Summary of the course

Advanced Quantum Theory | $\mathcal{AQT}$

Lecture notes by Noa Goedee

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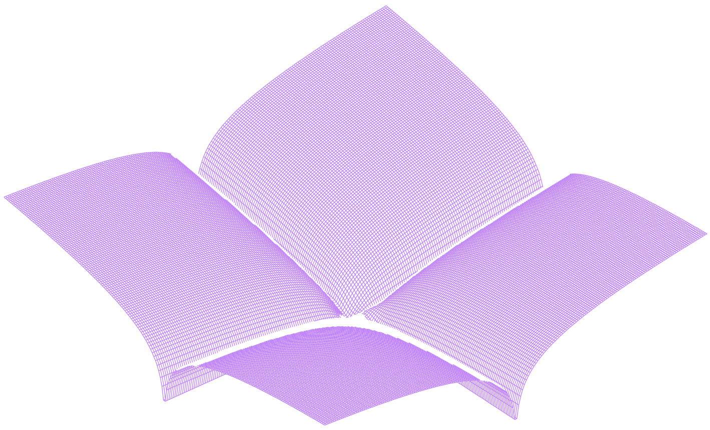


These notes are based on the lecture held by Prof. Manuel Drees and further sources which are not always mentioned specifically.

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 $\psi(\vec{x}_i, t)(i = 1, \ldots, N = \text{number of particles})$. ψ contains all 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 not be predicted with certainty. Just after 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
$$\Rightarrow \qquad u_n(t) = \int \mathrm{d}^3x_1 \ldots \mathrm{d}^3x_N \psi_n^\star(\vec{x}_i, t) \tag{4}$$

- Given a wavefunction $\psi(\vec{x}_i, t)$, the expectation value (in statistical sense) of observable Q is
$$\langle Q \rangle = \int \mathrm{d}^3x_1 \ldots \mathrm{d}^3x_N \psi_n^\star(\vec{x}_i, t) \tag{5}$$
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
$$\sum_n |u_n(t)|^2 + \int \mathrm{d}q |u(q,t)|^2 = 1 \tag{6}$$
$$\Rightarrow \qquad \langle \hat{Q} \rangle = \sum_n q_n |u_n(t)|^2 + \int \mathrm{d}qq |u(q,t)|^2 \tag{7}$$

- 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 $\vec{x}_0$

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

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

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

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

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

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

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

(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^*

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

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

(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):

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

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

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

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

$$\{\bar{q}_i, \bar{q}_k\} = 0;\ \{\bar{p}_i, \bar{p}_k\} = 0 \text{ from } (43)$$
$$\{\bar{q}_i, \bar{q}_k\} = \sum_l \left(\frac{\partial \bar{q}_i}{\partial q_l}\frac{\partial \bar{p}_k}{\partial p_l} - \frac{\partial \bar{q}_i}{\partial p_l}\frac{\partial \bar{p}_k}{\partial q_l}\right) \overset{42}{=} \sum_l \frac{\partial \bar{q}_i}{\partial q_l}\frac{\partial q_l}{\partial \bar{q}_k} = \frac{\partial \bar{q}_i}{\partial \bar{q}_k} = \delta_{ik}$$

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:

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

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):

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

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

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

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

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

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 1st 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)

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

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:

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

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

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

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

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

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

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)

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

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

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

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):

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

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

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

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:

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

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

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

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

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

Check the first equation (77):

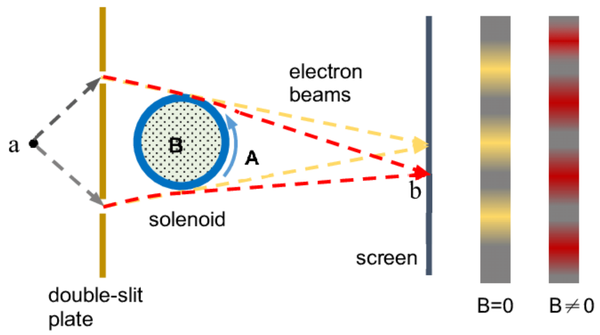
$$\left(-i\hbar\nabla - q\vec{A} - q\nabla\lambda\right)e^{i\alpha}\psi = e^{i\frac{q\lambda}{\hbar}}\left(-i\hbar\nabla - q\vec{A}\right)\psi$$

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:

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

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

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:

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

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

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:

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

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

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 $\int_{-\infty}^{\infty}\mathrm{d}x\,x^2e^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$

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

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

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:

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

$$S \to S_\lambda = S + \int_{t_s}^{t_d} \left(q\dot{\vec{x}} \cdot \nabla\lambda + q\frac{\partial\lambda}{\partial t} \right) \mathrm{d}t = S + q\int_{t_s}^{t_d} \frac{\mathrm{d}\lambda}{\mathrm{d}t}\mathrm{d}t \tag{111}$$
$$= S + \left[\lambda(\vec{x}_d, t_d) - \lambda(\vec{x}_s, t_s)\right] q \tag{112}$$

This does not change classical e.o.m., since in $\delta S, (\vec{x}_d, t_d)$ 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!

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

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

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

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

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,

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

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 <u>same</u> 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:

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

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

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

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

<u>Definition</u>: 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

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

$\forall|\psi_I(t_0)\rangle$

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

$\hat{H}_{1,I}$ 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 $\hat{H}_{1,I}$.

<u>Zeroth order:</u> 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.

<u>First order</u>: 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:

$$\hat{U}_I^{(n)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\hat{H}_{1,I}(t') + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}t' \int_{t_0}^{t'}\mathrm{d}t''\,\hat{H}_{1,I}(t')\hat{H}_{1,I}(t'') + \dots \tag{142}$$

$$+\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \dots \int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{H}_{1,I}(t_1)\hat{H}_{1,I}(t_2)\dots\hat{H}_{1,I}(t_n) \tag{143}$$

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:

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

(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:

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

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:

$$\hat{U}_S^{(0)}(t,t_0)\hat{U}_I^{(n)}(t,t_0) = \hat{U}_S^{(n)}(t,t_0)$$

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

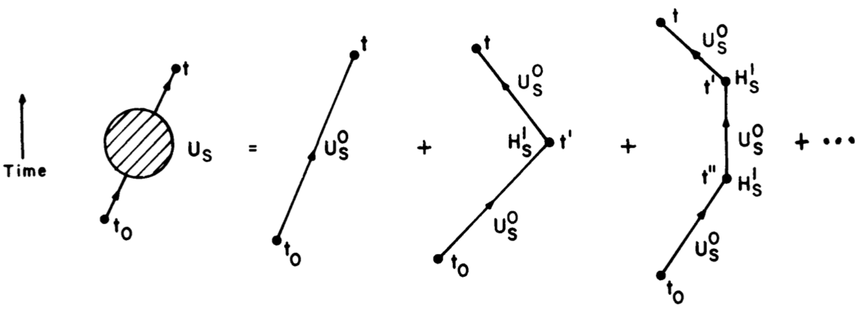
$$\hat{U} \text{ is unitary } \Rightarrow \left[\hat{U}(t,t_0)\right]^\dagger = \left[\hat{U}(t,t_0)\right]^{-1} = \hat{U}(t,t_0) \tag{151}$$

$$\text{Also: } \hat{U}(t_1,t_2)\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3) \tag{152}$$

$$\Rightarrow \hat{U}_S^{(n)}(t,t_0) = \hat{U}_S^{(0)}(t,t_0) - \frac{i}{\hbar}\int_{t_0}^{t} \hat{U}_S^{(0)}(t,t')\hat{H}_{1,S}(t')\hat{U}_S^{(0)}(t',t_0)\,\mathrm{d}t' \tag{153}$$

$$+\cdots+\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\cdots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\,\hat{U}_S^{(0)}(t,t_1)\hat{H}_{1,S}(t_1)\hat{U}_S^{(0)}(t,t_2)\cdots \tag{154}$$

$$\hat{U}_S^{(0)}(t_{n-1},t_n)\hat{H}_{1,S}(t_n)\hat{U}_S^{(0)}(t_n,t_0) \tag{155}$$



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

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

$$\Rightarrow \tilde{A}_{fi}(t) = e^{-iE_f^{(0)}(t-t_0)/\hbar}\left\{\delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\langle f^{(0)}|\hat{H}_{1,S}(t')|i^{(0)}\rangle e^{i\omega_{fi}(t'-t_0)}\right\} \tag{156}$$

$$+\left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\sum_n\langle f^{(0)}|\hat{H}_{1,S}(t')|n^{(0)}\rangle\langle n^{(0)}|\hat{H}_{1,S}(t'')|i^{(0)}\rangle \tag{157}$$

$$\cdot\exp\left\{\underbrace{\frac{i}{\hbar}\left(E_f^{(0)}-E_n^{(0)}\right)(t'-t_0)}_{i\omega_{fn}(t'-t_0)}+\underbrace{\frac{i}{\hbar}\left(E_n^{(0)}-E_i^{(0)}\right)(t''-t_0)}_{i\omega_{ni}(t''-t_0)}\right\}+\ldots \tag{158}$$

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

- 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 $t = 0$:

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

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

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

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

and $\Delta E_{\min}$ is the smallest relevant energy distance between states.
Let

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

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

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

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

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

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

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

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

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

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

$\left(\frac{\sin x}{x}\right)^2$ 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)

$$\mathcal{A}_{fi}(t) = -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \int \mathrm{d}t' e^{i(\omega_{fi}-\omega)t'}, \text{ use } t'' = t' - \frac{t}{2}$$

$$= -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle \int_{-t/2}^{t/2} \mathrm{d}t'' e^{i(\omega_{fi}-\omega)\frac{t}{2}} e^{i(\omega_{fi}-\omega)t''}$$

$$\underset{t\to\infty}{\to} -\frac{1}{\hbar}\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle e^{i(\omega_{fi}-\omega)\frac{t}{2}} \cdot 2\pi\delta(\omega_{fi}-\omega)$$

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

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 rate $\equiv$ 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:

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

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

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

Recall:

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

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

Propagating wave with velocity $c = \frac{\omega}{|\vec{k}|}$.
$\Rightarrow$ (Average) energy in electromagnetic radiation in volume V (SI units):

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

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

where N_γ is the number of photons in the volume.

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

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

where $\vec{\varepsilon}$ is the polarization vector (unit vector).
To correct for the absorption of a photon; for emission we need $N_\gamma \to N_\gamma + 1$:

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

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!
⇒ 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):

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

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)

$$\begin{aligned}[\hat{x}_e, \hat{\vec{P}}_e^2] &= [\hat{x}_e, \hat{P}_{x_e}^2 + \hat{P}_{y_e}^2 + \hat{P}_{z_e}^2] = [\hat{x}_e, \hat{P}_{x_e}^2] = \hat{x}_e\hat{P}_{x_e}\hat{P}_{x_e} - \hat{P}_{x_e}\hat{P}_{x_e}\hat{x}_e \\ &= \left(\cancel{\hat{P}_{x_e}\hat{x}_e} + \underbrace{[\hat{x}_e, \hat{P}_{x_e}]}_{i\hbar}\right)\hat{P}_{x_e} - \hat{P}_{x_e}\left(\cancel{\hat{x}_e\hat{P}_{x_e}} + \underbrace{[\hat{P}_{x_e}, \hat{x}_e]}_{-i\hbar}\right) = 2i\hbar\hat{P}_{x_e}\end{aligned}$$

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

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

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

<u>Selection rules:</u>
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 <u>different</u> 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:

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

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 <u>several</u> photons.
Numerical estimate for allowed transitions:

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

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

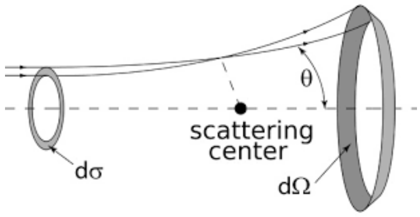
with $\hbar \approx 6.6 \times 10^{-22}\,\text{MeV s}$ and $M_e c^2 = 0.511\,\text{MeV}$.

[13.11.2024, Lecture 12]

[18.11.2024, Lecture 13]

Scattering Theory

<u>Problem</u>: 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 ≫ 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:

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

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 total 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:

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

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

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:

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

Because:

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

Green's function via Fourier transform:

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

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

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

Notes:
- $G_+(\vec{q})$ has a pole at $q^2 = k^2$, since $\nabla^2 + k^2$ has vanishing eigenvalues: not 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:

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

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:

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

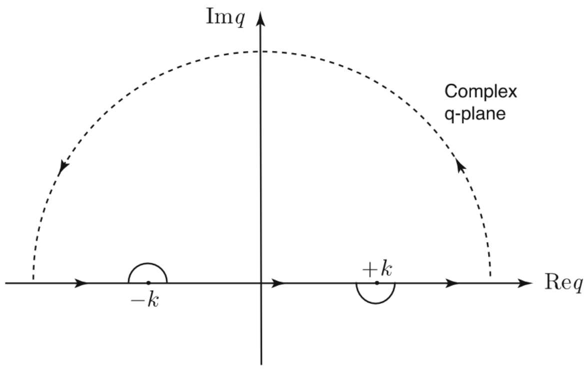
where z_e are the poles of $f(t)$. Let $f(t)$ be a complex function of $z \in \mathbb{C}$. If z_e is a pole, then:

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

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:

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

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:

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

Remarks:

* 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 no 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:

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

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

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):

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

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

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

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$^{\text{nd}}$ 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 (→ 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:

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

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:

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

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:

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

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:

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

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

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

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:

$$A_\ell j_\ell(qr_0) = B_\ell h_\ell^{(1)}(i\kappa r_0) \tag{251}$$

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:

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

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

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:

$$\cot(qr_0) \leq 0 \quad \Rightarrow \quad qr_0 \geq \frac{\pi}{2}$$

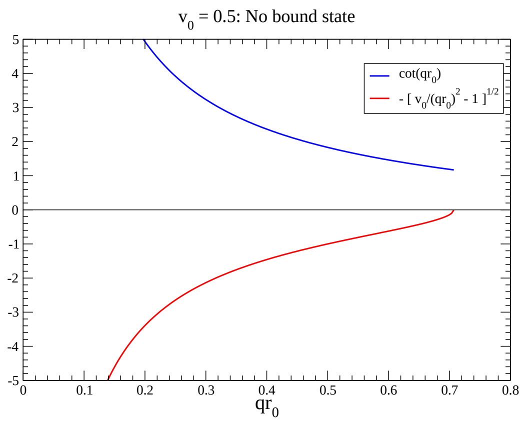
Additionally, if $q^2 < \frac{2MV_0}{\hbar^2}$, we have:

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

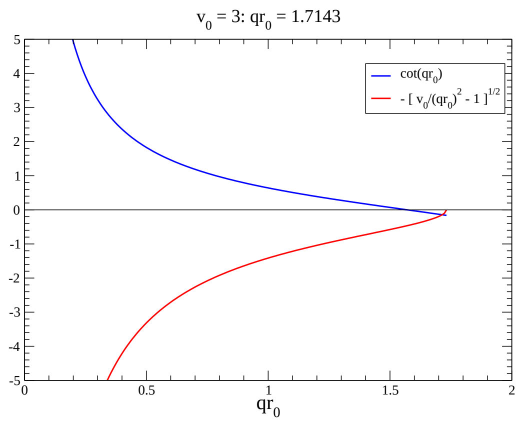
The first bound state appears at $qr_0 = \frac{\pi}{2}$, $\quad V_0 \overset{256}{=} \frac{\pi^2 \hbar^2}{8Mr_0^2}$ which implies $E = 0$. $\Rightarrow \kappa = 0$, i.e.

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

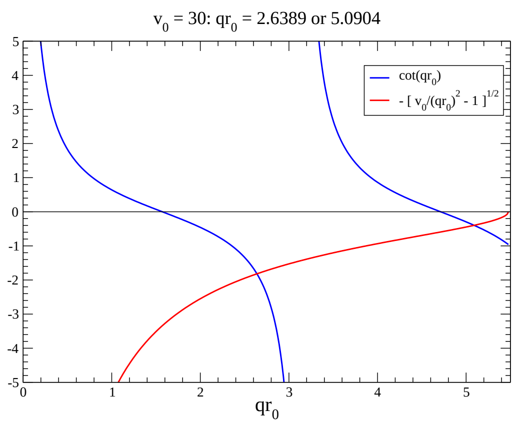
For larger $r_0^2 V_0$, i.e., a "large" well, more bound states can appear. The tightest bound state moves lower in E.



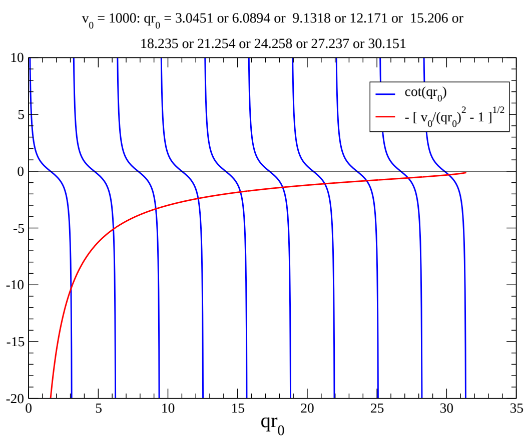
$v_0 = 0.05$



$v_0 = 3$

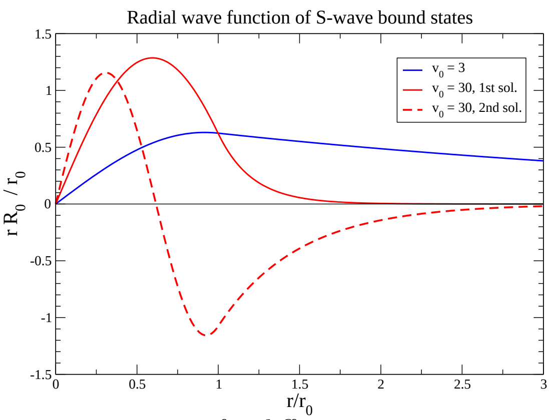


$v_0 = 30$

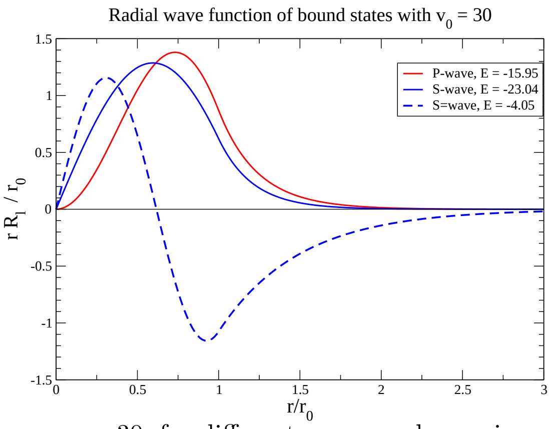


$v_0 = 1000$

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:

$$A j_\ell(qr_0) = B j_\ell(kr_0) + C n_\ell(kr_0), \tag{262}$$
$$qA j_\ell'(qr_0) = k\left[B j_\ell'(kr_0) + C n_\ell'(kr_0)\right] \tag{263}$$

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:

$$\frac{q\left(\frac{\cos(qr_0)}{qr_0} - \frac{\sin(qr_0)}{(qr_0)^2}\right)}{\frac{\sin(qr_0)}{qr_0}} = q\cot(qr_0) - \frac{1}{r_0}.$$

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

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

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 <u>resonance</u> 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

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

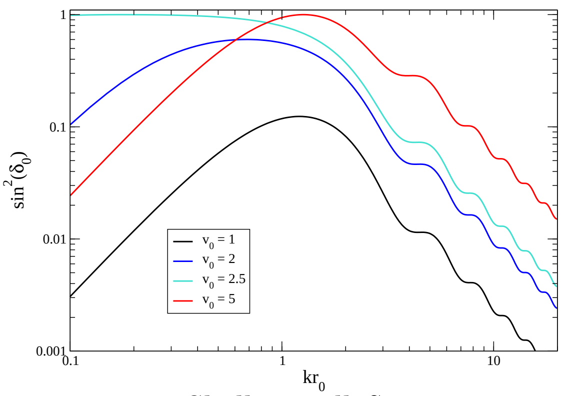
Resonance occurs <u>if</u> a bound state exists.

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

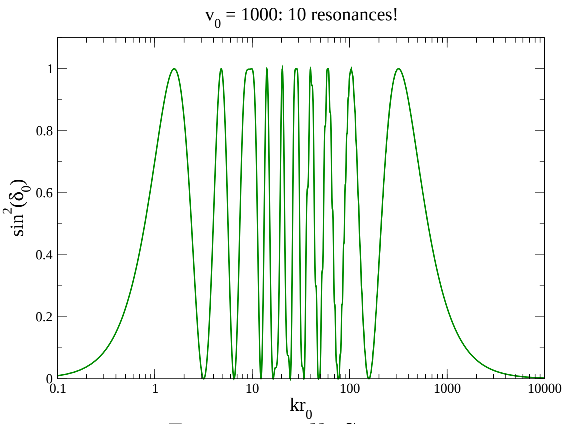
$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \quad j_1'(x) = \frac{2\cos x}{x^2} - \frac{2\sin x}{x^3} + \frac{\sin x}{x}.$$
$$n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \quad n_1'(x) = \frac{2\sin x}{x^2} + \frac{2\cos x}{x^3} - \frac{\cos x}{x}.$$

Phase shift from (265) (266)

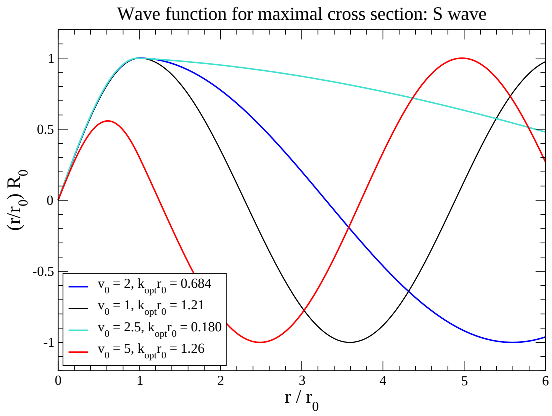
<u>S-wave scattering phase and S-wave unbound wave functions for spherical square well</u>



Shallow well; S-wave



Deeper well; S-wave



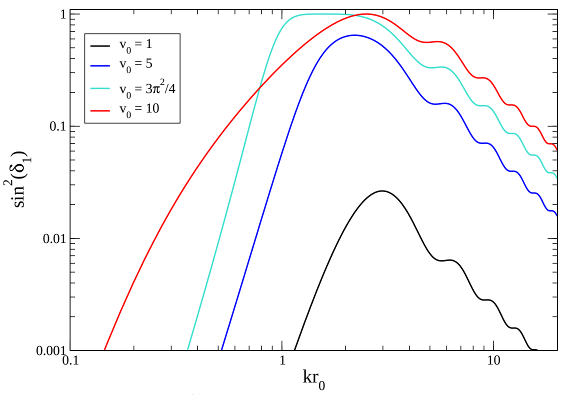
S-wave unbound wave functions

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 $\delta_0 = v_0/(2kr_0) - v_0 \sin(2kr_0)/(2kr_0)^2$.

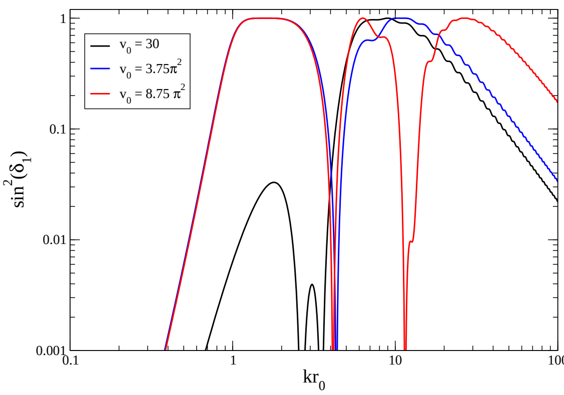
2. **Deeper well**; S-wave: There are now ten resonances. Note that this corresponds exactly to the number of bound states for this value of v_0, see $v_0 = 1000$!

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.

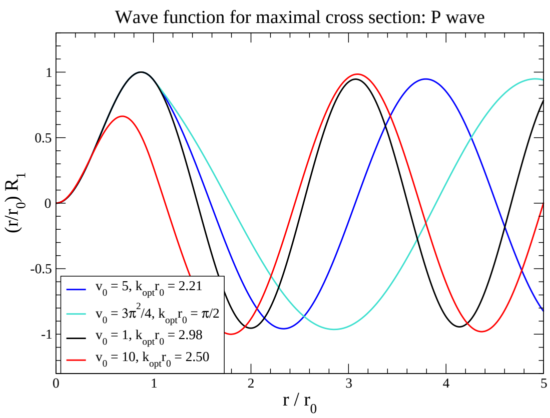
P-wave scattering phase and P-wave unbound wave functions for spherical square well



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 $r \leq r_0$.
  - 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 $\hat{P}^\dagger_{ik}$ is defined as usual:
$$\langle\varphi|\hat{P}_{ik}\psi\rangle = \langle\hat{P}^\dagger_{ik}\varphi|\psi\rangle \tag{278}$$
Since $\hat{P}^{-1}_{ik}$ is also a permutation, in fact $\hat{P}^{-1}_{ik} = \hat{P}_{ik}$:
$$\langle\varphi|\hat{P}_{ik}\psi\rangle \overset{277}{=} \langle\hat{P}^{-1}_{ik}\varphi|\hat{P}^{-1}_{ik}\hat{P}_{ik}\psi\rangle = \langle\hat{P}^{-1}_{ik}\varphi|\psi\rangle$$
but also $\langle\varphi|\hat{P}_{ik}\psi\rangle \overset{278}{=} \langle\hat{P}^\dagger_{ik}\varphi|\psi\rangle$
$$\Rightarrow \quad \hat{P}^\dagger_{ik} = \hat{P}^{-1}_{ik} \quad \Rightarrow \quad \hat{P}_{ik} \text{ is unitary} \tag{279}$$

iv For all symmetrical N-particle operators $\hat{S}(1,2,\dots,N)$, we have:
$$[\hat{P}_{ik}, \hat{S}] = 0, \quad \forall i,k \tag{280}$$
$$\Rightarrow \langle\hat{P}_{ik}\varphi|\hat{S}|\hat{P}_{ik}\Psi\rangle = \langle\varphi|\hat{P}^\dagger_{ik}\hat{S}\hat{P}_{ik}|\Psi\rangle \overset{280}{=} \langle\varphi|\overbrace{\hat{P}^\dagger_{ik}\hat{P}_{ik}}^{=\,1\ (279)}\hat{S}|\Psi\rangle = \langle\varphi|\hat{S}|\Psi\rangle \tag{281}$$
This shows that permutations do not change the matrix elements of a symmetric operator.

v Since the exchange of identical particles must <u>not</u> have observable consequences, all observables must correspond to completely symmetric operators:
$$\hat{O}. \tag{282}$$
Since (282) holds for <u>all</u> 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 <u>all</u> $\hat{P}_{ik}$ 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 <u>bosons</u>, described by ψ_s, or <u>fermions</u>, 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.

<u>Note</u>
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:
$$(1\,2\,4) \quad \text{means: particle 1 replaces particle 2, 2 replaces 4, 4 replaces 1.}$$
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:

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

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:

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

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):

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

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

$\Rightarrow n_i' = n_i - 1$: 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 $i \neq k$:

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

(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: $i = k$

$$\begin{aligned} \hat{b}_i \hat{b}_i^\dagger |n_1, n_2, \dots, n_i, \dots\rangle &\overset{323}{=} (1 - n_i)(-1)^{\sum_{k<i} n_k} \hat{b}_i |n_1, \dots, n_i + 1, \dots\rangle \\ &\overset{324}{=} \underbrace{(1 - n_i)(n_i + 1)}_{1 - n_i^2} \left[(-1)^{\sum_{k<i} n_k}\right]^2 |n_1, \dots, n_i, \dots\rangle \end{aligned}$$

$$\begin{aligned} \hat{b}_i^\dagger \hat{b}_i |n_1, n_2, \dots, n_i, \dots\rangle &\overset{324}{=} n_i (-1)^{\sum_{k<i} n_k} \hat{b}_i^\dagger |n_1, n_2, \dots, n_i - 1, \dots\rangle \\ &\overset{323}{=} = \underbrace{n_i (2 - n_i)}_{n_i} \left[(-1)^{\sum_{k<i} n_k}\right]^2 |n_1, n_2, \dots, n_i, \dots\rangle \end{aligned}$$

$$\{\hat{b}_i, \hat{b}_i^\dagger\} = 1 - n_i^2 + n_i = 1, \quad n_i \in \{0,1\}$$

$$\hat{n}_i^{(f)} = \hat{b}_i^\dagger \hat{b}_i \tag{327}$$

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 field operator:

$$\hat{\psi}(\vec{x}) = \sum_i \varphi_i(\vec{x})\hat{a}_i \tag{333}$$

$$\implies \hat{\psi}^\dagger(\vec{x}) = \sum_i \varphi_i^*(\vec{x})\hat{a}_i^\dagger \tag{334}$$

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 <u>higher</u> energy, which is not possible in thermal equilibrium. One <u>cannot</u> 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.:

$$n_{\vec{k}_\gamma}(t) = [n_{\vec{k}_\gamma}(0)+1]e^{An_2t}-1 \tag{351}$$

Exponential growth of photons with fixed $\vec{k}_\gamma$ and hence fixed E_γ.
<u>Possibilitiesto achieve $n_2>n_1$</u>

* 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:

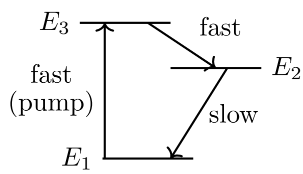


Figure 1: $A_{13}A_{23}>>A_{12}$

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:

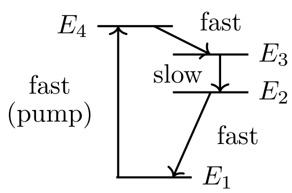


Figure 2: can get $n_3>>n_2$ even if $n_1>>n_3$

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 <u>not</u> work.

[18.12.2024, Lecture 21]

[23.12.2024, Lecture 22]

Bell's Inequalitiy

Hold for local alternatives to standard Quantum Mechanics ("hidden variable theories"), are violated 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 same 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** (not 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 always yields $-S_{z,1}$ with 100% probability, even if the two measurements have space-like separation. (Cannot 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 always 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 correlations 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:

$$P(\vec{a}, \vec{b}) = -\frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}(\cos\theta)\ \mathrm{sign}(\underbrace{\cos\theta}_{\vec{a}\cdot\vec{\lambda}})\mathrm{sign}[\underbrace{(\cos\varphi_b\cos\varphi + \sin\varphi_b\sin\varphi)}_{\underbrace{\cos(\varphi_b - \varphi)}_{\tilde{\varphi}}}\sin\theta_b\sin\theta + \cos\theta_b\cos\theta]$$

$$= -\frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}(\cos\theta)\, \mathrm{sign}(\cos\theta)\mathrm{sign}[\cos\tilde{\varphi}\sin\theta_b\sin\theta + \cos\theta_b\cos\theta]$$

If $\vec{a} = \vec{b}$, then $\cos\theta_b = 1$ and $\sin\theta_b = 0$, so:

$$P(\vec{a},\vec{a}) = -\frac{1}{4\pi}\int_0^{2\pi} \mathrm{d}\tilde{\varphi} \int_{-1}^{1} \mathrm{d}(\cos\theta)\, \underbrace{\left[\mathrm{sign}(\cos\theta)\right]^2}_{1} = -1 \quad \checkmark$$

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 $\vec{c}$:

$$\begin{aligned} P(\vec{a},\vec{b}) - P(\vec{a},\vec{c}) &= -\int \mathrm{d}\lambda\, \rho(\lambda)\left[A(\vec{a},\lambda)A(\vec{b},\lambda) - A(\vec{a},\lambda)A(\vec{c},\lambda)\right] \\ &= \int \mathrm{d}\lambda\, \rho(\lambda) A(\vec{a},\lambda)A(\vec{b},\lambda)\underbrace{\left[-1 + A(\vec{b},\lambda)A(\vec{c},\lambda)\right]}_{\leq 0}, \text{ used } \left[A(\vec{b},\lambda)\right]^2 = 1 \end{aligned}$$

Using the linearity of integration and the property $|f(x)| \leq \int |f(x)|dx$:

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \leq \int \mathrm{d}\lambda\, \rho(\lambda)\, \left|\cancelto{1}{A(\vec{a},\lambda)A(\vec{b},\lambda)}\right| \;\left[1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\right]$$

Since $A(\vec{b},\lambda)A(\vec{c},\lambda) \leq 1$:

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \leq 1 + P(\vec{b},\vec{c})$$

$$1 + P(\vec{b},\vec{c}) \geq \left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \quad \forall\, \vec{a},\vec{b},\vec{c} \tag{366}$$

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: $1 + P(\vec{b},\vec{c}) = 1 - \cos(45°) = 1 - \frac{\sqrt{2}}{2} \approx 0.293$

$$\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| = \left|-\cos(45°) + \cos(90°)\right| = \frac{\sqrt{2}}{2} \approx 0.707 > 0.293$$

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]

[8.01.2025, Lecture 23]

[13.01.2025, Lecture 24]

[13.01.2025, Lecture 24]

[15.01.2025, Lecture 25]

[15.01.2025, Lecture 25]

[20.01.2025, Lecture 26]

[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

$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} e^{i\omega(x'-x)} = \delta(x'-x) = \begin{cases} 0 & \text{for } x' \neq x, \\ \infty & \text{for } x' = x. \end{cases} \tag{368}$$

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 (368) 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

$$D\psi(x) = f(x) \tag{369}$$

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 (369)

$$\psi(x) = \psi_0(x) + \int \mathrm{d}x' G(x,x')f(x'), \tag{370}$$

where $\psi_0(x)$ is the general solution of the homogeneous differential equation

$$D\psi_0(x) = 0.$$

Equation (370) contains a particular solution of the inhomogeneous differential equation (369), 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

$$(\nabla^2+k^2)G(\mathbf{x}-\mathbf{x}') = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \tag{371}$$

The Fourier transform of $G(\mathbf{x}-\mathbf{x}')$

$$\tilde{G}(\mathbf{q}) = \int \mathrm{d}^3y\, e^{-i\mathbf{q}\cdot\mathbf{y}}G(\mathbf{y})$$

becomes, with (371),

$$(-q^2+k^2)\tilde{G}(\mathbf{q}) = 1.$$

Inverting the last two functions, one first obtains for the Green's function

$$G(\mathbf{y}) = \int \frac{\mathrm{d}^3q}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{y}}\frac{1}{-q^2+k^2}. \tag{372}$$

However, because of the poles at $\pm k$, the integral in (372) 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:

$$G_\pm(\mathbf{x}) = -\lim_{\varepsilon\to 0}\int \frac{\mathrm{d}^3q}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{q^2-k^2\mp i\varepsilon}. \tag{373}$$

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

$$G_\pm(\mathbf{x}) = -\frac{1}{4\pi 2ir}\int_{-\infty}^{+\infty}\frac{\mathrm{d}q\, qe^{iqr}}{q^2-k^2\mp i\varepsilon}.$$

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 (370) 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 (370) 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

$$\hat{C} = \hat{B} + \int_0^1 \mathrm{d}t\, g(e^{\mathrm{ad}\,\hat{A}\,t}e^{\mathrm{ad}\,\hat{B}})[\hat{A}], \tag{374}$$

and $g(z)$ is the function

$$g(z) \equiv \frac{\log z}{z-1} = \sum_{n=0}^{\infty}\frac{(1-z)^n}{n+1}, \tag{375}$$

and ad$B$ is the operator associated with $\hat{B}$ in the so-called *adjoint representation*, which is defined by

$$\mathrm{ad}B[\hat{A}] \equiv [\hat{B},\hat{A}]. \tag{376}$$

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. (374) and using the power series (375), one finds the explicit formula

$$\hat{C} = \hat{B} + \hat{A} + \sum_{n=1}^{\infty}\frac{(-1)^n}{n+1}\sum_{p_i,q_i;p_i+q_i\geq 1}\frac{1}{1+\sum_{i=1}^n p_i}\frac{(\mathrm{ad}A)^{p_1}}{p_1!}\frac{(\mathrm{ad}B)^{q_1}}{q_1!}\cdots\frac{(\mathrm{ad}A)^{p_n}}{p_n!}\frac{(\mathrm{ad}B)^{q_n}}{q_n!}[\hat{A}]. \tag{377}$$

The lowest expansion terms are

$$\begin{aligned}\hat{C} = \hat{B} + \hat{A} &- \frac{1}{2}\left[\frac{1}{2}\mathrm{ad}A + \mathrm{ad}B + \frac{1}{6}(\mathrm{ad}A)^2 + \frac{1}{2}\mathrm{ad}A\mathrm{ad}B + \frac{1}{2}(\mathrm{ad}B)^2 + \ldots\right][\hat{A}]\\ &+ \frac{1}{3}\left[\frac{1}{3}(\mathrm{ad}A)^2 + \frac{1}{2}\mathrm{ad}A\mathrm{ad}B + \frac{1}{2}\mathrm{ad}B\mathrm{ad}A + (\mathrm{ad}B)^2 + \ldots\right][\hat{A}]\end{aligned}$$

$$\Rightarrow \hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{12}([\hat{A},[\hat{A},\hat{B}]] + [\hat{B},[\hat{B},\hat{A}]]) + \frac{1}{24}[\hat{A},[[\hat{A},\hat{B}],\hat{B}]]\ldots \tag{378}$$

The result can be rearranged to the closely related *Zassenhaus formula*

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{\hat{Z}_2}e^{\hat{Z}_3}e^{\hat{Z}_4}\ldots, \tag{379}$$

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 (374) and thus the expansion (378), we proceed by deriving and solving a differential equation for the operator function

$$\hat{C}(t) = \log(e^{\hat{A}t}e^{\hat{B}}). \tag{380}$$

Its value at $t = 1$ will supply us with the desired result $\hat{C}$ in (377). The starting point is the observation that for any operator $\hat{M}$,

$$e^{\hat{C}(t)}\hat{M}e^{-\hat{C}(t)} = e^{\mathrm{ad}C(t)}[\hat{M}], \tag{381}$$

by definition of ad$C$. Inserting (380), 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 (376). Hence we have

$$e^{\mathrm{ad}C(t)} = e^{\mathrm{ad}At}e^{\mathrm{ad}B}. \tag{382}$$

Differentiation of (380) yields

$$e^{\hat{C}(t)}\frac{d}{dt}e^{-\hat{C}(t)} = -\hat{A}. \tag{383}$$

The left-hand side, on the other hand, can be rewritten in general as

$$e^{\hat{C}(t)}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{384}$$

where

$$f(z) \equiv \frac{e^z - 1}{z}. \tag{385}$$

It implies that

$$f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)] = \hat{A}. \tag{386}$$

We now define the function $g(z)$ as in (375) and see that it satisfies

$$g(e^z)f(z) \equiv 1. \tag{387}$$

We therefore have the trivial identity

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)]. \tag{388}$$

Using (386) and (382), this turns into the differential equation

$$\dot{\hat{C}}(t) = g(e^{\mathrm{ad}C(t)})[\hat{A}] = e^{\mathrm{ad}At}e^{\mathrm{ad}B}[\hat{A}], \tag{389}$$

from which we find directly the result (374).
To complete the proof we must verify (384). 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

$$\hat{O}(s,t) \equiv e^{\hat{C}(t)s}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)s}. \tag{390}$$

Differentiating this with respect to s gives

$$\partial_s\hat{O}(s,t) = e^{\hat{C}(t)s}\hat{C}(t)\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-\hat{C}(t)s}\right) - e^{\hat{C}(t)s}\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{C}(t)e^{-\hat{C}(t)s}\right), \tag{391}$$

$$= -e^{\hat{C}(t)s}\dot{\hat{C}}(t)e^{-\hat{C}(t)s} \tag{392}$$

$$= -e^{\mathrm{ad}C(t)s}[\dot{\hat{C}}(t)]. \tag{393}$$

Hence

$$\hat{O}(s,t) - \hat{O}(0,t) = \int_0^s \mathrm{d}s'\partial'_s\hat{O}(s',t) = -\sum_{n=0}^{\infty}\frac{s^{n+1}}{(n+1)!}(\mathrm{ad}C(t))^n[\dot{\hat{C}}(t)], \tag{394}$$

from which we obtain

$$\hat{O}(1,t) = e^{\hat{C}(t)}\frac{\mathrm{d}}{\mathrm{d}t}e^{-\hat{C}(t)} = -f(\mathrm{ad}C(t))[\dot{\hat{C}}(t)], \tag{395}$$

which is what we wanted to prove.
Note that the final form of the series for $\hat{C}$ in (378) 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

$$\hat{E} = \frac{1}{i\hbar}\int_{t_a}^{t_b} \mathrm{d}t_1 \hat{H}(t_1) + \frac{1}{2}\left(\frac{1}{i\hbar}\right)^2 \int_{t_a}^{t_b} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 [\hat{H}(t_2), \hat{H}(t_1)] \tag{396}$$

$$+ \frac{1}{4}\left(\frac{1}{i\hbar}\right)^3 \left\{\int_{t_a}^{t_b} \mathrm{d}t_3 \int_{t_a}^{t_3} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 \left[\hat{H}(t_3), \left[\hat{H}(t_2), \hat{H}(t_1)\right]\right]\right. \tag{397}$$

$$\left. + \frac{1}{3}\int_{t_a}^{t_b} \mathrm{d}t_3 \int_{t_a}^{t_3} \mathrm{d}t_2 \int_{t_a}^{t_2} \mathrm{d}t_1 \left[\left[\hat{H}(t_3), \hat{H}(t_2)\right], \hat{H}(t_1)\right]\right\} + \ldots, \tag{398}$$

which converges faster than the Neumann-Liouville expansion.

[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`).

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 (401). For this, we compute (note the summation convention)

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{1}{m}\left(p_i - \frac{e}{c}A_i(x,t)\right), \tag{399}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} = -\frac{1}{m}\left(p_j - \frac{e}{c}A_j(\mathbf{x},t)\right)\left(-\frac{e}{c}A_{j,i}\right) - e\Phi_{,i} = \dot{x}_j\frac{e}{c}A_{j,i} - e\Phi_{,i}, \tag{400}$$

with $f_{,i} \equiv \partial f/\partial x_i$. From (399, 400), 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.,

$$m\ddot{x}_i = \left(\frac{e}{c}\dot{\mathbf{x}} \times \mathbf{B} + e\mathbf{E}\right)_i. \tag{401}$$

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 (399) 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

$$x_\pm = x \pm iy. \tag{402}$$

The following commutation relations hold:

$$[L_z, x_\pm] = \pm\hbar x_\pm, \quad [L_\pm, x_\pm] = 0, \quad [L_\pm, x_\mp] = \pm 2\hbar z, \tag{403}$$
$$[\mathbf{L}^2, x_+] = L_z\hbar x_+ + \hbar x_+ L_z + \hbar^2 x_+ - 2\hbar z L_+ \tag{404}$$
$$= 2\hbar x_+ L_z + 2\hbar^2 x_+ - 2\hbar z L_+, \tag{405}$$

where $\mathbf{L}^2 = L_z^2 + \hbar L_z + L_- L_+$ has been used. It follows that

$$L_z x_+|l,l\rangle = x_+ L_z|l,l\rangle + \hbar x_+|l,l\rangle = \hbar(l+1)x_+|l,l\rangle \tag{406}$$
$$\mathbf{L}^2 x_+|l,l\rangle = \hbar^2 l(l+1)x_+|l,l\rangle + 2\hbar^2(l+1)x_+|l,l\rangle = \hbar^2(l+1)(l+2)x_+|l,l\rangle. \tag{407}$$

The quantity x_+ is thus the ladder operator for the states $|l,l\rangle$,

$$x_+|l,l\rangle = N|l+1,l+1\rangle. \tag{408}$$

Hence, the eigenstates of angular momentum can be represented as follows:

$$|l,m\rangle = N' L_-^{l-m}(x_+)^l|0,0\rangle. \tag{409}$$

N and N' in (408) 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

$$\psi_{00}(\mathbf{x}) = \langle\mathbf{x}|0,0\rangle \tag{410}$$

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

$$\psi_{00}(\mathbf{x}) = \frac{1}{\sqrt{4\pi}}. \tag{411}$$

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

$$I_l = \int_0^1\mathrm{d}\eta(1-\eta^2)^l = \eta(1-\eta^2)^l\Big|_0^1 + 2l\int_0^1\mathrm{d}\eta(1-\eta^2)^{l-1}\eta = -2lI_l + 2lI_{l-1},$$
$$I_l = \frac{2l}{2l+1}I_{l-1} = \frac{2l}{2l+1}\frac{2(l-1)}{2(l-1)+1}\cdots\frac{2\times 1}{2+1}I_0 = \frac{2l(2l-2)\ldots 2}{(2l+1)(2l-1)\ldots 3} = \frac{2^l(l!)^2}{(2l+1)!}, \quad I_0 = 1.$$

One thus has

$$\psi_{ll}(\mathbf{x}) = \frac{1}{\sqrt{4\pi I_l}}\sin^l\vartheta e^{il\varphi} \tag{412}$$

and the definition of the spherical harmonics

$$Y_l^m(\vartheta,\varphi) = (-1)^l \sqrt{\frac{(2l+1)!}{4\pi}} \frac{1}{2^l l!} \sin^l \vartheta e^{il\varphi}. \tag{413}$$

$Y_{ll}(\vartheta,\varphi)$ 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_-:

$$(L_-)^{l-m}|l,l\rangle = N'|l,m\rangle. \tag{414}$$

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

$$Y_{lm}(\vartheta,\varphi) = \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}(L_-/\hbar)^{l-m} Y_{ll}(\vartheta,\varphi). \tag{415}$$

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

$$Y_{lm}(\vartheta,\varphi) = (-1)^l\sqrt{\frac{(l+m)!(2l+1)}{(l-m)!4\pi}}\frac{1}{2^l l!} e^{im\varphi}\sin^{-m}\vartheta\frac{\mathrm{d}^{l-m}}{(\mathrm{d}\cos\vartheta)^{l-m}}\sin^{2l}\vartheta \tag{416}$$

$$= (-1)^{l+m}\frac{1}{2^l l!}\sqrt{\frac{(l-m)!(2l+1)}{(l+m)!4\pi}} e^{im\varphi}\sin^m\vartheta\frac{\mathrm{d}^{l+m}}{(\mathrm{d}\cos\vartheta)^{l+m}}\sin^{2l}\vartheta. \tag{417}$$

And the spherical harmonics obey

$$Y_{l,m}(\vartheta,\varphi) = (-1)^m Y^*_{l,-m}(\vartheta,\varphi). \tag{418}$$

This concludes the algebraic derivation of the angular momentum eigenfunctions.

Remark: In going from (416) over to the conventional representation (417), we have used the fact that the associated Legendre function

$$P_l^m(\eta) = \frac{1}{2^l l!}(1-\eta^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}\eta^{l+m}}(\eta^2-1)^l \tag{419}$$

satisfies the identity

$$P_l^{-m} = (-1)^m \frac{(l-m)!}{(l+m)!}P_l^m. \tag{420}$$

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 (420).
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

$$\mathbf{a}^{(l)} = i\hat{\mathbf{x}}\times\mathbf{L} - \hbar\hat{\mathbf{x}} = \begin{cases} \hat{x}_y L_z - \hat{x}_z L_y \\ \hat{x}_z L_x - \hat{x}_x L_z \\ \hat{x}_x L_y - \hat{x}_y L_x \end{cases} - \hbar\hat{\mathbf{x}} \tag{421}$$

where $\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|$ is the radial unit vector. It turns out to be useful to introduce the decomposition

$$a_\pm^{(l)} = a_x^{(l)} \pm i a_y^{(l)} = \mp\hat{x}_z L_\pm \pm \hat{x}_\pm(L_z \mp \hbar), \tag{422}$$

$$a_z^{(l)} = \hat{x}_- L_+ + \hat{x}_z(L_z - \hbar l) - \hat{\mathbf{x}}\cdot\mathbf{L} = \hat{x}_- L_+ + \hat{x}_z(L_z - \hbar l), \tag{423}$$

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

$$[a_+^{(l)}, a_-^{(l)}] = 2\hbar\hat{\mathbf{x}}^2 L_z = 2\hbar L_z, \tag{424}$$

$$[L_+, a_-^{(l)}] = 2\hbar a_z^{(l)}, \tag{425}$$

$$[L_z, a_-^{(l)}] = -\hbar a_-^{(l)}. \tag{426}$$

This then implies

$$a_+^{(l)}|l,l\rangle = 0 \tag{427}$$

$$\text{and } a_z^{(l)}|l,l\rangle = 0. \tag{428}$$

Together with the commutator (424), this yields

$$a_+^{(l)} a_-^{(l)}|l,l\rangle = 2\hbar^2 l\mathbf{x}^2|l,l\rangle. \tag{429}$$

Multiplication of (429) 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 (423) and (429) 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 (425) and (428), one finds

$$L_+ a_-^{(l)}|l,l\rangle = a_-^{(l)} L_+|l,l\rangle + 2\hbar a_z^{(l)}|l,l\rangle = 0 \tag{430}$$

and, from (426),

$$L_z a_-^{(l)}|l,l\rangle = \hbar(l-1)a_-^{(l)}|l,l\rangle. \tag{431}$$

With $\mathbf{L}^2 = L_-L_+ + \hbar L_z + L_z^2$, we obtain from (431) and (430)

$$\mathbf{L}^2 a_-^{(l)}|l,l\rangle = \hbar^2\big((l-1)+(l-1)^2\big)a_-^{(l)}|l,l\rangle = \hbar^2 l(l-1)a_-^{(l)}|l,l\rangle. \tag{432}$$

In summary, (431) and (432) imply

$$a_-^{(l)}|l,l\rangle \propto |l-1,l-1\rangle. \tag{433}$$

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:

$$\psi_B(\vec{x}) = \exp\left\{\frac{i2e}{\hbar c}\int_{\vec{x}_0}^{\vec{x}} \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s})\right\}\psi_0(\vec{x}) \tag{434}$$

The vector potential in (434) 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:

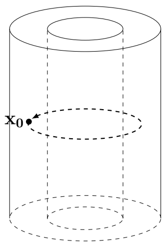


Figure 3: Flux quantization

$$\psi_B(\vec{x}_0) = \psi_0(\vec{x}_0) = \exp\left\{\frac{i2e}{\hbar c}\oint \mathrm{d}\vec{s}\cdot\mathbf{A}(\vec{s})\right\}\psi_0(\vec{x}_0)$$

$$\begin{aligned}
\Phi_B &= \Phi_0 n \quad , \quad n = 0, \pm 1, \ldots, \\
\Phi_0 &= \frac{\hbar c\pi}{e_0} = 2.07\times 10^{-7}\,\mathrm{G\ cm}^2 \quad \text{(the flux quantum)}.
\end{aligned}$$

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

$$H = H_\perp + \frac{p_3^2}{2m}. \tag{435}$$

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

$$H_\perp = \frac{m}{2}(\dot{x}_1^2 + \dot{x}_2^2). \tag{436}$$

The second term in (Equation 435) 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

$$[mx_1, mx_2] = i\hbar\frac{eB}{c}, \quad [x_1, x_1] = [\dot{x}_1, \dot{x}_2] = 0 \tag{437}$$

[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

$$\pi_i = \frac{m\dot{x}_i}{\sqrt{e_0 B/c}}. \tag{438}$$

Now, these operators satisfy the commutation relations

$$[\pi_2, \pi_1] = i\hbar, \quad [\pi_1, \pi_1] = [\pi_2, \pi_2] = 0, \tag{439}$$

and, in analogy to position and momentum, they represent canonical variables with the Hamiltonian

$$H_\perp = \frac{1}{2}\frac{e_0 B}{cm}(\pi_1^2 + \pi_2^2). \tag{440}$$

According to the theory of the harmonic oscillator using

$$a = \frac{\pi_2 + i\pi_1}{\sqrt{2\hbar}}, \tag{441}$$

this can be brought into the standard form

$$H_\perp = \hbar\omega_c\left(a^\dagger a + \frac{1}{2}\right), \tag{442}$$

where

$$\omega_c = \frac{e_0 B}{mc} \tag{443}$$

is the cyclotron frequency. Consequently, the energy eigenvalues of (436) are

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right), \tag{444}$$

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

$$(x_b t_b|x_a t_a) = \langle x_b|\hat{U}(t_b, t_a)|x_a\rangle, \quad t_b > t_a. \tag{445}$$

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 (445) could be sliced into a large number, say $N+1$, of time evolution operators, each acting across an infinitesimal time slice of thickness $\varepsilon = t_n - t_{n-1} = (t_b - t_a)/(N+1) > 0$:

$$(x_b t_b|x_a t_a) = \langle x_b|\hat{U}(t_b, t_N)\hat{U}(t_N, t_{N-1}) \cdots \hat{U}(t_2, t_1)\hat{U}(t_1, t_a)|x_a\rangle. \tag{446}$$

When inserting a complete set of states between each pair of $\hat{U}$'s,

$$\int_{-\infty}^{\infty} \mathrm{d}x_n |x_n\rangle\langle x_n| = 1, \quad n = 1, 2, \ldots, N, \tag{447}$$

the amplitude becomes a product of N-integrals

$$(x_b t_b|x_a t_a) = \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right]\prod_{n=1}^{N+1}(x_n t_n|x_{n-1}t_{n-1}), \tag{448}$$

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

$$\langle x_n t_n|x_{n-1}t_{n-1}\rangle = \langle x_n|e^{-i\varepsilon\hat{H}(t_n)/\hbar}|x_{n-1}\rangle, \tag{449}$$

with the Hamiltonian operator

$$\hat{H}(t) \equiv H(\hat{p}, \hat{x}, t). \tag{450}$$

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:

$$H(p, x, t) = T(p, t) + V(x, t). \tag{451}$$

For a sufficiently small slice thickness, the time evolution operator

$$e^{-i\varepsilon\hat{H}/\hbar} = e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar} \tag{452}$$

is factorizable as a consequence of the *Baker-Campbell-Hausdorff formula* (allready proved in Baker-Campbell-Hausdorff Formula and Magnus Expansion)

$$e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar} = e^{-i\varepsilon\hat{V}/\hbar}e^{-i\varepsilon\hat{T}/\hbar}e^{-i\varepsilon^2\hat{X}/\hbar^2}, \tag{453}$$

where the operator $\hat{X}$ has the expansion

$$\hat{X} \equiv \frac{i}{2}[\hat{V}, \hat{T}] - \frac{\varepsilon}{\hbar}\left(\frac{1}{6}[\hat{V}, [\hat{V}, \hat{T}]] - \frac{1}{3}[[\hat{V}, \hat{T}], \hat{T}]\right) + \mathcal{O}(\varepsilon^2). \tag{454}$$

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:

$$\langle x_n|e^{-i\varepsilon H(\hat{p},\hat{x},t_n)/\hbar}|x_{n-1}\rangle \approx \int_{-\infty}^{\infty} \mathrm{d}x \langle x_n|e^{-i\varepsilon V(\hat{x},t_n)/\hbar}|x\rangle\langle x|e^{-i\varepsilon T(\hat{p},t_n)/\hbar}|x_{n-1}\rangle. \tag{455}$$

Evaluating the local matrix elements,

$$\langle x_n | e^{-i\varepsilon V(\hat{x},t_n)/\hbar} | x \rangle = \delta(x_n - x) e^{-i\varepsilon V(x_n,t_n)/\hbar}, \tag{456}$$

this becomes

$$\langle x_n | e^{-i\varepsilon H(\hat{p},\hat{x},t_n)/\hbar} | x_{n-1} \rangle \approx \int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar} \exp\left\{ i p_n (x_n - x_{n-1})/\hbar - i\varepsilon [T(p_n,t_n) + V(x_n,t_n)]/\hbar \right\}. \tag{457}$$

Inserting this back into (448), we obtain *Feynman's path integral formula*, consisting of the multiple integral

$$(x_b t_b | x_a t_a) \approx \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \mathrm{d}x_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar} \right] \exp\left(\frac{i}{\hbar} \mathcal{A}^N \right), \tag{458}$$

where $\mathcal{A}^N$ is the sum

$$\mathcal{A}^N = \sum_{n=1}^{N+1} \left[p_n (x_n - x_{n-1}) - \varepsilon H(p_n, x_n, t_n) \right]. \tag{459}$$

$$\tag{460}$$

Zero-Hamiltonian Path Integral

Note that the path integral (458) with zero Hamiltonian produces the Hilbert space structure of the theory via a chain of scalar products:

$$(x_b t_b | x_a t_a) \approx \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \mathrm{d}x_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar} \right] e^{i \sum_{n=1}^{N+1} p_n (x_n - x_{n-1})/\hbar}, \tag{461}$$

which is equal to

$$(x_b t_b | x_a t_a) \approx \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \mathrm{d}x_n \right] \prod_{n=1}^{N+1} \langle x_n | x_{n-1} \rangle = \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} \mathrm{d}x_n \right] \prod_{n=1}^{N+1} \delta(x_n - x_{n-1}) = \delta(x_b - x_a). \tag{462}$$

Whose continuum limit is

$$(x_b t_b | x_a t_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i \int \mathrm{d}t p(t) \dot{x}(t)/\hbar} = \langle x_b | x_a \rangle = \delta(x_b - x_a). \tag{463}$$

In the operator expression (446), 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 (461) 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 $x(t)$:

$$[\hat{p}(t), x(t)] = -i\hbar. \tag{464}$$

These are the canonical *equal-time* commutation relations of Heisenberg.
This observation forms the basis for deriving, from the path integral (458), the Schrödinger equation for the time evolution amplitude.

Schrödinger Equation for Time Evolution Amplitude

Let us split from the product of integrals in (458) the final time slice as a factor, so that we obtain the recursion relation

$$(x_b t_b | x_a t_a) \approx \int_{-\infty}^{\infty} \mathrm{d}x_N (x_b t_b | x_N t_N)(x_N t_N | x_a t_a), \tag{465}$$

where

$$(x_b t_b | x_N t_N) \approx \int_{-\infty}^{\infty} \frac{\mathrm{d}p_b}{2\pi\hbar} e^{(i/\hbar)[p_b(x_b - x_N) - \varepsilon H(p_b, x_b, t_b)]}. \tag{466}$$

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

$$(x_b t_b | x_N t_N) \approx e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b)/\hbar} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_b}{2\pi\hbar} e^{i p_b (x_b - x_N)/\hbar} = e^{-i\varepsilon H(-i\hbar\partial_{x_b}, x_b, t_b)/\hbar} \delta(x_b - x_N). \tag{467}$$

Inserting this back into (465) we obtain

$$\left(x_b t_b | x_a t_a\right) \approx e^{-i\varepsilon H\left(-i\hbar\partial_{x_b}, x_b, t_b\right)/\hbar}\left(x_b t_b - \varepsilon | x_a t_a\right), \tag{468}$$

or

$$\frac{1}{\varepsilon}\left[\left(x_b t_b + \varepsilon | x_a t_a\right) - \left(x_b t_b | x_a t_a\right)\right] \approx \frac{1}{\varepsilon}\left[e^{-i\varepsilon H\left(-i\hbar\partial_{x_b}, x_b, t_b+\varepsilon\right)/\hbar} - 1\right]\left(x_b t_b | x_a t_a\right). \tag{469}$$

In the limit $\varepsilon \to 0$, this goes over into the differential equation for the time evolution amplitude

$$i\hbar\frac{\partial}{\partial t_b}\left(x_b t_b | x_a t_a\right) = H\left(-i\hbar\partial_{x_b}, x_b, t_b\right)\left(x_b t_b | x_a t_a\right), \tag{470}$$

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 (458) to the quantum-mechanical amplitude in the continuum limit, where the thickness of the time slices $\varepsilon = \left(t_b - t_a\right)/(N+1) \to 0$ 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

$$e^{-i\left(t_t - t_n\right)\hat{H}/\hbar} = \lim_{N\to\infty}\left(e^{-i\varepsilon\hat{V}/\hbar}e^{-i\varepsilon\hat{T}/\hbar}\right)^{N+1} \tag{471}$$

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 (471) as

$$e^{i\left(t_b - t_a\right)\hat{H}/\hbar} \equiv \left(e^{-i\varepsilon(\hat{T}+\hat{V})/\hbar}\right)^{N+1} \equiv \left(e^{-i\varepsilon\hat{V}/\hbar}e^{-i\varepsilon\hat{T}/\hbar}e^{-i\varepsilon^2\hat{X}/\hbar^2}\right)^{N+1}$$

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 (458), even in systems where the formula is known to be valid. In particular, the short-time amplitude may be different from (457). 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 (454) 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 (458) 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 (458) 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 (459) tends towards the integral

$$\mathcal{A}[p,x] = \int_{t_a}^{t_b}\mathrm{d}t[p(t)\dot{x}(t) - H(p(t),x(t),t)] \tag{472}$$

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 $x\left(t_b\right) = x_b, x\left(t_a\right) = x_a$.

In the same limit, the product of infinitely many integrals in (458) will be called a path integral. The limiting measure of integration is written as

$$\lim_{N\to\infty}\prod_{n=1}^{N}\left[\int_{-\infty}^{\infty}\mathrm{d}x_n\right]\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{\mathrm{d}p_n}{2\pi\hbar}\right] \equiv \int_{x\left(t_a\right)=x_a}^{x\left(t_b\right)=x_b}\mathcal{D}'x\int\frac{\mathcal{D}p}{2\pi\hbar}. \tag{473}$$

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 $\left(x_n, x_{n-1}\right)$ 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

$$\left(x_b t_b \mid x_a t_a\right) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}'x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{i\mathcal{A}[p,x]/\hbar} \tag{474}$$

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,

$$\left(x_b t_b \mid x_a t_a\right) = \sum_{\substack{\text{all histories} \\ (x_a,t_a)\rightsquigarrow(x_b,t_b)}} e^{i\mathcal{A}[p,x]/\hbar} \tag{475}$$

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

$$\left(p_b t_b \mid p_a t_a\right) \equiv \langle p_b| \hat{U}\left(t_b, t_a\right) |p_a\rangle \tag{476}$$

The time slicing proceeds as in (446)-(448), with all x's replaced by p's, except in the completeness relation (447) which we shall take as

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} |p\rangle\langle p| = 1 \tag{477}$$

corresponding to the choice of the normalization of states

$$\langle p_b \mid p_a\rangle = 2\pi\hbar\delta\left(p_b - p_a\right) \tag{478}$$

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

$$\left(p_b t_b \mid p_a t_a\right) \approx \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar}\right] \prod_{n=0}^{N}\left[\int_{-\infty}^{\infty} dx_n\right] \tag{479}$$

$$\times \exp\left\{\frac{i}{\hbar} \sum_{n=0}^{N}\left[-x_n\left(p_{n+1} - p_n\right) - \varepsilon H\left(p_n, x_n, t_n\right)\right]\right\} \tag{480}$$

The relation between this and the x-space amplitude (458) is simple: By taking in (458) 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 $\sum_{n=1}^{N+1} p_n\left(x_n - x_{n-1}\right)$ as follows

$$\sum_{n=1}^{N+1} p_n\left(x_n - x_{n-1}\right) = p_{N+1}\left(x_{N+1} - x_N\right) + p_N\left(x_N - x_{N-1}\right) + \ldots + p_2\left(x_2 - x_1\right) + p_1\left(x_1 - x_0\right) \tag{481}$$

$$= p_{N+1}x_{N+1} - p_1 x_0 - \left(p_{N+1} - p_N\right)x_N - \left(p_N - p_{N-1}\right)x_{N-1} - \ldots - \left(p_2 - p_1\right)x_1 \tag{482}$$

$$= p_{N+1}x_{N+1} - p_1 x_0 - \sum_{n=1}^{N}\left(p_{n+1} - p_n\right)x_n \tag{483}$$

the remaining product of integrals looks as in Eq. (480), except that the lowest index n is one unit larger than in the sum in Eq. (480). In the limit $N \to \infty$ this does not matter, and we obtain the Fourier transform

$$\left(x_b t_b \mid x_a t_a\right) = \int \frac{\mathrm{d}p_b}{2\pi\hbar} e^{ip_b x_b/\hbar} \int \frac{\mathrm{d}p_a}{2\pi\hbar} e^{-ip_a x_a/\hbar} \left(p_b t_b \mid p_a t_a\right). \tag{484}$$

The inverse relation is

$$\left(p_b t_b \mid p_a t_a\right) = \int \mathrm{d}x_b e^{-ip_b x_b/\hbar} \int \mathrm{d}x_a e^{ip_a x_a/\hbar} \left(x_b t_b \mid x_a t_a\right). \tag{485}$$

In the continuum limit, the amplitude (480) can be written as a path integral

$$\left(p_b t_b \mid p_a t_a\right) = \int_{p(t_a)=p_a}^{p(t_b)=p_b} \frac{\mathcal{D}' p}{2\pi\hbar} \int \mathcal{D}x e^{i\bar{\mathcal{A}}[p,x]/\hbar} \tag{486}$$

where

$$\bar{\mathcal{A}}[p,x] = \int_{t_a}^{t_b} dt[-\dot{p}(t)x(t) - H(p(t),x(t),t)] = \mathcal{A}[p,x] - p_b x_b + p_a x_a. \tag{487}$$

If the Hamiltonian is independent of x and t, the sliced path integral (480) 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 $\prod_{n=0}^{N} e^{-i\varepsilon H(p_a)/\hbar}$, which is equal to $e^{-i(t_b-t_a)H(p)/\hbar}$. Hence we obtain:

$$\left(p_b t_b \mid p_a t_a\right) = 2\pi\hbar\delta\left(p_b - p_a\right) e^{-i(t_b-t_a)H(p)/\hbar} \tag{488}$$

Inserting this into Eq. (484), we find a simple Fourier integral for the time evolution amlitude in x-space:

$$\left(x_b t_b \mid x_a t_a\right) = \int \frac{\mathrm{d}p}{2\pi\hbar} e^{ip(x_b-x_a)/\hbar - i(t_b-t_a)H(p)/\hbar} \tag{489}$$

Note that in (488) contains an equal sign rather than the $\approx$-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

$$Z_{\mathrm{QM}}\left(t_b, t_a\right) = \operatorname{Tr}\left(e^{-i(t_b-t_a)\hat{H}/\hbar}\right). \tag{490}$$

In the local basis, the trace becomes an integral over the amplitude $\left(x_b t_b \mid x_a t_a\right)$ with $x_b = x_a$:

$$Z_{\mathrm{QM}}\left(t_b, t_a\right) = \int_{-\infty}^{\infty} \mathrm{d}x_a \left(x_a t_b \mid x_a t_a\right). \tag{491}$$

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 :

$$\int_{-\infty}^{\infty} \mathrm{d}x_{N+1} \prod_{n=1}^{N}\left[\int_{-\infty}^{\infty} \mathrm{d}x_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_n}{2\pi\hbar}\right] = \prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty} \frac{\mathrm{d}x_n \mathrm{d}p_n}{2\pi\hbar}\right] \tag{492}$$

In the continuum limit, the right-hand side is written as

$$\lim_{N\to\infty} \prod_{n=1}^{N+1}\left[\iint_{-\infty}^{\infty} \frac{\mathrm{d}x_n \mathrm{d}p_n}{2\pi\hbar}\right] \equiv \oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar}, \tag{493}$$

and the measures are related by

$$\int_{-\infty}^{\infty} \mathrm{d}x_a \int_{x(t_a)=x_a}^{x(t_b)=x_a} \mathcal{D}' x \int \frac{\mathcal{D}p}{2\pi\hbar} \equiv \oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar}. \tag{494}$$

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

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p_a}{2\pi\hbar} \int_{p(t_a)=p_a}^{p(t_b)=p_a} \frac{\mathcal{D}' p}{2\pi\hbar} \int \mathcal{D}x \equiv \oint \frac{\mathcal{D}p}{2\pi\hbar} \int \mathcal{D}x, \tag{495}$$

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

$$Z_{\mathrm{QM}}\left(t_b, t_a\right) = \oint \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} e^{iA[p,x]/\hbar} = \oint \frac{\mathcal{D}p}{2\pi\hbar} \int \mathcal{D}x e^{i\overline{\mathcal{A}}[p,x]/\hbar} \tag{496}$$

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 (487) are removed by the periodic boundary conditions. In the time-sliced expression, the equality is easily derived from the rearrangement of the sum (483), which shows that

$$\sum_{n=1}^{N+1} p_n \left(x_n - x_{n-1}\right)\bigg|_{x_{N+1}=x_0} = -\sum_{n=0}^{N} \left(p_{n+1} - p_n\right) x_n\bigg|_{p_{N+1}=p_0} . \tag{497}$$

In the path integral expression (496) 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_BT}. 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.