\text{out}}(r,\theta) = \frac{k}{5}\left(-\frac{3R^2}{r^2}P_1(\cos\theta) + \frac{8R^4}{r^4}P_3(\cos\theta)\right) \tag{728}$$

Laguerre polynomials

Edmond Laguerre (1834 - 1886) introduced Laguerre polynomials, which are the solution of Laguerre's equation of order n

$$x\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + (1-x)\frac{\mathrm{d}y}{\mathrm{d}x} + ny = 0, \quad n \text{ being a positive integer} \tag{729}$$

- Laguerre polynomials are used to numerically compute integrals of the form $\int_0^\infty f(x)e^{-x}\mathrm{d}x$ in Gaussian quadrature.
- In quantum mechanics, they are seen in the radial part of the solution of the Schrödinger equation for a one-electron atom.
- They are also used to describe the static Wigner functions of oscillator systems in quantum mechanics in phase space.

We use Frobenius method to solve (729). Let

$$y = \sum_{m=0}^{\infty} c_m x^{k+m}, \quad c_0 \neq 0 \tag{730}$$

be the series solution of (729). We differentiate (730) to get $\frac{\mathrm{d}y}{\mathrm{d}x}, \frac{\mathrm{d}^2y}{\mathrm{d}x^2}$ and substitute them in (729) to obtain

$$x\sum_{m=0}^{\infty} c_m(k+m)(k+m-1)x^{k+m-2} + (1-x)\sum_{m=0}^{\infty} c_m(k+m)x^{k+m-1} + n\sum_{m=0}^{\infty} c_m x^{k+m} = 0 \tag{731}$$

$$\Longrightarrow \sum_{m=0}^{\infty} c_m(k+m)^2 x^{k+m-1} - \sum_{m=0}^{\infty} c_m(k+m-n)x^{k+m} = 0 \tag{732}$$

The indicial equation is (obtained by equating to zero the smallest power of x in (732), namely x^{k-1})

$$c_0k^2 = 0 \Longrightarrow k = 0, 0 \quad (\text{since } c_0 \neq 0).$$

We now equate the coefficient of x^{k+m-1} to zero in (732) and get

$$c_m(k+m)^2 - c_{m-1}(k+m-1-n) = 0$$
$$\Longrightarrow c_m = \frac{(k+m-1-n)}{(k+m)^2}c_{m-1}$$

In this case, the two independent solutions are given by $(y)_{k=0}$ and $\left(\frac{\partial y}{\partial k}\right)_{k=0}$. However,

$$\left(\frac{\partial y}{\partial k}\right)_{k=0} = \sum_{m=0}^{\infty} c_m x^{k+m}\log x,$$

which contains $\log x$ and is undefined at $x = 0$. Hence, we consider the solution $(y)_{k=0}$, which implies

$$y = \sum_{m=0}^{\infty} c_m x^m, \tag{733}$$

$$\text{where, } c_m = \frac{(m-1-n)}{m^2}c_{m-1} \quad (k=0) \tag{734}$$

Substituting $m = 1, 2, 3, \ldots$ in (734), we get

$$c_1 = -\frac{n}{1^2}c_0 = \frac{-1}{(1!)^2}nc_0$$
$$c_2 = \frac{1-n}{2^2}c_1 = -\frac{(n-1)}{(2)^2}(-1)nc_0 = (-1)^2\frac{n(n-1)}{(2!)^2}c_0$$
$$c_3 = \frac{2-n}{3^2}c_2 = (-1)^3\frac{n(n-1)(n-2)}{(3!)^2}c_0$$
$$c_r = (-1)^r\frac{n(n-1)(n-2)\cdots(n-r+1)}{(r!)^2}c_0, quad\text{for } r \leq n.$$

And $c_{n+1} = c_{n+2} = c_{n+3} = \cdots = 0 (r > n)$. Thus, (733) reduces to

$$\begin{aligned}
y &= c_0 \sum_{r=0}^{\infty} (-1)^r \frac{n(n-1)\cdots(n-r+1)}{(r!)^2} x^r \\
&= c_0 \sum_{r=0}^{n} (-1)^r \frac{n(n-1)\cdots(n-r+1)(n-r)(n-r-1)\cdots 3\cdot 2\cdot 1}{(n-r)(n-r-1)\cdots 3\cdot 2\cdot 1 (r!)^2} x^r \\
&= c_0 \sum_{r=0}^{n} (-1)^r \frac{n!}{(n-r)!(r!)^2} x^r
\end{aligned}$$

By taking $c_0 = 1$, this solution of Laguerre's equation is defined as the Laguerre polynomial of order n and is denoted by

$$L_n(x) = \sum_{r=0}^{n} (-1)^r \frac{n!}{(n-r)!(r!)^2} x^r$$

Alternatively, one may take $c_0 = n!$ and obtain another definition of Laguerre polynomial as

$$L_n(x) = \sum_{r=0}^{n} (-1)^r \frac{(n!)^2}{(n-r)!(r!)^2} x^r$$

Laguerre polynomial of order n is given by:

$$L_n(x) = \sum_{r=0}^{n} (-1)^r \frac{n!}{(n-r)!(r!)^2} x^r$$

Therefore,

$$\begin{aligned}
L_0(x) &= \sum_{r=0}^{0} (-1)^r \frac{0!}{(0-0)!(0!)^2} x^0 = 1 \\
L_1(x) &= \sum_{r=0}^{1} (-1)^r \frac{1!}{(1-r)!(r!)^2} x^r \\
&= (-1)^0 \frac{1!}{(1-0)!(0!)^2} x^0 + (-1)^1 \frac{1!}{(1-1)!(1!)^2} x^1 = 1 - x \\
L_2(x) &= \sum_{r=0}^{2} (-1)^r \frac{2!}{(2-r)!(r!)^2} x^r \\
&= (-1)^0 \frac{2!}{(2-0)!(0!)^2} x^0 + (-1)^1 \frac{2!}{(2-1)!(1!)^2} x^1 + (-1)^2 \frac{2!}{(2-2)!(2!)^2} x^2 = \frac{1}{2!}(2 - 4x + x^2) \\
L_3(x) &= \sum_{r=0}^{3} (-1)^r \frac{3!}{(3-r)!(r!)^2} x^r \\
&= (-1)^0 \frac{3!}{(3-0)!(0!)^2} x^0 + (-1)^1 \frac{3!}{(3-1)!(1!)^2} x^1 + (-1)^2 \frac{3!}{(3-2)!(2!)^2} x^2 + (-1)^3 \frac{3!}{(3-3)!(3!)^2} x^3 \\
&= \frac{1}{3!}(6 - 18x + 9x^2 - x^3)
\end{aligned}$$

Alternative expression for the Laguerre polynomials

Proposition: The Laguerre polynomials $L_n(x)$ can also be expressed as

$$l_n(x) = \frac{e^x}{n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(x^n e^{-x}\right)$$

Proof: Using Leibnitz's theorem, we get

$$\begin{aligned}
D^n(uv) &= \frac{\mathrm{d}^n}{\mathrm{d}x^n}(uv) = D^n u \cdot v + \binom{n}{1} D^{n-1} u \cdot Dv + \cdots + \binom{n}{r} D^{n-r} u \cdot D^r v + \cdots + u \cdot D^n v \\
\Longrightarrow D^n(uv) &= \sum_{r=0}^{n} \binom{n}{r} D^{n-r} u \cdot D^r v
\end{aligned}$$

Now,

$$\begin{aligned}
\frac{e^x}{n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(x^n e^{-x}\right) &= \frac{e^x}{n!} \sum_{r=0}^{n} \binom{n}{r} D^{n-r}\left(x^n\right) \cdot D^r\left(e^{-x}\right) \\
&= \frac{e^x}{n!} \sum_{r=0}^{n} \binom{n}{r} \frac{n!}{(n-(n-r))!} x^{n-(n-r)} (-1)^r e^{-x}
\end{aligned}$$

Using the result $D^n x^m = \frac{m!}{(m-n)!}x^{m-n}$ and $D^n e^{ax} = a^n e^{ax}$, we get

$$\begin{aligned}
&= \sum_{r=0}^{n} \frac{e^x}{n!} \frac{n!}{(n-r)!\,r!} \frac{n!}{r!} \cdot x^r \cdot (-1)^r e^{-x} \\
&= \sum_{r=0}^{n} \frac{(-1)^r n!}{(r!)^2 (n-r)!} x^r = L_n(x), \quad \text{(by definition)}
\end{aligned}$$

Putting $n = 0,1,2,3$ in $L_n(x) = e^x \frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^n e^{-x})$, we obtain the first few Laguerre polynomials as follows:

$$\begin{aligned}
L_0(x) &= \frac{e^x}{0!}\frac{\mathrm{d}^0}{\mathrm{d}x^0}\left(x^0 e^{-x}\right) = 1, \\
L_1(x) &= \frac{e^x}{1!}\frac{\mathrm{d}}{\mathrm{d}x}\left(x e^{-x}\right) = e^x\left(e^{-x} - x e^{-x}\right) = 1 - x, \\
L_2(x) &= \frac{e^x}{2!}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(x^2 e^{-x}\right) = \frac{1}{2!}\left(2 - 4x + x^2\right), \\
L_3(x) &= \frac{e^x}{3!}\frac{\mathrm{d}^3}{\mathrm{d}x^3}\left(x^3 e^{-x}\right) = \frac{1}{3!}\left(6 - 18x + 9x^2 - x^3\right).
\end{aligned}$$

Example 1: Express the polynomial $x^3 + x^2 - 3x + 2$ in a series of Laguerre polynomials.
Solution: From the results $L_0(x) = 1$, $L_1(x) = 1 - x$, $L_2(x) = \frac{2-4x+x^2}{2}$, and $L_3(x) = \frac{6-18x+9x^2-x^3}{6}$, we can calculate:

$$\begin{aligned}
L_0(x) = 1, \quad x &= 1 - L_1(x), \\
x^2 &= 4x - 2 + 2L_2(x) = 4(1 - L_1(x)) - 2 + 2L_2(x) = 2 - 4L_1(x) + 2L_2(x), \\
x^3 &= 6 - 18x + 9x^2 - 6L_3(x) = 6 - 18(1 - L_1(x)) + 9(2 - 4L_1(x) + 2L_2(x)) - 6L_3(x) \\
&= 6 - 18L_1(x) + 18L_2(x) - 6L_3(x),
\end{aligned}$$

Therefore,

$$\begin{aligned}
&x^3 + x^2 - 3x + 2 = (6 - 18L_1(x) + 18L_2(x) - 6L_3(x)) + (2 - 4L_1(x) + 2L_2(x)) - 3(1 - L_1(x)) + 2L_0(x) \\
\implies &x^3 + x^2 - 3x + 2 = 7 - 19L_1(x) + 20L_2(x) - 6L_3(x).
\end{aligned}$$

Laguerre polynomials - generating function

Proposition: The generating function for Laguerre polynomials is

$$\frac{\exp\{-xt/(1-t)\}}{(1-t)}.$$

Proof: Here, we show that the coefficient of t^n in the expansion of $\frac{\exp\{-xt/(1-t)\}}{1-t}$ is $L_n(x)$.
Now,

$$\begin{aligned}
\frac{\exp\{-xt/(1-t)\}}{(1-t)} &= \frac{1}{1-t}\sum_{r=0}^{\infty}\frac{1}{r!}\left(\frac{-xt}{1-t}\right)^r \\
&= \sum_{r=0}^{\infty}\frac{(-1)^r}{r!}x^r t^r (1-t)^{-(r+1)}.
\end{aligned}$$

Using the binomial expansion for $(1-t)^{-(r+1)}$, we write:

$$\begin{aligned}
&= \sum_{r=0}^{\infty}\frac{(-1)^r}{r!}x^r t^r \sum_{s=0}^{\infty}\frac{(r+s)!}{r!s!}t^s \\
&= \sum_{r=0}^{\infty}\sum_{s=0}^{\infty}\frac{(-1)^r}{r!}\binom{r+s}{s}x^r t^{r+s}.
\end{aligned}$$

Substituting $n = r + s$, where $s = n - r$, and reordering terms:

$$= \sum_{n=0}^{\infty}\sum_{r=0}^{n}\frac{(-1)^r}{r!}\binom{n}{r}x^r t^n.$$

Thus, the coefficient of t^n is:

$$\frac{(-1)^r n!}{(r!)^2(n-r)!}x^r.$$

Now, $s \geq 0$ implies $r \leq n$, giving all possible values of r. Hence, all the coefficients of t^n is given by:

$$\sum_{r=0}^{n} \frac{(-1)^r n!}{(r!)^2(n-r)!}x^r,$$

which by definition is the Laguerre polynomial $L_n(x)$ of order n. Example 2: Show that $\int_0^\infty e^{-st}L_n(t)\,\mathrm{d}t = \frac{1}{s}\left\{1-\frac{1}{s}\right\}^n$.
Solution:

$$\begin{aligned}\int_0^\infty e^{-st}L_n(t)\,\mathrm{d}t &= \int_0^\infty e^{-st}\left\{\sum_{r=0}^{n}\frac{(-1)^r n!\,t^r}{(n-r)!\,(r!)^2}\right\}\mathrm{d}t \quad \text{(by definition)}\\ &= \sum_{r=0}^{n}\frac{(-1)^r n!}{(n-r)!\,(r!)^2}\int_0^\infty e^{-st}t^r\,dt\end{aligned}$$

The integral can be solved using the Gamma function:

$$\int_0^\infty e^{-st}t^r\,\mathrm{d}t = \frac{\Gamma(r+1)}{s^{r+1}}.$$

Substituting:

$$\begin{aligned}&= \sum_{r=0}^{n}\frac{(-1)^r n!}{(n-r)!\,(r!)^2}\underbrace{\frac{\Gamma(r+1)}{s^{r+1}}}_{\frac{r!}{s^{r+1}}}\\ &= \frac{1}{s}\sum_{r=0}^{n}\frac{(-1)^r n!}{(n-r)!\,r!}\left(\frac{1}{s}\right)^r\\ &= \frac{1}{s}\sum_{r=0}^{n}\binom{n}{r}\left(-\frac{1}{s}\right)^r\\ &= \frac{1}{s}\left[1-\frac{1}{s}\right]^n.\end{aligned}$$

Example 3: Prove that

(i) $L_n'(0) = -n$,

(ii) $L_n''(0) = \frac{1}{2}n(n-1)$.

Solution: (i) $L_n(x)$, being a solution of the Laguerre's equation, satisfies it. Hence, we have:

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0.$$

Substitute $x = 0$ and $L_n(0) = 1$:

$$0 + (1-0)L_n'(0) + n\cdot 1 = 0 \implies L_n'(0) = -n.$$

(ii) The generating function for Laguerre polynomials is given by:

$$\frac{1}{1-t}e^{-tx/(1-t)} = \sum_{n=0}^{\infty} t^n L_n(x).$$

Differentiating twice with respect to x gives:

$$\frac{1}{1-t}e^{-tx/(1-t)}\left\{-\frac{t}{1-t}\right\}^2 = \sum_{n=0}^{\infty} L_n''(x)t^n.$$

By putting $x = 0$, we get:

$$\sum_{n=0}^{\infty} L_n''(0)t^n = t^2(1-t)^{-3}.$$

We now equate the coefficient of t^n from both sides to obtain:

$$L_n''(0) = \text{coefficient of } t^n \text{ in the expansion of } t^2(1-t)^{-3}$$
$$L_n''(0) = \text{coefficient of } t^{n-2} \text{ in the expansion of } (1-t)^{-3}$$

$$\begin{aligned}
\implies L_n''(0) &= (-3)(-3-1)\cdots(-3-(n-2)+1)(-1)^{n-2}/(n-2)! \\
&= (-3)(-4)\dots(-n)(-1)^{n-2}/(n-2)! \\
&= (3\cdot 4\cdot 5\cdot\dots\cdot n)(-1)^{n-2}(-1)^{n-2}/(n-2)! \\
&= \frac{1\cdot 2\cdot 3\cdot\dots\cdot n}{1\cdot 2\cdot (n-2)!}(-1)^{2n-2} \\
&= \frac{n!}{2(n-2)!} = \frac{n(n-1)}{2}
\end{aligned}$$

Eigenvalues, Eigenvectors and Diagonalization

Eigenvalues and Eigenvectors

In quantum mechanics, a physical state is represented by a vector in a vector space. Physically measurable quantities are represented by linear operators that operate on the state vector. If the state represents a system with a specific value of the physical quantity, applying the linear operator to the state results in that state being multiplied by the value of the quantity. Mathematically, such a state is called an *eigenvector* of the operator, and the numerical value, that results is called the *eigenvalue.* The word 'eigen' is German for 'own', so an eigenvalue is a value 'owned' by the operator. Here, we'll examine eigenvalues and eigenvectors from a purely mathematical viewpoint, as it's useful to have an underlying understanding of the mathematics when applying it to quantum theory.
We start with a vector space V and an operator T. Suppose there is a one-dimensional subspace U of V which has the property that for any vector $u \in U, Tu = \lambda u$. That is, the operator T maps any vector u back into another vector in the same subspace U. In that case, U is said to be an *invariant subspace* under the operator T.
You can think of this in geometric terms. Suppose we have some n-dimensional vector space V, and a one-dimensional subspace U consisting of all vectors parallel to some straight line within V. Let the operator T acting on any vector u parallel to that line produce another vector which is also parallel to the same line. In other words, T multiplies a vector u in U by some number λ, which results in another vector λu parallel to u. Of course we can't push the geometric illustration too far, since in general V and U can be complex vector spaces, so the result of acting on u with T might give you some complex number λ multiplied by u.
The equation

$$Tu = \lambda u \tag{735}$$

is called an eigenvalue equation, and the number $\lambda \in \mathbb{F}$ is called the eigenvalue. The vector u itself is called the eigenvector corresponding to the eigenvalue λ. Since we can multiply both sides of this equation by any number c, any multiple of u is also an eigenvector corresponding to λ, so any vector 'parallel' to u is also an eigenvector. (I've put 'parallel' in quotes, since we're allowing for multiplication of u by complex as well as real numbers.)
It can happen that, for a particular value of λ, there are two or more linearly independent (that is, non-parallel) eigenvectors. In that case, the subspace spanned by the eigenvectors is two- or higer-dimensional.
Another way of writing (735) is by introducing the identity operator I:

$$(T - \lambda I)u = 0 \tag{736}$$

If this equation has a solution other than $u = 0$, then the operator $T - \lambda I$ has a non-trivial null space, which in turn means that $T - \lambda I$ is not injective (not one-to-one) and therefore not invertible. Also, the eigenvectors of T with eigenvalue λ are those vectors u in the null space of $T - \lambda I$.
An important result is

Theorem 1. *Suppose $\lambda_1, \dots, \lambda_m$ are distinct eigenvalues of T and $v_1, \dots, v_m$ are the corresponding non-zero eigenvectors. Then the set $v_1, \dots, v_m$ is linearly independent.*

Proof. Suppose to the contrary that $v_1, \dots, v_m$ is linearly dependent. Then there must be some subset that is linearly independent. Suppose that k is the smallest positive integer such that v_k can be written in terms of $v_1, \dots, v_{k-1}$. That is, the set $v_1, \dots, v_{k-1}$ is a linearly independent subset of $v_1, \dots, v_m$. In that case, there are numbers $a_1, \dots, a_{k-1} \in \mathbb{F}$ such that

$$v_k = \sum_{i=1}^{k-1} a_i v_i \tag{737}$$

If we apply the operator T to both sides and use the eigenvalues equation, we have

$$\begin{aligned} Tv_k &= \lambda_k v_k & (738)\\ &= \sum_{i=1}^{k-1} a_i T v_i & (739)\\ &= \sum_{i=1}^{k-1} a_i \lambda_i v_i & (740) \end{aligned}$$

That is

$$\lambda_k v_k = \sum_{i=1}^{k-1} a_i \lambda_i v_i \tag{741}$$

We cam multiply both sides of (737) by λ_k and subtract from (741) to get

$$\begin{aligned} (\lambda_k - \lambda_k) v_k &= \sum_{i=1}^{k-1} a_i (\lambda_i - \lambda_k) v_i & (742)\\ &= 0 & (743) \end{aligned}$$

Since the set of vectors $v_1, \dots, v_{k-1}$ is linearly independent, and $\lambda_k \neq \lambda_i$ for $i = 1, \dots, k-1$, the only solution of this equation is $a_i = 0$ for $i = 1, \dots, k-1$. But (from 737) this would make $v_k = 0$, contrary to our assumption that v_k is a non-zero eigenvector of T. Therefore the set $v_1, \dots, v_m$ is linearly independent. □

It turns out that there are some operators on real vector spaces that don't have any eigenvalues. A simple

example is the 2-dimensional vector space consisting of the xy-plane. The rotation operator which rotates any vector about the origin (by some angle other than 2π) doesn't leave any vector parallel to itself and thus has no eigenvalues or eigenvectors.
However, in a complex vector space, things are a bit neater. This leads to the following theorem:

Theorem 2. *Every operator on a finite-dimensional, non-zero, complex vector space has at least one eigenvalue.*

Proof. Suppose V is a complex vector space with dimension $n > 0$. For some vector $v \in V$ we can write the $n+1$ vectors

$$v, Tv, T^2 v, \dots, T^n v \tag{744}$$

Because we have $n+1$ vectors in an n-dimensional vector space, these vectors must be linearly dependent, which means we can find complex numbers $a_0, \dots, a_n \in \mathbb{C}$, not all zero, such that

$$0 = a_0 v + a_1 T v + \cdots + a_n T^n v \tag{745}$$

We can consider a polynomial in z with the a_i as coefficients:

$$p(z) = a_0 + a_1 z + \cdots + a_n z^n \tag{746}$$

The Fundamental Theorem of Algebra states that any polynomial of degree n can be factored into n linear factors. In our case, the actual degree of $p(z)$ is $m \leq n$ since a_n could be zero. So we can factor $p(z)$ as follows:

$$p(z) = c(z - \lambda_1) \cdots (z - \lambda_m) \tag{747}$$

where $c \neq 0$.
Comparing this to (745), we can write that equation as

$$0 = a_0 v + a_1 T v + \dots + a_n T^n v \tag{748}$$
$$= (a_0 I + a_1 T + \dots + a_n T^n) v \tag{749}$$
$$= c(T - \lambda_1 I) \cdots (T - \lambda_m I) v \tag{750}$$

All the $T - \lambda_i I$ operators in the last line commute with each other since I commutes with everything and T commutes with itself, so n order for the last line to be zero, there has to be at least one λ_i such that $(T - \lambda_i I)v = 0$. That is, there is at least one λ_i such that $T - \lambda_i I$ has a nonzero null space, which means λ_i is an eigenvalue. □

References

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(3) Landi, Giovanni & Zampini, Alessandro (2018), *Linear Algebra and Analytic Geometry for Physical Sciences*, Chapter 9.

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Diagonalization of matrices

Suppose we have an operator T that has a matrix representation $T(v)$ in some basis v. In some cases (not all!) it is possible to transform to a different basis u in which $T(u)$ is a diagonal matrix. If the operator A transforms from the basis v to u, then we can see that T transforms according to

$$T(u) = A^{-1} T(v) A \tag{751}$$

The diagonalization problem is therefore to find the matrix A (if it exists) so that $T(u)$ is diagonal.
Assuming A does exist, we can look at the situation in two ways.

(1) The matrix representation of T is diagonal in the u basis.

(2) The operator $A^{-1}TA$ is diagonal in the original v basis.

To prove (2), we start with the fact that T is diagonal in the u basis, so that (no implied sums in what follows):

$$T u_i = \lambda_i u_i \tag{752}$$
$$T A v_i = \lambda_i A v_i \tag{753}$$
$$A^{-1} T A v_i = \lambda_i A^{-1} A v_i \tag{754}$$
$$= \lambda_i v_i \tag{755}$$

From the last line, we see that v_i is an eigenvector of the operator $A^{-1}TA$ with the same eigenvalue λ_i as the eigenvector u_i of the operator T. Thus we can write, in the original basis v, the equation

$$D_T \equiv A^{-1} T A \tag{756}$$

where D_T is the diagonlized version of the matrix T in the v basis. This is known as a *similarity transformation.*
All this is fine, but we still haven't seen how to find A. It turns out that the columns of A are the eigenvectors of T. We can see this from the following argument.
In the basis v, each v_i has the form of a column vector with a 1 in the i-th position and zeroes everywhere else. Thus the transformation to the u basis can be written as

$$u_k = A v_k = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix} \cdot \begin{bmatrix} \vdots \\ 1 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{1k} \\ \vdots \\ A_{nk} \end{bmatrix} \tag{757}$$

The 1 is in the k-th position in the column vector representing v_k and picks out the elements in th column k of A in the product Av_k. Since u_k is the k-th eigenvector of T, the columns of A are the eigenvectors of T. Suppose we have

$$T = \begin{bmatrix} 1 & 2 \\ 3 & 1 \end{bmatrix} \tag{758}$$

The eigenvalues are found in the usual way, from the characteristic determinant, which is

$$(1-\lambda)^2 - 6 = 0 \tag{759}$$

$$\lambda = 1 \pm \sqrt{6} \tag{760}$$

We can find the eigenvectors by solving $Tu_i = \lambda_i u_i$ for each eigenvalue, where u_i is a 2-element column vector. (I won't go through this, since it's just algebra.) Placing the eigenvectors as the columns in a matrix A, we have

$$A = \begin{bmatrix} \frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{3} \\ 1 & 1 \end{bmatrix} \tag{761}$$

The inverse of a 2×2 matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is

$$A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \tag{762}$$

So for our matrix, we have

$$A^{-1} = \begin{bmatrix} \frac{\sqrt{6}}{4} & \frac{1}{2} \\ -\frac{\sqrt{6}}{4} & \frac{1}{2} \end{bmatrix} \tag{763}$$

Doing the matrix products (just a lot of arithmetic) we get

$$A^{-1}TA = \begin{bmatrix} 1+\sqrt{6} & 0 \\ 0 & 1-\sqrt{6} \end{bmatrix} \tag{764}$$

The resulting matrix is diagonal, and the diagonal entries are the eigenvalues of T. It's worth verifying that the traces of $A^{-1}TA$ and T are the same (both = 2), as are the determinants (both = −5).

References

(1) Zwiebach, Barton, Online course *Mastering Quantum Mechanics Part 1: Wave Mechanics.* Archive available here

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Gram-Schmidt orthogonalization

TBA

Spectral Theorem for normal operators

We'll now look at a central theorem about normal operators, known as the *spectral theorem.*
We've seen that if a matrix M has a set v of eigenvectors that span the space, then we can diagonilze M by means of the similarity transformation

$$D_M = A^{-1}MA \tag{765}$$

where D_M is diagonal and the columns of A are the eigenvectors of M. In the general case, there's no guarentee that the eigenvectors of M are orthonormal. However, if there *is* an orthonormal basis in which M is diagonal, then M is said to be *unitarily diagonalizable.* Suppose we start with some arbitrary orthonormal basis $(e_1, \dots, e_n)$ (we can always construct such a basis using the Gram-Schmidt procedure). Then if the set of eigenvectors of M form an orthonormal basis $(u_1, \dots, u_n)$, there is a unitary matrix U that transforms the e_i basis into the u_i basis (since unitary operators preserve inner products):

$$u_i = U e_i = \sum_j U_{ji} e_j \tag{766}$$

Using this unitary operator, we therefore have for a unitarily diagonalizable operator M

$$D_M = U^{-1} M U = U^\dagger M U \tag{767}$$

The *spectral theorem* now states:

Theorem 1. *An operator M in a complex vector space has an orthonormal basis of eigenvectors (that is, it's unitarily diagonalizable) if and only if M is normal.*

Proof. Since this is an 'if and only if' theorem, we need to prove it in both directions. First, suppose that M is unitarily diagonalizable, so that (767) holds for some U. Then

$$M = U D_M U^\dagger \tag{768}$$

$$M^\dagger = U D_M^\dagger U^\dagger \tag{769}$$

The commutator is then, since $U^\dagger U = I$

$$\left[M^\dagger, M\right] = U D_M^\dagger D_M U^\dagger - U D_M D_M^\dagger U^\dagger \tag{770}$$

$$= U\left[D_M^\dagger, D_M\right] U^\dagger \tag{771}$$

$$= 0 \tag{772}$$

where the result follows because all diagonal matrices commute and, since D_M is diagonal, so is its hermitian conjugate $D_M^\dagger$. Thus M is normal, and this completes one direction of the proof.
Going the other way is a bit trickier. We need to show that for any normal matrix M with elements defined on some arbitrary orthonormal basis (that is, a basis that is not necessarily composed of eigenvectors of M), there is a unitary matrix U such that $U^\dagger M U$ is diagonal. Since we started with an orthonormal basis and U preserves inner products, the new basis is also orthonormal which will prove the theorem.
The proof uses mathematical induction, in which we first prove that the result is true for one specific dimension of vector space, say $\dim V = 1$. We can then assume the result is true for some dimension $n-1$ and from that assumption, prove it is also true for the next higher dimension n.
Since any 1×1 matrix is diagonal (it consists of only one element), the result is true for $\dim V = 1$. So we now assume it's true for a dimension of $n-1$ and prove it's true for a dimension of n.
We take an arbitrary orthonormal basis of the n-dimensional vector space V to be $(|1\rangle, \dots, |n\rangle)$. In that basis, the matrix M has elements $M_{ij} = \langle i|M|j\rangle$. We know that M has at least one eigenvalue λ_1 with a normalized eigenvector $|x_1\rangle$:

$$M|x_1\rangle = \lambda_1 |x_1\rangle \tag{773}$$

and, since M is normal, the eigenvector $|x_1\rangle$ is also an eigenvector of $M^\dagger$:

$$M^\dagger |x_1\rangle = \lambda_1^* |x_1\rangle \tag{774}$$

Starting with a basis of V containing $|x_1\rangle$, we can use Gram-Schmidt to generate an orthonormal basis $(|x_1\rangle, \dots, |x_n\rangle)$. We now define an operator U_1 as follows:

$$U_1 \equiv \sum_i |x_i\rangle\langle i| \tag{775}$$

where $|i\rangle$ is a vector in the original orthonormal basis defined above. U_1 is unitary, since

$$U_1^\dagger = \sum_i |i\rangle\langle x_i| \tag{776}$$

$$U_1^\dagger U = \sum_i \sum_j |i\rangle\langle x_i|x_j\rangle\langle j| \tag{777}$$

$$= \sum_i \sum_j |i\rangle \delta_{ij} \langle j| \tag{778}$$

$$= \sum_i \sum_j |i\rangle\langle i| \tag{779}$$

$$= I \tag{780}$$

From its definition

$$U_1|1\rangle = |x_1\rangle \tag{781}$$
$$U_1^\dagger|x_1\rangle = |1\rangle \tag{782}$$
$$\tag{783}$$

Now consider the matrix M_1 defined as

$$M_1 \equiv U_1^\dagger M U_1 \tag{784}$$

M_1 is also normal, as can be verified by calculating the commutator and using $\left[M^\dagger, M\right] = 0$. Further

$$M_1|1\rangle = U_1^\dagger M U_1|1\rangle \tag{785}$$
$$= U_1^\dagger M|x_1\rangle \tag{786}$$
$$= \lambda_1 U_1^\dagger|x_1\rangle \tag{787}$$
$$= \lambda_1|1\rangle \tag{788}$$

where we used (773) to get the third line. Thus $|1\rangle$ is an eigenvector of M_1 with eigenvalue λ_1.
The matrix elements in the first column of M_1 in the original basis $(|1\rangle, \ldots, |n\rangle)$ are

$$\langle j|M_1|1\rangle = \lambda_1\langle j|1\rangle = \lambda_1\delta_{1j} \tag{789}$$

Thus all entries in the first column are zero except for the first row, where it is λ_1. How about the first row? Using (774) we have

$$\langle 1|M_1|j\rangle = \left(\langle j|M_1^\dagger|1\rangle\right)^* \tag{790}$$
$$= (\lambda_1^*\langle j|1\rangle)^* \tag{791}$$
$$= \lambda_1\delta_{1j} \tag{792}$$

Thus all entries in the first row, except the first, are also zero. Thus in the original basis $(|1\rangle, \ldots, |n\rangle)$ we have

$$M_1 = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & M' & \\ 0 & & & \end{bmatrix} \tag{793}$$

where M' is an $(n-1)\times(n-1)$ matrix. We have

$$M_1^\dagger = \begin{bmatrix} \lambda_1^* & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & M'^\dagger & \\ 0 & & & \end{bmatrix} \tag{794}$$

$$M_1^\dagger M_1 = \begin{bmatrix} |\lambda_1|^2 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & M'^\dagger M' & \\ 0 & & & \end{bmatrix} \tag{795}$$

$$M_1 M_1^\dagger = \begin{bmatrix} |\lambda_1|^2 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & M' M'^\dagger & \\ 0 & & & \end{bmatrix} \tag{796}$$

Since M_1 is normal, we must have $M_1 M_1^\dagger = M_1^\dagger M_1$, which implies

$$M'^\dagger M' = M' M'^\dagger \tag{797}$$

so that M' is also a normal matrix. By the induction hypotheses, since M' is an $(n-1)\times(n-1)$ normal matrix, it is unitarily diagonalizable by some unitary matrix U', that is

$$U'^\dagger M' U' = D_{M'} \tag{798}$$

is diagonal. We can extend U' to an $n \times n$ unitary matrix by adding a 1 to the upper left:

$$U = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U' & \\ 0 & & & \end{bmatrix} \tag{799}$$

We can check that U is unitary by direct calculation, using $U'^\dagger U' = I$

$$U^\dagger U = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U'^\dagger & \\ 0 & & & \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U' & \\ 0 & & & \end{bmatrix} \tag{800}$$

$$= \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U'^\dagger U' & \\ 0 & & & \end{bmatrix} \tag{801}$$

$$= \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & \\ \vdots & & 1 & \\ 0 & & & 1 \end{bmatrix} = I \tag{802}$$

We then have, using (798)

$$U^\dagger M_1 U = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U'^\dagger & \\ 0 & & & \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & M' & \\ 0 & & & \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U' & \\ 0 & & & \end{bmatrix} \tag{803}$$

$$= \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & U'^\dagger M' U' & \\ 0 & & & \end{bmatrix} \tag{804}$$

$$= \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & D_{M'} & \\ 0 & & & \end{bmatrix} \tag{805}$$

That is, $U^\dagger M_1 U$ is diagonal. From the definition (784) of M_1, we now have

$$U^\dagger M_1 U = U^\dagger U_1^\dagger M U_1 U \tag{806}$$

$$= (U_1 U)^\dagger M (U_1 U) \tag{807}$$

Since the product of two Unitary matrices is unitary, we have found a unitary operator $U_1 U$ that diagonalizes M, which proves the result.

□

Notice that the proof didn't assume that the eigenvalues are nondegenerate, so that even if there are several

linearly independent eigenvectors corresponding to one eigenvalue, it is still possible to find an orthonormal basis consisting of the eigenvectors. In other words, for any hermitian or unitary operator, it is always possible to find an orthonormal basis of the vector space consisting of eigenvectors of the operator.
In the general case, a normal matrix M in an n-dimensional vector space can have m distinct eigenvalues, where $1 \leq m \leq n$. If $n = m$, there is no degeneracy and each eigenvalue has a unique (up to a scalar multiple) eigenvector. If $m < n$, then one or more of the eigenvalues occurs more than once, and the eigenvector subspace corresponding to a degenerate eigenvalue has a dimension larger than 1. However, the spectral theorem guarentees that it is possible to choose an orthonormal basis within each subspace, and that each subspace is orthogonal to all other subspaces.
More precisely, the vector space V can be decomposed into m subspaces U_k for $k = 1, \ldots, m$, with the dimension d_k of subspace U_k equal to the degeneracy of eigenvalue λ_k. The full space V is the direct sum of

these subspaces

$$V = U_1 \oplus U_2 \oplus \cdots \oplus U_m \tag{808}$$

$$n = \sum_{k=1}^{m} d_k \tag{809}$$

It's usually most convenient to order the eigenvectors as follows:

$$\left(u_1^{(1)}, \ldots, u_{d_1}^{(1)}, u_1^{(2)}, \ldots, u_{d_2}^{(2)}, \ldots, u_1^{(m)}, \ldots, u_{d_m}^{(m)}\right) \tag{810}$$

The notation $u_j^{(k)}$ means the j-th eigenvector belonging to eigenvalue k.
In practice, there is a lot of freedom in choosing orthonormal eigenvectors for degenerate eigenvalues, since we can pick any d_k mutually orthogonal vectors within the subspace of dimension d_k. For example, in 3-d space we usually choose the x, y, z unit vectors as the orthonormal set, but we can pivot these three vectors about the origin, or even reflect them in a plane passing through the origin, and still get an orthonormal set of 3 vectors.
The diagonal form of the normal matrix M in this orthonormal basis is

$$D_M = \begin{bmatrix} \lambda_1 & & & & & & \\ & \ddots & & & & & \\ & & \lambda_1 & & & & \\ & & & \ddots & & & \\ & & & & \lambda_m & & \\ & & & & & \ddots & \\ & & & & & & \lambda_m \end{bmatrix} \tag{811}$$

Here, eigenvalue λ_k occurs d_k times along the diagonal.

References

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Tensor Analysis

TBA

Asymptotic Analysis

TBA

Probabilty Theory

TBA

Appendix B

Canonical and Kinetic Momentum

In this appendix, we collect some formulae from the classical mechanics of charged particles moving in an electromagnetic field and determine the eigenfunctions of the orbital angular momentum.

We first recall that the Hamiltonian

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(x,t)\right)^2 + e\Phi(\mathbf{x},t)$$

leads to the classical equations of motion (814). For this, we compute (note the summation convention)

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{1}{m}\left(p_i - \frac{e}{c}A_i(x,t)\right), \tag{812}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} = -\frac{1}{m}\left(p_j - \frac{e}{c}A_j(\mathbf{x},t)\right)\left(-\frac{e}{c}A_{j,i}\right) - e\Phi_{,i} = \dot{x}_j\frac{e}{c}A_{j,i} - e\Phi_{,i}, \tag{813}$$

with $f_{,i} \equiv \partial f/\partial x_i$. From (812, 813), the Newtonian equation of motion

$$m\ddot{x}_i = \dot{p}_i - \frac{e}{c}A_{i,j}\dot{x}_j - \frac{e}{c}\dot{A}_i = \frac{e}{c}\dot{x}_jA_{j,i} - e\Phi_{,i} - \frac{e}{c}\dot{x}_jA_{i,j} - \frac{e}{c}\dot{A}_i$$

follows, i.e.,

$$m\ddot{x}_i = \left(\frac{e}{c}\dot{\mathbf{x}} \times \mathbf{B} + e\mathbf{E}\right)_i. \tag{814}$$

Here, we have also used

$$(\dot{\mathbf{x}} \times \mathbf{B})_i = \epsilon_{ijk}\dot{x}_j\epsilon_{krs}A_{s,r} = \dot{x}_j(A_{j,i} - A_{i,j}),$$

and

$$(\mathrm{curl}\,\mathbf{A})_k = B_k, \quad \mathbf{E} = -\mathrm{grad}\,\Phi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}.$$

One refers to $\mathbf{p}$ as the canonical momentum and $m\dot{\mathbf{x}}$ from (812) as the kinetic momentum.
We obtain the Lagrangian

$$L = \mathbf{p}\cdot\dot{\mathbf{x}} - H = m\dot{\mathbf{x}}^2 + \frac{e}{c}\mathbf{A}\cdot\dot{\mathbf{x}} - \frac{m}{2}\dot{\mathbf{x}}^2 - e\Phi,$$
$$L = \frac{m}{2}\dot{\mathbf{x}}^2 + \frac{e}{c}\mathbf{A}\cdot\dot{\mathbf{x}} - e\Phi.$$

The Lagrange equations of motion

$$\frac{d}{dt}\frac{\partial L}{\partial\dot{\mathbf{x}}} = \frac{\partial L}{\partial\mathbf{x}}$$

with

$$\frac{\partial L}{\partial\dot{\mathbf{x}}} = m\dot{\mathbf{x}} + \frac{e}{c}\mathbf{A}, \quad \left(\frac{\partial L}{\partial\mathbf{x}}\right)_i = \frac{e}{c}\dot{x}_jA_{j,i} - e\Phi_{,i},$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\mathbf{x}}}\right)_i = m\ddot{x}_i + \frac{e}{c}A_{i,j}\dot{x}_j + \frac{e}{c}\dot{A}_i$$

lead again to Newton's second law with the Lorentz force:

$$m\ddot{\mathbf{x}} = e\mathbf{E} + \frac{e}{c}\dot{\mathbf{x}} \times \mathbf{B}.$$

Algebraic Determination of the Orbital Angular Momentum Eigenfunctions

We now determine the eigenfunctions of orbital angular momentum algebraically. For this we define

$$x_\pm = x \pm iy. \tag{815}$$

The following commutation relations hold:

$$[L_z, x_\pm] = \pm\hbar x_\pm, \quad [L_\pm, x_\pm] = 0, \quad [L_\pm, x_\mp] = \pm 2\hbar z, \tag{816}$$

$$[\mathbf{L}^2, x_+] = L_z \hbar x_+ + \hbar x_+ L_z + \hbar^2 x_+ - 2\hbar z L_+ \tag{817}$$

$$= 2\hbar x_+ L_z + 2\hbar^2 x_+ - 2\hbar z L_+, \tag{818}$$

where $\mathbf{L}^2 = L_z^2 + \hbar L_z + L_- L_+$ has been used. It follows that

$$L_z x_+ |l,l\rangle = x_+ L_z |l,l\rangle + \hbar x_+ |l,l\rangle = \hbar(l+1) x_+ |l,l\rangle \tag{819}$$

$$\mathbf{L}^2 x_+ |l,l\rangle = \hbar^2 l(l+1) x_+ |l,l\rangle + 2\hbar^2 (l+1) x_+ |l,l\rangle = \hbar^2 (l+1)(l+2) x_+ |l,l\rangle. \tag{820}$$

The quantity x_+ is thus the ladder operator for the states $|l,l\rangle$,

$$x_+ |l,l\rangle = N |l+1, l+1\rangle. \tag{821}$$

Hence, the eigenstates of angular momentum can be represented as follows:

$$|l,m\rangle = N' L_-^{l-m} (x_+)^l |0,0\rangle. \tag{822}$$

N and N' in (821) and (**??**) are constants. Since $\mathbf{L}|0,0\rangle = 0$, it follows that

$$\langle \mathbf{x} | U_{\delta\varphi} |0,0\rangle = \langle U_{\delta\varphi}^{-1} \mathbf{x} |0,0\rangle = \langle \mathbf{x}|0,0\rangle,$$

and thus

$$\psi_{00}(\mathbf{x}) = \langle \mathbf{x}|0,0\rangle \tag{823}$$

does not depend on the polar angles ϑ, φ. The norm of $|0,0\rangle$

$$\langle 0,0|0,0\rangle = \int \mathrm{d}\Omega \langle 0,0|\mathbf{x}\rangle\langle \mathbf{x}|0,0\rangle$$

is unity for

$$\psi_{00}(\mathbf{x}) = \frac{1}{\sqrt{4\pi}}. \tag{824}$$

The norm of the state $|l,l\rangle \propto \left(\frac{x_+}{r}\right)^l |0,0\rangle$, whose coordinate representation is

$$\langle x| \left(\frac{x_+}{r}\right)^l |0,0\rangle = \frac{1}{\sqrt{4\pi}} \sin^l \vartheta e^{il\varphi},$$

becomes

$$\langle 0,0| \left(\frac{x_-}{r}\right)^l \left(\frac{x_+}{r}\right)^l |0,0\rangle = \langle 0,0| \left(\frac{x^2+y^2}{r^2}\right)^l |0,0\rangle = \langle 0,0| \left(1 - \frac{z^2}{r^2}\right)^2 |0,0\rangle = \langle 0,0| \sin^{2l}\vartheta |0,0\rangle$$

$$= \int_0^{2\pi} \mathrm{d}\varphi \int_0^\pi \mathrm{d}\vartheta \sin\vartheta \frac{1}{4\pi} \sin^{2l}\vartheta = \frac{1}{2}\int_{-1}^1 \mathrm{d}(\cos\vartheta) \sin^{2l}\vartheta = I_l,$$

where

$$I_l = \int_0^1 \mathrm{d}\eta (1-\eta^2)^l = \eta(1-\eta^2)^l \Big|_0^1 + 2l \int_0^1 \mathrm{d}\eta (1-\eta^2)^{l-1}\eta = -2l I_l + 2l I_{l-1},$$

$$I_l = \frac{2l}{2l+1} I_{l-1} = \frac{2l}{2l+1} \frac{2(l-1)}{2(l-1)+1} \cdots \frac{2\times 1}{2+1} I_0 = \frac{2l(2l-2)\ldots 2}{(2l+1)(2l-1)\ldots 3} = \frac{2^l (l!)^2}{(2l+1)!}, \quad I_0 = 1.$$

One thus has

$$\psi_{ll}(\mathbf{x}) = \frac{1}{\sqrt{4\pi I_l}} \sin^l \vartheta e^{il\varphi} \tag{825}$$

and the definition of the spherical harmonics

$$Y_l^m(\vartheta,\varphi) = (-1)^l \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l l!} \sin^l \vartheta e^{il\varphi}. \tag{826}$$

$Y_{ll}(\vartheta,\varphi)$ can also be found directly from the equations

$$L_z Y_{ll} = \hbar l Y_{ll} \quad \text{and} \quad L_+ Y_{ll} = 0 = e^{i\varphi}\left(\frac{\partial}{\partial\vartheta} + i\cot\vartheta \frac{\partial}{\partial\varphi}\right) e^{il\varphi} f(\vartheta).$$

The first implies

$$Y_{ll} = e^{il\varphi} f(\vartheta),$$

and the second implies

$$\begin{aligned}
\frac{\partial}{\partial\vartheta} f(\vartheta) &= l\cot\vartheta f(\vartheta),\\
\frac{df}{f} &= l\cot\vartheta \mathrm{d}\vartheta,\\
\log|f| &= l\log\sin\vartheta + A,\\
f &= \alpha\sin^l\vartheta \quad \text{q.e.d.}
\end{aligned}$$

The remaining eigenfunctions are obtained by application of L_-:

$$(L_-)^{l-m}|l,l\rangle = N'|l,m\rangle. \tag{827}$$

In order to determine N', we start from

$$L_-|l,m\rangle = \hbar\sqrt{(l+m)(l-m+1)}|l,m-1\rangle,$$

hence,

$$(L_-)^{l-m}|l,l\rangle = [2l\times 1\times(2l-1)\times 2\ldots(l+m+1)(l-m)]^{1/2}\hbar^{l-m}|l,m\rangle,$$

and

$$Y_{lm}(\vartheta,\varphi) = \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}(L_-/\hbar)^{l-m} Y_{ll}(\vartheta,\varphi). \tag{828}$$

We now apply the operator L_-:

$$\begin{aligned}
(L_-/\hbar) f(\vartheta) e^{im\varphi} &= e^{-i\varphi}\left(-\frac{\partial}{\partial\vartheta} + i\cot\vartheta\frac{\partial}{\partial\varphi}\right) f(\vartheta) e^{im\varphi},\\
&= e^{i(m-1)\varphi}(-1)(f'(\vartheta) + m\cot\vartheta f).
\end{aligned}$$

Comparing this with

$$\frac{\mathrm{d}}{\mathrm{d}\cos\vartheta}(f\sin^m\vartheta) = -(f' + mf\cot\vartheta)\sin^{m-1}\vartheta,$$

we see that

$$(L_-/\hbar) f(\vartheta) e^{im\varphi} = e^{i(m-1)\varphi}\sin^{1-m}\vartheta\frac{\mathrm{d}(f\sin^m\vartheta)}{\mathrm{d}\cos\vartheta}.$$

Applying L_- $(l-m)$ times yields

$$(L_-/\hbar)^{l-m} e^{il\varphi}\sin^l\vartheta = e^{im\varphi}\sin^{-m}\vartheta\frac{\mathrm{d}^{l-m}}{(\mathrm{d}\cos\vartheta)^{l-m}}\sin^{2l}\vartheta,$$

and

$$Y_{lm}(\vartheta,\varphi) = (-1)^l\sqrt{\frac{(l+m)!(2l+1)}{(l-m)!4\pi}}\frac{1}{2^l l!} e^{im\varphi}\sin^{-m}\vartheta\frac{\mathrm{d}^{l-m}}{(\mathrm{d}\cos\vartheta)^{l-m}}\sin^{2l}\vartheta \tag{829}$$

$$= (-1)^{l+m}\frac{1}{2^l l!}\sqrt{\frac{(l-m)!(2l+1)}{(l+m)!4\pi}} e^{im\varphi}\sin^m\vartheta\frac{\mathrm{d}^{l+m}}{(\mathrm{d}\cos\vartheta)^{l+m}}\sin^{2l}\vartheta. \tag{830}$$

And the spherical harmonics obey

$$Y_{l,m}(\vartheta,\varphi) = (-1)^m Y^*_{l,-m}(\vartheta,\varphi). \tag{831}$$

This concludes the algebraic derivation of the angular momentum eigenfunctions.

Remark: In going from (829) over to the conventional representation (830), we have used the fact that the associated Legendre function

$$P_l^m(\eta) = \frac{1}{2^l l!}(1-\eta^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}\eta^{l+m}}(\eta^2-1)^l \tag{832}$$

satisfies the identity

$$P_l^{-m} = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m. \tag{833}$$

For the derivation of this identity, we note that both P_l^m and P_l^{-m} are l-th order polynomials in η for even m; for odd m, they are polynomials of order $(l-1)$, multiplied by $\sqrt{1-\eta^2}$. Further, the differential equation for P_l^m contains the coefficient m only quadratically, and therefore P_l^{-m} is also a solution and must be proportional to the regular solution P_l^m which we began with. In order to determine the coefficient of proportionality, we compare the highest powers of η in the expressions for P_l^{-m} and P_l^m, multiplied by $(1-\eta^2)^{m/2}$.
This yields (833).
We now prove algebraically that for the angular momentum operator the quantum number l is a nonnegative integer. To this end, we construct a "ladder operator", which lowers the quantum number l by 1; for half-integral l-values, it would then take us out of the region $l \geq 0$. We introduce the definition

$$\mathbf{a}^{(l)} = i\hat{\mathbf{x}} \times \mathbf{L} - \hbar\hat{\mathbf{x}} = \begin{cases} \hat{x}_y L_z - \hat{x}_z L_y \\ \hat{x}_z L_x - \hat{x}_x L_z \\ \hat{x}_x L_y - \hat{x}_y L_x \end{cases} - \hbar\hat{\mathbf{x}} \tag{834}$$

where $\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|$ is the radial unit vector. It turns out to be useful to introduce the decomposition

$$a_\pm^{(l)} = a_x^{(l)} \pm i a_y^{(l)} = \mp\hat{x}_z L_\pm \pm \hat{x}_\pm(L_z \mp \hbar), \tag{835}$$

$$a_z^{(l)} = \hat{x}_- L_+ + \hat{x}_z(L_z - \hbar l) - \hat{\mathbf{x}}\cdot\mathbf{L} = \hat{x}_- L_+ + \hat{x}_z(L_z - \hbar l), \tag{836}$$

where we have used $\hat{\mathbf{x}}\cdot\mathbf{L} = 0$, a property valid specifically for orbital angular momentum, and where we have defined $\hat{x}_\pm = \hat{x}_x \pm i\hat{x}_y$. The commutation relations read

$$[a_+^{(l)}, a_-^{(l)}] = 2\hbar\hat{\mathbf{x}}^2 L_z = 2\hbar L_z, \tag{837}$$

$$[L_+, a_-^{(l)}] = 2\hbar a_z^{(l)}, \tag{838}$$

$$[L_z, a_-^{(l)}] = -\hbar a_-^{(l)}. \tag{839}$$

This then implies

$$a_+^{(l)}|l,l\rangle = 0 \tag{840}$$

$$\text{and } a_z^{(l)}|l,l\rangle = 0. \tag{841}$$

Together with the commutator (837), this yields

$$a_+^{(l)} a_-^{(l)}|l,l\rangle = 2\hbar^2 l\mathbf{x}^2|l,l\rangle. \tag{842}$$

Multiplication of (842) by $\langle l,l|$ thus yields $a_-^{(l)}|l,l\rangle \neq 0$ for all $l \neq 0$. For the state $|0,0\rangle$, both (836) and (842) imply

$$a_-^{(0)}|0,0\rangle = (\hat{x}_z L_- - \hat{x}_-(L_z + 0))|0,0\rangle = 0.$$

We now determine the eigenvalues of the state $a_-^{(l)}|l,l\rangle$: Using (838) and (841), one finds

$$L_+ a_-^{(l)}|l,l\rangle = a_-^{(l)} L_+|l,l\rangle + 2\hbar a_z^{(l)}|l,l\rangle = 0 \tag{843}$$

and, from (839),

$$L_z a_-^{(l)}|l,l\rangle = \hbar(l-1)a_-^{(l)}|l,l\rangle. \tag{844}$$

With $\mathbf{L}^2 = L_-L_+ + \hbar L_z + L_z^2$, we obtain from (844) and (843)

$$\mathbf{L}^2 a_-^{(l)}|l,l\rangle = \hbar^2((l-1)+(l-1)^2)a_-^{(l)}|l,l\rangle = \hbar^2 l(l-1)a_-^{(l)}|l,l\rangle. \tag{845}$$

In summary, (844) and (845) imply

$$a_-^{(l)}|l,l\rangle \propto |l-1,l-1\rangle. \tag{846}$$

If half-integral l were to occur, then starting from $|l,l\rangle$ with $a_-^{(l)}|l,l\rangle \propto |l-1,l-1\rangle, \ldots a_-^{(l-1)}a_-^{(l)}|l,l\rangle \propto |l-2,l-2\rangle$, and so on, one would eventually encounter negative half-integral l. Together with ($l = 0,1,2,3,\ldots$ or $l = \frac{1}{2},\frac{3}{2},\frac{5}{2},\ldots$), this implies that the *orbital angular momentum eigenvalues* l are given by the nonnegative integers 0, 1, 2, ...[3]

[3]Further literature concerning this can be found in C.C. Noack: Phys. Bl. **41**, 283 (1985)

Appendix C

Flux Quantization in Superconductors

A number of metals and oxidic semiconductors have been observed to exhibit superconducting properties below a critical temperature T_c, which is characteristic of each particular substance. The electrons form Cooper pairs. Lets consider a type-I superconductor in the form of a hollow cylinder situated within an external magnetic field that is parallel to the cylinder's axis. Experimentally, the Meissner effect has been observed, whereby the magnetic field is expelled from the superconductor and thus vanishes within it, except for a thin boundary layer. The doubly charged Cooper pairs thus move in a field-free region, and therefore the wave function can be used to describe them. If the wave function of the Cooper pairs in the absence of a field is given by $\psi_0(x)$, then in the presence of a field it becomes:

$$\psi_B(\vec{x}) = \exp\left\{\frac{i2e}{\hbar c}\int_{\vec{x}_0}^{\vec{x}} \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s})\right\}\psi_0(\vec{x}) \tag{847}$$

The vector potential in (847) has the property that within the superconductor curl $\mathbf{A} = 0$ (i.e., for any curve within the superconductor which can be shrunk to a point, $\oint \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s}) = 0$), whereas $\Phi_B = \int \mathrm{d}\vec{a}\cdot \operatorname{curl}\mathbf{A} = \oint \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s})$ gives the magnetic flux through the hollow cylinder (i.e., for curves encircling the cavity, $\oint \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s}) = \Phi_B$). A closed path about the cylinder starting at the point x_0 (Figure 3) gives
The requirement that the wave function $\psi_B(\vec{x})$ be single valued implies the quantization of the enclosed flux:

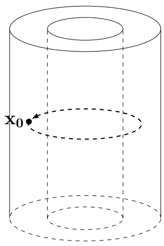

Figure 3: Flux quantization

$$\psi_B(\vec{x}_0) = \psi_0(\vec{x}_0) = \exp\left\{\frac{i2e}{\hbar c}\oint \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s})\right\}\psi_0(\vec{x}_0)$$

$$\Phi_B = \Phi_0 n \quad , \quad n = 0, \pm1, \dots,$$
$$\Phi_0 = \frac{\hbar c\pi}{e_0} = 2.07\times10^{-7}\,\mathrm{G\ cm}^2 \quad \text{(the flux quantum).}$$

This quantization has also been observed experimentally[4]. The occurrence of twice the electronic charge in the quantization represents an important test of the existence of Cooper pairs, which are the basis of BCS (Bardeen–Cooper–Schrieffer) theory.

Free Electrons in a Magnetic Field

We now investigate free electrons in a magnetic field oriented in the x_3-direction. The vector potential ($\mathbf{A} = -\frac{1}{2}[\mathbf{x}\times\mathbf{B}]$) has only components perpendicular to $\mathbf{B}$, so that the p_3-contribution to the kinetic energy is the same as that of free particles, and the Hamiltonian is given by

$$H = H_\perp + \frac{p_3^2}{2m}. \tag{848}$$

Expressed in terms of the components of the kinetic momentum ($m\dot{\mathbf{x}} = \mathbf{p} - \frac{e}{c}\mathbf{A}$), the transverse part of the Hamiltonian takes the form

$$H_\perp = \frac{m}{2}(\dot{x}_1^2 + \dot{x}_2^2). \tag{849}$$

The second term in (Equation 848) is diagonalized by $\exp\{ip_3x_3/\hbar\}$, corresponding to free motion in the x_3-direction, which can be separated off, since p_3 commutes with the $\dot{x}_i$. We now turn to the transverse part, which contains the magnetic effects. For electrons, $e = -e_0$, and the commutation relations

$$[mx_1, mx_2] = i\hbar\frac{eB}{c}, \quad [x_1, x_1] = [\dot{x}_1, \dot{x}_2] = 0 \tag{850}$$

[4]R. Doll, M. Näbauer: Phys. Rev. Lett. **7**, 51 (1961); B.S. Deaver, Jr., W.M. Fairbank: Phys. Rev. Lett. **7**, 43 (1961).

suggest the introduction of

$$\pi_i = \frac{m\dot{x}_i}{\sqrt{e_0 B/c}}. \tag{851}$$

Now, these operators satisfy the commutation relations

$$[\pi_2, \pi_1] = i\hbar, \quad [\pi_1, \pi_1] = [\pi_2, \pi_2] = 0, \tag{852}$$

and, in analogy to position and momentum, they represent canonical variables with the Hamiltonian

$$H_\perp = \frac{1}{2}\frac{e_0 B}{cm}(\pi_1^2 + \pi_2^2). \tag{853}$$

According to the theory of the harmonic oscillator using

$$a = \frac{\pi_2 + i\pi_1}{\sqrt{2\hbar}}, \tag{854}$$

this can be brought into the standard form

$$H_\perp = \hbar\omega_c\left(a^\dagger a + \frac{1}{2}\right), \tag{855}$$

where

$$\omega_c = \frac{e_0 B}{mc} \tag{856}$$

is the cyclotron frequency. Consequently, the energy eigenvalues of (849) are

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right), \tag{857}$$

with $n = 0, 1, \ldots$. We have thus found the energy levels for free electrons in a homogeneous magnetic field – also known as *Landau levels*. These play an important role in solid state physics. The problem is not yet completely solved, since for example we have not yet determined the degeneracy and the wave function of our particles. Formally it is clear that, beginning with the four canonical operators x_1, x_2, p_1, p_2, we need two more operators, in addition to π_1, π_2 introduced above, for a complete characterization. In the Heisenberg representation these are given by

$$X = x - \frac{1}{\omega_c}\tau\dot{x},$$

where

$$\tau = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

In classical mechanics, X is the center of the circular orbits $(x - X)^2 = \dot{x}^2/\omega_c^2 = \text{const}$. In quantum mechanics, X_1 and X_2 are canonical variables and cannot simultaneously be specified with arbitrary accuracy. X is also referred to as the "guiding center."

Path Integrals – Elementary Properties and Simple Solutions

The following derivation of the path integral is presented as an alternative to the one discussed in the lecture.

The operator formalism of quantum mechanics and quantum statistics may not always lead to the most transparent understanding of quantum phenomena. There exists another, equivalent formalism in which operators are avoided by the use of infinite products of integrals, called *path integrals*. In contrast to the Schrödinger equation, which is a differential equation determining the properties of a state at a time from their knowledge at an infinitesimally earlier time, path integrals yield the quantum-mechanical amplitudes in a global approach involving the properties of a system at *all times*.

Path Integral Representation of Time Evolution Amplitudes

The path integral approach to quantum mechanics was developed by Feynman in 1942. In its original form, it applies to a point particle moving in a Cartesian coordinate system and yields the transition amplitudes of the time evolution operator between the localized states of the particle

$$(x_b t_b | x_a t_a) = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle, \quad t_b > t_a. \tag{858}$$

For simplicity, we shall at first assume the space to be one-dimensional. The extension to D Cartesian dimensions will be given later. The introduction of curvilinear coordinates will require a little more work. A further generalization to spaces with nontrivial geometry, in which curvature and torsion are present, will extend beyond the scope of the course's objective.

Sliced Time Evolution Amplitude

We shall be interested mainly in the causal or retarded time evolution amplitudes. These contain all relevant quantum-mechanical information and possess, in addition, pleasant analytic properties in the complex energy plane. This is why we shall always assume, from now on, the causal sequence of time arguments $t_b > t_a$. Feynman realized that due to the fundamental composition law of the time evolution operator, the amplitude (858) could be sliced into a large number, say $N+1$, of time evolution operators, each acting across an infinitesimal time slice of thickness $\varepsilon = t_n - t_{n-1} = (t_b - t_a)/(N+1) > 0$:

$$(x_b t_b | x_a t_a) = \langle x_b | \hat{U}(t_b, t_N) \hat{U}(t_N, t_{N-1}) \cdots \hat{U}(t_2, t_1) \hat{U}(t_1, t_a) | x_a \rangle. \tag{859}$$

When inserting a complete set of states between each pair of $\hat{U}$'s,

$$\int_{-\infty}^{\infty} \mathrm{d}x_n |x_n\rangle\langle x_n| = 1, \quad n = 1, 2, \ldots, N, \tag{860}$$

the amplitude becomes a product of N-integrals

$$(x_b t_b | x_a t_a) = \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \mathrm{d}x_n \right] \prod_{n=1}^{N+1} (x_n t_n | x_{n-1} t_{n-1}), \tag{861}$$

where we have set $x_b \equiv x_{N+1}, x_a \equiv x_0, t_b \equiv t_{N+1}, t_a \equiv t_0$. The symbol $\prod[\cdots]$ denotes the product of the quantities within the brackets. The integrand is the product of the amplitudes for the infinitesimal time intervals

$$\langle x_n t_n | x_{n-1} t_{n-1} \rangle = \langle x_n | e^{-i\varepsilon \hat{H}(t_n)/\hbar} | x_{n-1} \rangle, \tag{862}$$

with the Hamiltonian operator

$$\hat{H}(t) \equiv H(\hat{p}, \hat{x}, t). \tag{863}$$

The further development becomes simplest under the assumption that the Hamiltonian has the standard form, being the sum of a kinetic and a potential energy:

$$H(p, x, t) = T(p, t) + V(x, t). \tag{864}$$

For a sufficiently small slice thickness, the time evolution operator

$$e^{-i\varepsilon \hat{H}/\hbar} = e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar} \tag{865}$$

is factorizable as a consequence of the *Baker-Campbell-Hausdorff formula* (allready proved in Baker-Campbell-Hausdorff Formula and Magnus Expansion)

$$e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar} = e^{-i\varepsilon\hat{V}/\hbar} e^{-i\varepsilon\hat{T}/\hbar} e^{-i\varepsilon^2 \hat{X}/\hbar^2}, \tag{866}$$

where the operator $\hat{X}$ has the expansion

$$\hat{X} \equiv \frac{i}{2}[\hat{V}, \hat{T}] - \frac{\varepsilon}{\hbar}\left(\frac{1}{6}[\hat{V}, [\hat{V}, \hat{T}]] - \frac{1}{3}[[\hat{V}, \hat{T}], \hat{T}]\right) + \mathcal{O}(\varepsilon^2). \tag{867}$$

The omitted terms of order $\varepsilon^4, \varepsilon^5, \ldots$ contain higher commutators of $\hat{V}$ and $\hat{T}$. If we neglect, for the moment, the $\hat{X}$-term which is suppressed by a factor ε^2, we calculate for the local matrix elements of $e^{-i\varepsilon\hat{H}/\hbar}$ the following simple expression:

$$\langle x_n | e^{-i\varepsilon H(\hat{p}, \hat{x}, t_n)/\hbar} | x_{n-1} \rangle \approx \int_{-\infty}^{\infty} \mathrm{d}x \langle x_n | e^{-i\varepsilon V(\hat{x}, t_n)/\hbar} | x \rangle \langle x | e^{-i\varepsilon T(\hat{p}, t_n)/\hbar} | x_{n-1} \rangle. \tag{868}$$

Evaluating the local matrix elements,

$$\langle x_n|e^{-i\varepsilon V(\hat{x},t_n)/\hbar}|x\rangle = \delta(x_n - x)e^{-i\varepsilon V(x_n,t_n)/\hbar}, \tag{869}$$

this becomes

$$\langle x_n|e^{-i\varepsilon H(\hat{p},\hat{x},t_n)/\hbar}|x_{n-1}\rangle \approx \int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar} \exp\{ip_n(x_n - x_{n-1})/\hbar - i\varepsilon[T(p_n,t_n) + V(x_n,t_n)]/\hbar\}. \tag{870}$$

Inserting this back into (861), we obtain *Feynman's path integral formula*, consisting of the multiple integral

$$(x_b t_b|x_a t_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{\mathrm{d}p_n}{2\pi\hbar}\right]\exp\left(\frac{i}{\hbar}\mathcal{A}^N\right), \tag{871}$$

where $\mathcal{A}^N$ is the sum

$$\mathcal{A}^N = \sum_{n=1}^{N+1}\left[p_n(x_n - x_{n-1}) - \varepsilon H(p_n, x_n, t_n)\right]. \tag{872}$$

$$\tag{873}$$

Zero-Hamiltonian Path Integral

Note that the path integral (871) with zero Hamiltonian produces the Hilbert space structure of the theory via a chain of scalar products:

$$(x_b t_b|x_a t_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{\mathrm{d}p_n}{2\pi\hbar}\right]e^{i\sum_{n=1}^{N+1}p_n(x_n - x_{n-1})/\hbar}, \tag{874}$$

which is equal to

$$(x_b t_b|x_a t_a) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right]\prod_{n=1}^{N+1}\langle x_n|x_{n-1}\rangle = \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right]\prod_{n=1}^{N+1}\delta(x_n - x_{n-1}) = \delta(x_b - x_a). \tag{875}$$

Whose continuum limit is

$$(x_b t_b|x_a t_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\int \mathrm{d}t p(t)\dot{x}(t)/\hbar} = \langle x_b|x_a\rangle = \delta(x_b - x_a). \tag{876}$$

In the operator expression (859), the right-hand side follows from the fact that for zero Hamiltonian the time evolution operators $\hat{U}(t_n, t_{n-1})$ are all equal to unity.
At this point we make the important observation that a momentum variable p_n *inside* the product of momentum integrations in the expression (874) can be generated by a derivative $\hat{p}_n \equiv -i\hbar\partial_{x_n}$ *outside* of it. Later we shall go to the continuum limit of time slicing in which the slice thickness ε goes to zero. In this limit, the discrete variables x_n and p_n become functions $x(t)$ and $p(t)$ of the continuous time t, and the momenta p_n become differential operators $p(t) = -i\hbar\partial_{x(t)}$, satisfying the commutation relations with $x(t)$:

$$[\hat{p}(t), x(t)] = -i\hbar. \tag{877}$$

These are the canonical *equal-time* commutation relations of Heisenberg.
This observation forms the basis for deriving, from the path integral (871), the Schrödinger equation for the time evolution amplitude.

Schrödinger Equation for Time Evolution Amplitude

Let us split from the product of integrals in (871) the final time slice as a factor, so that we obtain the recursion relation

$$(x_b t_b|x_a t_a) \approx \int_{-\infty}^{\infty} \mathrm{d}x_N (x_b t_b|x_N t_N)(x_N t_N|x_a t_a), \tag{878}$$

where

$$(x_b t_b|x_N t_N) \approx \int_{-\infty}^{\infty}\frac{\mathrm{d}p_b}{2\pi\hbar} e^{(i/\hbar)[p_b(x_b - x_N) - \varepsilon H(p_b, x_b, t_b)]}. \tag{879}$$

The momentum p_b *inside* the integral can be generated by a differential operator $\hat{p}_b \equiv -i\hbar\partial_{x_b}$ *outside* of it. The same is true for any function of p_b, so that the Hamiltonian can be moved before the momentum integral yielding

$$(x_b t_b|x_N t_N) \approx e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b)/\hbar}\int_{-\infty}^{\infty}\frac{\mathrm{d}p_b}{2\pi\hbar} e^{ip_b(x_b - x_N)/\hbar} = e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b)/\hbar}\delta(x_b - x_N). \tag{880}$$

Inserting this back into (878) we obtain

$$(x_b t_b | x_a t_a) \approx e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b)/\hbar}(x_b t_b - \varepsilon | x_a t_a), \tag{881}$$

or

$$\frac{1}{\varepsilon}\left[(x_b t_b + \varepsilon | x_a t_a) - (x_b t_b | x_a t_a)\right] \approx \frac{1}{\varepsilon}\left[e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b+\varepsilon)/\hbar} - 1\right](x_b t_b | x_a t_a). \tag{882}$$

In the limit $\varepsilon \to 0$, this goes over into the differential equation for the time evolution amplitude

$$i\hbar \frac{\partial}{\partial t_b}(x_b t_b | x_a t_a) = H(-i\hbar\partial_{x_b}, x_b, t_b)(x_b t_b | x_a t_a), \tag{883}$$

which is precisely the Schrödinger equation of operator quantum mechanics.

Convergence of the Time-Sliced Evolution Amplitude

Some remarks are necessary concerning the convergence of the time-sliced expression (871) to the quantum-mechanical amplitude in the continuum limit, where the thickness of the time slices $\varepsilon = (t_b - t_a)/(N+1) \to 0$ goes to zero and the number N of slices tends to ∞. This convergence can be proved for the standard kinetic energy $T = p^2/2M$ only if the potential $V(x,t)$ is sufficiently *smooth*. For timeindependent potentials this is a consequence of the *Trotter product formula* which reads

$$e^{-i(t_t - t_n)\hat{H}/\hbar} = \lim_{N\to\infty}\left(e^{-i\varepsilon\hat{V}/\hbar}e^{-i\varepsilon\hat{T}/\hbar}\right)^{N+1} \tag{884}$$

If T and V are c-numbers, this is trivially true. If they are operators, we use Eq. (2.9) to rewrite the left-hand side of (884) as

$$e^{i(t_b - t_a)\hat{H}/\hbar} \equiv \left(e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar}\right)^{N+1} \equiv \left(e^{-i\varepsilon\hat{V}/\hbar}e^{-i\varepsilon\hat{T}/\hbar}e^{-i\varepsilon^2\hat{X}/\hbar^2}\right)^{N+1}$$

The Trotter formula implies that the commutator term $\hat{X}$ proportional to ε^2 does not contribute in the limit $N \to \infty$. The mathematical conditions ensuring this require functional analysis too technical to be presented here. For us it is sufficient to know that the Trotter formula holds for operators which are bounded from below and that for most physically interesting potentials, it cannot be used to derive Feynman's time-sliced path integral representation (871), even in systems where the formula is known to be valid. In particular, the short-time amplitude may be different from (870). Take, for example, an attractive Coulomb potential $V(x) \propto -1/|x|$ for which the Trotter formula has been proved to be valid. Feynman's time-sliced formula, however, diverges even for two time slices. Similar problems will be found for other physically relevant potentials such as $V(x) \propto l(l+D-2)\hbar^2/|x|^2$ (centrifugal barrier) and $V(\theta) \propto m^2\hbar^2/\sin^2\theta$ (angular barrier near the poles of a sphere). In all these cases, the commutators in the expansion (867) of $\hat{X}$ become more and more singular. In fact, as we shall see, the expansion does not even converge, even for an infinitesimally small ε. All atomic systems contain such potentials and the Feynman formula (871) cannot be used to calculate an approximation for the transition amplitude. A new path integral formula has to be found. Fortunately, it is possible to eventually reduce the more general formula via some transformations back to a Feynman type formula with a bounded potential in an auxiliary space. After this it serves as an independent starting point for all further quantum-mechanical calculations.

In the sequel, the symbol $\approx$ in all time-sliced formulas such as (871) will imply that an equality emerges in the *continum limit* $N \to \infty, \varepsilon \to 0$ unless the potential has singularities of the above type. In the action, the continuum limit is without subtleties. The sum $\mathcal{A}^N$ in (872) tends towards the integral

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b} \mathrm{d}t[p(t)\dot{x}(t) - H(p(t), x(t), t)] \tag{885}$$

under quite general circumstances. This expression is recognized as the classical canonical action for the path $x(t), p(t)$ in phase space. Since the position variables x_{N+1} and x_0 are fixed at their initial and final values x_b and x_a, the paths satisfy the boundary condition $x(t_b) = x_b, x(t_a) = x_a$.

In the same limit, the product of infinitely many integrals in (871) will be called a path integral. The limiting measure of integration is written as

$$\lim_{N\to\infty}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}\mathrm{d}x_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{\mathrm{d}p_n}{2\pi\hbar}\right] \equiv \int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}'x\int\frac{\mathcal{D}p}{2\pi\hbar}. \tag{886}$$

By definition, there is always one more p_n-integral than x_n-integrals in this product. While x_0 and x_{N+1} are held fixed and the x_n-integrals are done for $n = 1, \ldots, N$, each pair (x_n, x_{n-1}) is accompanied by one

p_n-integral for $n = 1, \ldots, N+1$. The situation is recorded by the prime on the functional integral $\mathcal{D}'x$. With this definition, the amplitude can be written in the short form

$$(x_b t_b \mid x_a t_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\mathcal{A}[p,x]/\hbar} \tag{887}$$

The path integral has a simple intuitive interpretation: Integrating over all paths corresponds to summing over all histories along which a physical system can possibly evolve. The exponential $e^{i\mathcal{A}[p,x]/\hbar}$ is the quantum analog of the Boltzmann factor $e^{-E/k_B T}$ in statistical mechanics. Instead of an exponential probability, a pure phase factor is assigned to each possible history: The total amplitude for going from x_a, t_a to x_b, t_b is obtained by adding up the phase factors for all these histories,

$$(x_b t_b \mid x_a t_a) = \sum_{\substack{\text{all histories} \\ (x_a,t_a)\rightsquigarrow(x_b,t_b)}} e^{i\mathcal{A}[p,x]/\hbar} \tag{888}$$

where the sum comprises all paths in phase space with fixed endpoints x_b, x_a in x-space.

Time Evolution Amplitude in Momentum Space

The above observed asymmetry in the functional integrals over x and p is a consequence of keeping the endpoints fixed in position space. There exists the possibility of proceeding in a conjugate way keeping the initial and final *momenta* p_b and p_a fixed. The associated time evolution amplitude can be derived by going through the same steps as before but working in the momentum space representation of the Hilbert space, starting from the matrix elements of the time evolution operator

$$(p_b t_b \mid p_a t_a) \equiv \langle p_b | \hat{U}(t_b, t_a) | p_a \rangle \tag{889}$$

The time slicing proceeds as in (859)-(861), with all x's replaced by p's, except in the completeness relation (860) which we shall take as

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} |p\rangle\langle p| = 1 \tag{890}$$

corresponding to the choice of the normalization of states

$$\langle p_b \mid p_a \rangle = 2\pi\hbar\delta(p_b - p_a) \tag{891}$$

In the resulting product of integrals, the integration measure has an opposite asymmetry: there is now one more x_n-integral than p_n-integrals. The sliced path integral reads

$$(p_b t_b \mid p_a t_a) \approx \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar}\right] \prod_{n=0}^{N} \left[\int_{-\infty}^{\infty} dx_n\right] \tag{892}$$

$$\times \exp\left\{\frac{i}{\hbar} \sum_{n=0}^{N} \left[-x_n(p_{n+1} - p_n) - \varepsilon H(p_n, x_n, t_n)\right]\right\} \tag{893}$$

The relation between this and the x-space amplitude (871) is simple: By taking in (871) the first and last integrals over p_1 and p_{N+1} out of the product, renaming them as p_a and p_b, and rearranging the sum $\sum_{n=1}^{N+1} p_n(x_n - x_{n-1})$ as follows

$$\sum_{n=1}^{N+1} p_n(x_n - x_{n-1}) = p_{N+1}(x_{N+1} - x_N) + p_N(x_N - x_{N-1}) + \ldots + p_2(x_2 - x_1) + p_1(x_1 - x_0) \tag{894}$$

$$= p_{N+1}x_{N+1} - p_1 x_0 - (p_{N+1} - p_N)x_N - (p_N - p_{N-1})x_{N-1} - \ldots - (p_2 - p_1)x_1 \tag{895}$$

$$= p_{N+1}x_{N+1} - p_1 x_0 - \sum_{n=1}^{N} (p_{n+1} - p_n)x_n \tag{896}$$

the remaining product of integrals looks as in Eq. (893), except that the lowest index n is one unit larger than in the sum in Eq. (893). In the limit $N \to \infty$ this does not matter, and we obtain the Fourier transform

$$(x_b t_b \mid x_a t_a) = \int \frac{\mathrm{d}p_b}{2\pi\hbar} e^{ip_b x_b/\hbar} \int \frac{\mathrm{d}p_a}{2\pi\hbar} e^{-ip_a x_a/\hbar} (p_b t_b \mid p_a t_a). \tag{897}$$

The inverse relation is

$$(p_b t_b \mid p_a t_a) = \int \mathrm{d}x_b e^{-ip_b x_b/\hbar} \int \mathrm{d}x_a e^{ip_a x_a/\hbar} (x_b t_b \mid x_a t_a). \tag{898}$$

In the continuum limit, the amplitude (893) can be written as a path integral

$$\left(p_b t_b \mid p_a t_a\right)=\int_{p(t_a)=p_a}^{p(t_b)=p_b} \frac{\mathcal{D}' p}{2 \pi \hbar} \int \mathcal{D} x e^{i \bar{\mathcal{A}}[p, x] / \hbar} \tag{899}$$

where

$$\bar{\mathcal{A}}[p, x]=\int_{t_a}^{t_b} d t[-\dot{p}(t) x(t)-H(p(t), x(t), t)]=\mathcal{A}[p, x]-p_b x_b+p_a x_a . \tag{900}$$

If the Hamiltonian is independent of x and t, the sliced path integral (893) becomes trivial. Then the $N+1$ integrals over $x_n(n=0, \ldots, N)$ can be done yielding a product of δ-functions $\delta\left(p_b-p_N\right) \cdots \delta\left(p_1-p_0\right)$. As a conseqence, the integrals over the N momenta $p_n(n=1, \ldots, N)$ are all squeezed to the initial momentum $p_N=p_{N-1}=\cdots=p_1=p_a$. A single final δ-function $2 \pi \hbar \delta\left(p_b-p_a\right)$ remains, accompanied by the product of $N+1$ factors $\prod_{n=0}^N e^{-i \varepsilon H\left(p_a\right) / \hbar}$, which is equal to $e^{-i\left(t_b-t_a\right) H(p) / \hbar}$. Hence we obtain:

$$\left(p_b t_b \mid p_a t_a\right)=2 \pi \hbar \delta\left(p_b-p_a\right) e^{-i\left(t_b-t_a\right) H(p) / \hbar} \tag{901}$$

Inserting this into Eq. (897), we find a simple Fourier integral for the time evolution amlitude in x-space:

$$\left(x_b t_b \mid x_a t_a\right)=\int \frac{\mathrm{d} p}{2 \pi \hbar} e^{i p\left(x_b-x_a\right) / \hbar-i\left(t_b-t_a\right) H(p) / \hbar} \tag{902}$$

Note that in (901) contains an equal sign rather than the ≈-sign since the right-hand sign is the same for any number of time slices.

Quantum-Mechanical Partition Function

A path integral symmetric in p and x arises when considering the quantummechanical partition function defined by the trace

$$Z_{\mathrm{QM}}\left(t_b, t_a\right)=\operatorname{Tr}\left(e^{-i\left(t_b-t_a\right) \hat{H} / \hbar}\right) . \tag{903}$$

In the local basis, the trace becomes an integral over the amplitude $\left(x_b t_b \mid x_a t_a\right)$ with $x_b=x_a$:

$$Z_{\mathrm{QM}}\left(t_b, t_a\right)=\int_{-\infty}^{\infty} \mathrm{d} x_a\left(x_a t_b \mid x_a t_a\right) . \tag{904}$$

The additional trace integral over $x_{N+1} \equiv x_0$ makes the path integral for Z_{QM} symmetric in p_n and x_n :

$$\int_{-\infty}^{\infty} \mathrm{d} x_{N+1} \prod_{n=1}^N\left[\int_{-\infty}^{\infty} \mathrm{d} x_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{\mathrm{d} p_n}{2 \pi \hbar}\right]=\prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty} \frac{\mathrm{d} x_n \mathrm{d} p_n}{2 \pi \hbar}\right] \tag{905}$$

In the continuum limit, the right-hand side is written as

$$\lim _{N \rightarrow \infty} \prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty} \frac{\mathrm{d} x_n \mathrm{d} p_n}{2 \pi \hbar}\right] \equiv \oint \mathcal{D} x \int \frac{\mathcal{D} p}{2 \pi \hbar}, \tag{906}$$

and the measures are related by

$$\int_{-\infty}^{\infty} \mathrm{d} x_a \int_{x(t_a)=x_a}^{x(t_b)=x_a} \mathcal{D}' x \int \frac{\mathcal{D} p}{2 \pi \hbar} \equiv \oint \mathcal{D} x \int \frac{\mathcal{D} p}{2 \pi \hbar} . \tag{907}$$

The symbol $\oint$ indicates the periodic boundary condition $x\left(t_a\right)=x\left(t_b\right)$. In the momentum representation we would have similarly

$$\int_{-\infty}^{\infty} \frac{\mathrm{d} p_a}{2 \pi \hbar} \int_{p(t_a)=p_a}^{p(t_b)=p_a} \frac{\mathcal{D}' p}{2 \pi \hbar} \int \mathcal{D} x \equiv \oint \frac{\mathcal{D} p}{2 \pi \hbar} \int \mathcal{D} x, \tag{908}$$

with the periodic boundary condition $p\left(t_a\right)=p\left(t_b\right)$, and the same right-hand side. Hence, the quantum-mechanical partition function is given by the path integral

$$Z_{\mathrm{QM}}\left(t_b, t_a\right)=\oint \mathcal{D} x \int \frac{\mathcal{D} p}{2 \pi \hbar} e^{i A[p, x] / \hbar}=\oint \frac{\mathcal{D} p}{2 \pi \hbar} \int \mathcal{D} x e^{i \overline{\mathcal{A}}[p, x] / \hbar} \tag{909}$$

In the right-hand exponential, the action $\bar{\mathcal{A}}[p,x]$ can be replaced by $\mathcal{A}[p,x]$, since the extra terms in (900) are removed by the periodic boundary conditions. In the time-sliced expression, the equality is easily derived from the rearrangement of the sum (896), which shows that

$$\sum_{n=1}^{N+1} p_n \left(x_n - x_{n-1}\right)\Big|_{x_{N+1}=x_0} = -\sum_{n=0}^{N} \left(p_{n+1} - p_n\right) x_n\Big|_{p_{N+1}=p_0} . \tag{910}$$

In the path integral expression (909) for the partition function, the rules of quantum mechanics appear as a natural generalization of the rules of classical statistical mechanics, as formulated by Planck. According to these rules, each volume element in phase space $\mathrm{d}x\mathrm{d}p/h$ is occupied with the exponential probability $e^{-E/k_B T}$. In the path integral formulation of quantum mechanics, each volume element in the *path phase space* $\Pi_n \mathrm{d}x\left(t_n\right)\mathrm{d}p\left(t_n\right)/h$ is associated with a pure phase factor $e^{i\mathcal{A}[p,x]/h}$. We see here a manifestation of the correspondence principle which specifies the transition from classical to quantum mechanics. In path integrals, it looks somewhat more natural than in the historic formulation, where it requires the replacement of all classical phase space variables p, x by operators, a rule which was initially hard to comprehend.

Appendix D

Numerical Techniques

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Common Software Tools

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Appendix E

Density Matrix Formalism

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Entanglement and Quantum Information

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Adiabatic Theorem and Berry Phase

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Additional Refernce Material

Physical Constants and Conversion Factors

A table of constants such as $\hbar, c$, and particle masses.
Here is a table of common constants: TBA

Constant	**Symbol**	**Value**
Reduced Planck constant	$\hbar$	1.054×10^{-34} J·s
Speed of light	c	3.00×10^{8} m/s
Electron mass	m_e	9.11×10^{-31} kg

Table 1: Common Physical Constants

Historical Notes

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Worked Examples

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Common Mistakes

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Further Reading

Recommended textbooks, articles, and lecture series for deeper exploration. Recommended books:

- *Principles of Quantum Mechanics* by R. Shankar.
- *Quantum Mechanics and Path Integrals* by Feynman and Hibbs.