Quantum Mechanics I Review Notes

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Reference: Cohen-Tannoudji Volume 1 [CT]

1 Waves and particles. Introduction to the ideas of fundamental QM

[CT 7-90]

1.1 Waves and particles

The quantization of light and energy was first suggested by Planck to explain blackbody radiation. They are defined by the Planck-Einstein relations

$$E = hv = \hbar\omega, \qquad \mathbf{p} = \hbar\mathbf{k} \tag{1}$$

However, Young's double-slit experiment suggested that light must behave like a wave. This led to the concept of wave-particle duality which is summarized as: (1) Light behaves simultaneously like a wave and like a flux of particles, (2) predictions about the behavior of a photon can only be probabilistic, and (3) The information about a photon at time t is given by the wave $E(\mathbf{r}, t)$, which is a solution of Maxwell's equation.

Another implication is that light measurement devices can only give certain results, called eigenvalues. These eigenvalues correspond to eigenstates of the wave function. When we predict the behavior of a light wave, we are assigning probabilities to each of its possible eigenstates.

De Broglie found that matter with energy E and momentum $\mathbf{p}$ also can behave like a wave, with its de Broglie wavelength given by

$$\lambda = \frac{2\pi}{|\mathbf{k}|} = \frac{h}{|\mathbf{p}|} \tag{2}$$

1.2 Schrodinger equation and solutions

We describe the quantum state of a particle by a wave function $\psi(\mathbf{r}, t)$. It is interpreted as the probability amplitude of the particle's presence such that the probability density $dP(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 d^3r$. We assume that the wave functions are normalized such that $\int |\psi(\mathbf{r}, t)|^2 d^3r = 1$.

When the particle of mass m is subjected to the influence of a potential $V(\mathbf{r}, t)$, the Schrodinger equation takes on the form

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla\psi(\mathbf{r}, t) + V(\mathbf{r}, t)\psi(\mathbf{r}, t) \tag{3}$$

1.2.1 Free particle

When $V(\mathbf{r}, t) = 0$, the Schrodinger equation has solutions of the form

$$\psi(\mathbf{r}, t) = Ae^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}, \qquad \omega = \frac{\hbar\mathbf{k}^2}{2m}, \qquad E = \hbar\omega = \frac{\mathbf{p}^2}{2m} \tag{4}$$

where the ω expression is called the *dispersion relation*. Because any superposition of solutions is also a solution, the wave function can be written as a superposition across all $\mathbf{k}$ to represent any square-integrable function $g(\mathbf{k})$.

$$\psi(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}} \int g(\mathbf{k}) e^{i[\mathbf{k}\cdot\mathbf{r}-\omega(k)t]} d^3k \tag{5}$$

Assuming the wave packet is one-dimensional and $g(k)$ is the Fourier transform of $\psi(x,0)$.

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int g(k) e^{ikx} dk, \qquad g(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0) e^{-ikx} dx \tag{6}$$

The time evolution of a plane wave can be described by

$$v_\phi(k) = \frac{\omega}{k} = \frac{c}{n(k)} = \frac{\hbar k}{2m}, \qquad v_G(k) = \frac{d\omega}{dk} = \frac{\hbar k}{m} = 2v_\phi \tag{7}$$

where v_ϕ is the phase velocity, v_G is the group velocity, $n(k)$ is the dispersive index of the medium.

1.2.2 Uncertainty relation

CT derives this from the form of the wave packet in [CT 23-28], but the explanation isn't necessary.

$$\Delta x \Delta p = \sigma_x \sigma_p \geq \hbar \tag{8}$$

1.3 Time-independent scalar potential

In a potential $V(\mathbf{r})$, we can use separation of variables, $\psi(\mathbf{r},t) = \phi(\mathbf{r})\chi(t)$ to simplify the Schrodinger equation

$$H\phi(\mathbf{r}) = \Big[-\frac{\hbar^2}{2m}\nabla + V(\mathbf{r}) \Big] \phi(\mathbf{r}) = E\phi(\mathbf{r}), \qquad i\hbar \frac{d\chi(t)}{dt} = E\chi(t) \tag{9}$$

The solution to the second ODE is simply $\chi(t) = Ae^{-i\omega t}$. This allows us to describe $\psi(\mathbf{r},0)$ as a linear combination of energy eigenstates and multiply them by their energy-based time dependence to describe

$$\psi(\mathbf{r},t) = \sum_n c_n \phi_n(\mathbf{r}) e^{-iE_n t/\hbar} \tag{10}$$

2 The mathematical tools of QM

[CT 91-210]

2.1 One-particle wave function space

Wave functions live in Hilbert space (also called L^2). This is described as a vector space where $\int d^3r |f|^2 = 1$ if $f \in L^2$. We will refer to F as the set of all wave functions composed of sufficiently regular functions of L^2. $F \subset L^2$.

A **vector space** is a set that is closed under vector addition and scalar multiplication. F is a vector space and $\psi_1, \psi_2 \in F$

$$\psi_1 + \psi_2 = \psi_2 + \psi_1 \in F, \qquad (\lambda_1 + \lambda_2)\psi_1 = \lambda_1\psi_1 + \lambda_2\psi_2 \in F \tag{11}$$

where λ_1 and λ_2 are arbitrary complex scalars.

The **scalar product** of two elements $\psi(\mathbf{r})$ and $\phi(\mathbf{r})$ is defined as

$$(\phi, \psi) = \int d^3r \ \phi^*(\mathbf{r})\psi(\mathbf{r}) \tag{12}$$

From this definition follows the following properties

$$(\phi, \psi) = (\psi, \phi)^*, \qquad (\phi, \lambda_1\psi_1 + \lambda_2\psi_2) = \lambda_1(\phi, \psi_1) + \lambda_2(\phi, \psi_2) \tag{13}$$

where λ_1 and λ_2 are arbitrary complex scalars. It is important to note that Shwarz inequality states $|(\psi_1, \psi_2)| \leq \sqrt{(\psi_1, \psi_1)}\sqrt{(\psi_2, \psi_2)}$.

A **linear operator**, A, transforms any function $\psi \in F$ to another function $\psi' \in F$ in a vector space.

$$\psi'(\mathbf{r}) = A\psi(\mathbf{r}), \qquad A[\lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r})] = \lambda_1 A\psi_1(\mathbf{r}) + \lambda_2 A\psi_2(\mathbf{r}) \tag{14}$$

The product of two linear operators, A and B, goes as $(AB)\psi(\mathbf{r}) = A[B\psi(\mathbf{r})]$. The commutator of linear operators is defined as $[A, B] = AB - BA$.

2.1.1 Discrete basis

A countable set of functions $\{u_i(\mathbf{r})\} \subset F$ is orthonormal if

$$(u_i, u_j) = \int d^3r \ u_i^*(\mathbf{r})u_j(\mathbf{r}) = \delta_{ij} \tag{15}$$

The orthonormal set $\{u_i(\mathbf{r})\}$ constitutes a basis of F if every function $\psi(\mathbf{r}) \in F$ can be expanded in one and only one way in terms of $u_i(\mathbf{r})$

$$\psi(\mathbf{r}) = \sum_i c_i u_i(\mathbf{r}), \qquad c_i = (u_i, \psi) \tag{16}$$

The inner product then can be calculated using the representation coefficients of the same basis

$$(\phi, \psi) = \sum_i b_i^* c_i, \qquad (\psi, \psi) = \sum_i |c_i|^2 \tag{17}$$

The closure relation shows that there exists an expansion for every function $\psi(\mathbf{r}) \in F$ in terms of $\{u_i(\mathbf{r})\}$. This is stated

$$\sum_i u_i(\mathbf{r})u_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{18}$$

2.1.2 Continuous basis

All the formulas established for the discrete basis $\{u_i(\mathbf{r})\}$ can be generalized for the continuous basis $\{\xi_{\mathbf{r_0}}(\mathbf{r})\}$. This is particularly relevant to descriptions of plane waves, which have continuous energy eigenstates. Skipping some of the formal description, here's a table of important formulas

	Discrete basis $\{u_i(\mathbf{r})\}$	**Continuous basis** $\{w_\alpha(\mathbf{r})\}$
Orthonormalization relation	$(u_i, u_j) = \delta_{ij}$	$(w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha')$
Closure relation	$\sum_i u_i(\mathbf{r}) u_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$	$\int d\alpha\ w_\alpha(\mathbf{r}) w_\alpha^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$
Expansion of a wave function $\psi(\mathbf{r})$	$\psi(\mathbf{r}) = \sum_i c_i u_i(\mathbf{r})$	$\psi(\mathbf{r}) = \int d\alpha\ c(\alpha) w_\alpha(\mathbf{r})$
Expression for the components of $\psi(\mathbf{r})$	$c_i = (u_i, \psi)$	$c(\alpha) = (w_\alpha, \psi)$
Scalar product	$(\phi, \psi) = \sum_i b_i^* c_i$	$(\phi, \psi) = \int d\alpha\ b^*(\alpha) c(\alpha)$
Square of the norm	$(\psi, \psi) = \sum_i \lvert c_i \rvert^2$	$(\psi, \psi) = \int d\alpha\ \lvert c(\alpha) \rvert^2$

2.2 Dirac notation

To make notation easier, we will write wave functions, operators, and relations in bra-ket notation. We can associate each $\psi(\mathbf{r}) \in F$ to a ket vector $|\psi\rangle \in S_r$. We will then define the dual space of S as S^* and its elements as bra vectors $\langle\phi| \in S^*$. Bra vectors act as linear functionals and applying it on kets go as

$$\chi(\lambda_1 |\psi_1\rangle + \lambda_2 |\psi_2\rangle) = \lambda_1 \langle\chi|\psi_1\rangle + \lambda_2 \langle\chi|\psi_2\rangle \tag{19}$$

where λ_1 and λ_2 are arbitrary complex numbers. Each ket has an accompanying bra.

Applying a bra to a ket is equivalent to taking the scalar product with its associated ket.

$$(|\psi\rangle)^* = \langle\psi|, \qquad \langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle) \tag{20}$$

Linear operations and scalar multiplication function the same way as on functions in state space $\psi(\mathbf{r}) \in F$.

The **projection operator** will take the orthogonal projection of a given vector into another state space.

$$P_q = \sum_{i=1}^{q} |\phi_i\rangle \langle\phi_i| \tag{21}$$

The **adjoint** or **Hermitian conjugate** $A^\dagger$ of a linear operator A is defined by the relations

$$\langle A\psi| = \langle\psi| A^\dagger, \qquad (\langle\psi'| A^\dagger |\psi\rangle)^* = \langle\psi| A |\psi'\rangle \tag{22}$$

An operator A is **Hermitian** if $A = A^\dagger$. All observables are represented by Hermitian operators. Also, note the following identities:

$$(AB)^\dagger = B^\dagger A^\dagger, \qquad P_\psi^\dagger = P_\psi \tag{23}$$

2.3 Representations in the state space

The same relationships established previously can be represented using Dirac notation

$\{\|u_i\rangle\}$ **representation**	$\{\|w_\alpha\rangle\}$ **representation**
$\langle u_i \| u_j \rangle = \delta_{ij}$	$\langle w_\alpha \| w_{\alpha'} \rangle = \delta(\alpha - \alpha')$
$P_{\{u_i\}} = \sum_i \|u_i\rangle \langle u_i\| = I$	$P_{\{w_\alpha\}} = \int d\alpha \ \|w_\alpha\rangle \langle w_\alpha\| = I$

We can represent linear operators with square matrices. Given a linear operator A, we can, in a $\{|u_i\rangle\}$ or $\{|w_\alpha\rangle\}$ basis, associate with it a series of numbers defined by

$$A_{ij} = \langle u_i | A | u_j \rangle , \qquad A(\alpha, \alpha') = \langle w_\alpha | A | w_{\alpha'} \rangle \tag{24}$$

As a result of this, the adjoint of a operator matrix A is its conjugate transpose $A^\dagger = (A^*)^T$. This also implies that the diagonal elements of a Hermitian matrix are always real numbers.

Eigenvalue equations in these vector spaces can thus be written

$$A | \psi \rangle = \lambda | \psi \rangle , \qquad \mathrm{Det}[A - \lambda I] = 0 \tag{25}$$

2.4 Sets of commuting observables

If two operators A and B commute, and if $|\psi\rangle$ is an eigenvector of A, $B|\psi\rangle$ is also an eigenvector of A, with the same eigenvalue. If a is a nondegenerate eigenvalue of A, $|\psi\rangle$ is an eigenvector of B.

$$A(B|\psi\rangle) = a(B|\psi\rangle) \tag{26}$$

If two observables A and B commute, and if $|\psi_1\rangle$ and $|\psi_2\rangle$ are two eigenvectors of A with different eigenvalues, the matrix element $\langle \psi_1 | B | \psi_2 \rangle = 0$.

If two observables A and B commute, one can construct an orthonormal basis of the state space with eigenvectors common to A and B.

2.5 Functions of operators

The function of an operator $F(A)$ can be expanded in a power series like a function of a scalar variable.

$$F(A) = \sum_{n=0}^{\infty} f_n A^n, \qquad e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \mathbb{I} + A + A^2/2! + \dots \tag{27}$$

If $|\psi_a\rangle$ is an eigenvector of A,

$$F(A)|\psi_a\rangle = F(a)|\psi_a\rangle \tag{28}$$

Here are some other useful relations

$$[A, F(A)] = 0, \qquad det(e^X) = e^{Tr(X)}, \qquad A^{-1} = \frac{1}{det(A)} A^\dagger \tag{29}$$

2.6 Unitary operators

An operator U is unitary if $U^\dagger = U^{-1}$. This leads to $U^\dagger U = \mathbb{I}$. An infinitesimal unitary operator can be represented like $U(\epsilon) = \mathbb{I} + \epsilon\ G$ where ϵ is small and G is U's generator. If U is unitary, G must be Hermitian.

2.7 The $\{|r\rangle\}$ and $\{|p\rangle\}$ representations

We'll introduce two bases of F that are particular relevance to wavefunctions.

$$\xi_{\mathbf{r_0}}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r_0}) \Leftrightarrow |\mathbf{r_0}\rangle\,, \qquad v_{\mathbf{p_0}}(\mathbf{r_0}) = (2\pi\hbar)^{-3/2} e^{i\mathbf{p_0}\cdot\mathbf{r}/\hbar} \Leftrightarrow |\mathbf{p_0}\rangle \tag{30}$$

These bases are subject to the same closure and orthonormalization relations as stated for previous bases. Their application on kets produce wavefunctions.

$$\langle\mathbf{r}|\psi\rangle = \psi(\mathbf{r}), \qquad \langle\mathbf{p}|\psi\rangle = \bar{\psi}(\mathbf{p}) \tag{31}$$

We introduce operators which multiply wavefunctions by the underlying variables. $\mathbf{R} = (X, Y, Z)$ is for position space and $\mathbf{P} = (P_x, P_y, P_z)$ is for momentum space. They interact with wavefunctions as follows.

$$\langle\mathbf{r}|\,X\,|\psi\rangle = x\,\langle\mathbf{r}|\psi\rangle\,, \qquad \langle\mathbf{r}|\,Y\,|\psi\rangle = y\,\langle\mathbf{r}|\psi\rangle\,, \qquad \langle\mathbf{r}|\,Z\,|\psi\rangle = z\,\langle\mathbf{r}|\psi\rangle \tag{32}$$

$$\langle\mathbf{p}|\,P_x\,|\psi\rangle = p_x\,\langle\mathbf{r}|\psi\rangle\,, \qquad \langle\mathbf{p}|\,P_y\,|\psi\rangle = p_y\,\langle\mathbf{r}|\psi\rangle\,, \qquad \langle\mathbf{p}|\,P_z\,|\psi\rangle = p_z\,\langle\mathbf{r}|\psi\rangle \tag{33}$$

Here are the commutation relations

$$[R_i, R_j] = 0, \qquad [P_i, P_j] = 0, \qquad [R_i, P_j] = i\hbar\delta_{ij} \tag{34}$$

Some other useful relations

$$\langle\mathbf{r}|\,\mathbf{R}\,|\mathbf{r}'\rangle = \mathbf{r}'\delta(\mathbf{r} - \mathbf{r}'), \qquad \langle\mathbf{p}|\,\mathbf{P}\,|\mathbf{p}'\rangle = \mathbf{p}'\delta(\mathbf{p} - \mathbf{p}') \tag{35}$$

$$\langle\mathbf{r}|\,P_x\,|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(\mathbf{r}), \qquad \langle\mathbf{p}|\,X\,|\psi\rangle = i\hbar\frac{\partial}{\partial p_x}\psi(\mathbf{p}) \tag{36}$$

2.8 Tensor product of state spaces

We will the tensor product to relate two independent spaces E_1 and E_2 with associated vectors $|\phi(1)\rangle$ and $|\chi(2)\rangle$. The tensor state is then denoted $|\phi(1)\chi(2)\rangle = |\phi(1)\rangle \otimes |\chi(2)\rangle$. It is linear with respect to scalar multiplication and distributive with respect to vector addition.

$$[\lambda\,|\phi(1)\rangle] \otimes [|\chi_1(2)\rangle + |\chi_2(2)\rangle] = \lambda[|\phi(1)\rangle \otimes |\chi_1(2)\rangle + |\phi(1)\rangle \otimes |\chi_2(2)\rangle] \tag{37}$$

Subjecting a tensor product to scalar products or operators goes just as you'd expect. Vectors and operators only operate within their own space.

$$\big\langle\phi'(1)\chi'(2)\big|\phi(1)\chi(2)\big\rangle = \big\langle\phi'(1)\big|\phi(1)\big\rangle\,\big\langle\chi'(2)\big|\chi(2)\big\rangle \tag{38}$$

$$(A(1) + B(2))\,|\phi_n(1)\chi_p(2)\rangle = (a_n + b_p)\,|\phi_n(1)\chi_p(2)\rangle \tag{39}$$

3 The Postulates of QM

[CT 211-384]

3.1 The postulates

1. At a fixed time t_0, the state of a physical system is defined by specifying a ket $|\psi(t_0)\rangle$ belonging to the state space S.

2. Every measurable physical quantity A is described by an operator A acting in S; this is an observable.

3. The only possible result of the measurement of a physical quantity A is one of the eigenvalues of the corresponding observable A.

4. When the physical quantity A is measured on a discrete spectrum system in the normalized state $|\psi\rangle$, the probability $P(a_n)$ of obtaining eigenvalue a_n of the corresponding observable A is

$$P(a_n) = \sum_{i=1}^{g_n} |\left\langle u_n^i \middle| \psi \right\rangle|^2 \tag{40}$$

   where g_n is the degree of degeneracy of a_n and $\{\left|u_n^i\right\rangle\}(i = 1, 2, \ldots, g_n)$ is an orthonormal set of vectors which forms a basis in the eigensubspace S_n associated with the eigenvalue a_n of A. For the case of a continuous spectrum,

$$dP(\alpha) = |\left\langle v_\alpha | \psi \right\rangle|^2 d\alpha \tag{41}$$

   where $|v_\alpha\rangle$ is the eigenvector corresponding to the eigenvalue α of the observable A.

5. If the measurement of the physical quantity A on the system in the state $|\psi\rangle$ gives the result a_n, the state of the system immediately after the measurement is the normalized projection, $\frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$, of $|\psi\rangle$ onto the eigensubspace associated with a_n.

6. The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrodinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \tag{42}$$

3.2 Physical implications

The expectation value of some observable A is given by

$$\langle A \rangle_\psi = \langle \psi | A | \psi \rangle \tag{43}$$

The root-mean-square deviation ΔA is given by

$$\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} \tag{44}$$

Solutions to the Schrodinger equation are linearly superposable. We can define a probability density $\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$. We also can define a probability current $\mathbf{J}(\mathbf{r}, t)$ such that

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0 \tag{45}$$

This is analogous to conservation of electrical charge in E/M. $\mathbf{J}(\mathbf{r},t)$ is then defined as the expectation of some r-dependent operator $\mathbf{K}(\mathbf{r})$.

$$\mathbf{J}(\mathbf{r},\mathbf{t}) = \langle\psi|\mathbf{K}(\mathbf{r})|\psi\rangle\,, \qquad \mathbf{K}(\mathbf{r}) = \frac{1}{2m}[|\mathbf{r}\rangle\langle\mathbf{r}|\,\mathbf{P} + \mathbf{P}\,|\mathbf{r}\rangle\langle\mathbf{r}|] \tag{46}$$

We can also derive the evolution of an expectation value of an observable from Schrodinger's equation. This relationship is called Ehrenfest theorem.

$$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle[A,H(t)]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle \tag{47}$$

Applied to basic observables $\mathbf{R}$ and $\mathbf{P}$

$$\frac{d}{dt}\langle\mathbf{R}\rangle = \frac{1}{m}\langle\mathbf{P}\rangle\,, \qquad \frac{d}{dt}\langle\mathbf{P}\rangle = -\langle\nabla V(\mathbf{R})\rangle \tag{48}$$

When H does not depend explicitly on time (conservative), to find $|\psi(t)\rangle$, given $|\psi(t_0)\rangle$,

$$|\psi(t)\rangle = \sum_n\sum_\tau c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}\,|\phi_{n,\tau}\rangle\,, \qquad c_{n,\tau}(t_0) = \langle\phi_{n,\tau}|\phi(t_0)\rangle \tag{49}$$

where each τ is a degenerate state of eigenvalue E_n.

CT derives a time-energy uncertainty relation [CL 250-252]

$$\Delta E\Delta t \geq \hbar \tag{50}$$

3.3 Infinite potential well

$$\phi_n(x) = \sqrt{\frac{2}{a}}sin\Big(\frac{2\pi x}{a}\Big), \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{51}$$

where a is the width of the well and n is any positive integer.

3.4 The density operator

We'll introduce the density operator ρ to make it easier to describe mixtures of states. It can be described as a density matrix ρ_{ij} in some given $\{|u_n\rangle\}$ basis.

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)|\,, \qquad \rho_{ij}(t) = \langle u_i|\,\rho(t)\,|u_j\rangle \tag{52}$$

The density operator has a number of useful properties such as

$$Tr\ \rho(t) = 1, \qquad \langle A\rangle(t) = Tr\ \{A\rho(t)\}, \qquad P(a_n) = Tr\ \{P_n\rho(t)\} \tag{53}$$

where $P(a_n)$ is the probability of measuring a_n and P_n is the projector onto the eigensubspace associated with a_n. Some other properties of $\rho(t)$ include

$$\rho^\dagger(t) = \rho(t), \qquad \rho^2(t) = \rho(t), \qquad Tr\ \rho^2(t) = 1 \tag{54}$$

Now, in a mixture of k states $\{|\psi_i\rangle\}$ with various probabilities $p_1, p_2, \dots$ we define the general ρ as

$$\rho = \sum_k p_k \rho_k \tag{55}$$

We can also use a density operator to describe the behavior of a global system $S = S(1) \otimes S(2)$. The operator matrix is formed in a basis $\{|\psi(1)\phi(1)\rangle, |\psi(1)\phi(2)\rangle, |\psi(2)\phi(1)\rangle, \dots\}$. We then define partial traces as

$$\rho(1) = Tr_2\{\rho\}, \qquad \langle A(1)\rangle = Tr\ \{\rho(1)A(1)\} \tag{56}$$

4 Application of postulates to simple cases: spin 1/2 and two-level systems

[CT 385-480]

The Stern-Gerlach apparatus is used to study the deflection of a beam of neutral paramagnetic atoms in an inhomogenous magnetic field. We assume that the magnetic field acts exclusively in one cartesian direction (usually $+\hat{z}$). Here's equations for the potential energy in a $\mathbf{B}$ field.

$$W = -\mathbf{M}\cdot\mathbf{B}, \qquad \mathbf{M} = \gamma s, \qquad \mathbf{F} = \nabla(\mathbf{M}\cdot\mathbf{B}) \tag{57}$$

where $\mathbf{M}$ is the magnetization of the particle, γ is the gyromagnetic ratio of the particle, and s is the spin (usually $\pm\hbar/2$ for a spin 1/2 particle).

4.1 Theoretical description

We'll introduce an observable S_z, which has two eigenvalues $\pm\hbar/2$. We'll associate these eigenvalues with two orthonormal, non-degenerate eigenvectors $|+\rangle_z$ and $|-\rangle_z$.

$$S_z|\pm\rangle_z = \pm\frac{\hbar}{2}|\pm\rangle_z, \qquad (S_z) = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{58}$$

There are other spin observables, for both the x and y direction as well as some arbitrary u direction. Here they are in the $\{|\pm\rangle_z\}$ basis

$$(S_x) = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad (S_y) = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad (S_u) = \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\phi}\\ \sin\theta e^{i\phi} & -cos\theta\end{pmatrix} \tag{59}$$

where θ and ϕ are from spherical coordinates. It is also useful to note the basis eigenvectors of these operators.

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}[|+\rangle_z \pm |-\rangle_z], \qquad |\pm\rangle_y = \frac{1}{\sqrt{2}}[|+\rangle_z \pm i|-\rangle_z] \tag{60}$$

$$|+\rangle_u = \cos\frac{\theta}{2}e^{-i\phi/2}|+\rangle_z + \sin\frac{\theta}{2}e^{i\phi/2}|-\rangle_z, \qquad |-\rangle_u = -\sin\frac{\theta}{2}e^{-i\phi/2}|+\rangle_z + \cos\frac{\theta}{2}e^{i\phi/2}|-\rangle_z \tag{61}$$

The expectation value of S_i given an arbitrary state $|+\rangle_u$ is derived by CT

$$\langle S_x\rangle_u = \frac{\hbar}{2}\sin\theta\cos\phi, \qquad \langle S_y\rangle_u = \frac{\hbar}{2}\sin\theta\sin\phi, \qquad \langle S_z\rangle_u = \frac{\hbar}{2}\cos\theta \tag{62}$$

4.2 Evolution in a uniform magnetic field

The Hamiltonian which describes the evolution of the spin of the atom in the field $\mathbf{B_0}$ is given by

$$H = \omega_0 S_z, \qquad \omega_0 = -\gamma B_0 \tag{63}$$

Since this operator is time-independent, we can derive the time-dependence of the wave function as described in chapter 3. For an arbitrarily polarized particle, it's $\psi(t)$ is

$$|\psi(t)\rangle = \cos\frac{\theta}{2}e^{-i(\phi+\omega_0 t)/2}|+\rangle_z + \sin\frac{\theta}{2}e^{i(\phi+\omega_0 t)/2}|-\rangle_z \tag{64}$$

This system is defined by the polar angles $\theta(t) = \theta$ and $\phi(t) = \phi + \omega_0 t$. The polarization vector rotates around the z-axis. This movement is called Larmor precession.

4.3 Spin 1/2 density matrix

The density matrix of an arbitrary polarized, pure system of particles is given

$$\rho(\theta,\phi) = \begin{pmatrix} \cos^2\frac{\theta}{2} & \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{i\phi} & \sin^2\frac{\theta}{2} \end{pmatrix} \tag{65}$$

The most common problem is the case of unpolarized spin, in which the density matrix is given by

$$\rho = \frac{1}{4\pi}\int d\Omega\ \rho(\theta,\phi) = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\ d\theta\ \rho(\theta,\phi) \tag{66}$$

5 The one-dimensional harmonic oscillator

[CT 481-639]

5.1 Quantum mechanical Hamiltonian

The classical quantities x and p are replaced by the observables X and P which satisfy $[X,P] = i\hbar$.

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \tag{67}$$

Important derivations from this Hamiltonian are that (i) its eigenvalues are positive, (ii) its eigenfunctions have a definite parity, and (iii) the energy spectrum is discrete. We will redefine the Hamiltonian in terms of raising and lowering operators. First, let's introduce some useful notation.

$$\hat{X} = \sqrt{\frac{m\omega}{\hbar}}X, \qquad \hat{P} = \frac{1}{\sqrt{m\hbar\omega}}P, \qquad \hat{H} = \frac{1}{\hbar\omega}H = \frac{1}{2}(\hat{X}^2 + \hat{P}^2) \tag{68}$$

where $[\hat{X}, \hat{P}] = i$. We use these to define the raising and lowering operators.

$$a = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}), \qquad a^\dagger = \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}), \qquad \hat{X} = \frac{1}{\sqrt{2}}(a^\dagger + a), \qquad \hat{P} = \frac{i}{\sqrt{2}}(a^\dagger - a) \tag{69}$$

where $[a, a^\dagger] = 1$. We then see that $\hat{H}$ can be written as

$$\hat{H} = a^\dagger a + \frac{1}{2} = aa^\dagger - \frac{1}{2} \tag{70}$$

5.2 Eigenstates

CT does all the heavy lifting in proving lemmas about this Hamiltonian in 491-501. He shows that the eigenstates $|\psi_n\rangle$ are discrete, $n \in \mathbb{R}$, and non-degenerate. Therefore H forms a C.S.C.O.. Orthonormalization and closure relations are given by the typical forms

$$\langle\psi_{n'}|\psi_n\rangle = \delta_{nn'}, \qquad \sum_n |\psi_n\rangle \langle\psi_n| = 1 \tag{71}$$

The action of various operators are as follows

$$H|\psi_n\rangle = \hbar\omega\Big(n + \frac{1}{2}\Big)|\psi_n\rangle, \qquad a^\dagger|\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle, \qquad a|\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle \tag{72}$$

It immediately follows that the energy spectrum is $E_n = \Big(n + \frac{1}{2}\Big)\hbar\omega$.

The actions of X and P can be easily derived from their definitions above. CT gives the general form for the eigenstates in the x basis as

$$\psi_n(x) = \langle x|\psi_n\rangle = \Big[\frac{1}{2^n n!}\Big(\frac{\hbar}{m\omega}\Big)^n\Big]^{1/2}\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}\Big[\frac{m\omega}{\hbar}x - \frac{d}{dx}\Big]^n e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{73}$$

The first few states are

$$\psi_0(x) = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}, \qquad \psi_1(x) = \Big[\frac{4}{\pi}\Big(\frac{m\omega}{\hbar}\Big)^3\Big]^{1/4} x e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}, \tag{74}$$

$$\psi_2(x) = \Big(\frac{m\omega}{4\pi\hbar}\Big)^{1/4}\Big[2\frac{m\omega}{\hbar}x^2 - 1\Big]e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} \tag{75}$$

Expectation values can be calculated in the standard way. Some highlights:

$$\Delta X \Delta P = \Big(n + \frac{1}{2}\Big)\hbar, \qquad \frac{d}{dt}\langle X\rangle = \frac{\langle P\rangle}{m}, \qquad \frac{d}{dt}\langle P\rangle = -m\omega^2\langle X\rangle \tag{76}$$

5.3 Two coupled harmonic oscillators

Consider two particles of the same mass m moving in harmonic oscillators and connected by a third, coupling oscillator.

$$H = T + U, \qquad T = \frac{1}{2m}(P_1^2 + P_2^2), \qquad U = \frac{1}{2}m\omega^2[(X_1 - a)^2 + (X_2 + a)^2 + 2\lambda(X_1 - X_2)^2] \tag{77}$$

We define new operators which commute to define vibrational states. This eliminates the coupling. [CT 575-580] derives these by finding eigenstates from the classical equations of motion.

$$X_G = \frac{1}{2}(X_1 + X_2), \qquad P_G = P_1 + P_2, \qquad X_R = X_1 - X_2, \qquad P_R = \frac{1}{2}(P_1 - P_2) \tag{78}$$

where $[X_G, X_R] = [P_G, P_R] = [X_G, P_R] = [X_R, P_G] = 0$ and $[X_G, P_G] = [X_R, P_R] = i\hbar$. We can create an un-coupled Hamiltonian.

$$H = H_G + H_R + m\omega^2 a^2 \frac{4\lambda}{1+4\lambda}, \qquad H_G = \frac{P_G^2}{2\mu_G} + \frac{1}{2}\mu_G \omega_G^2 X_G^2, \qquad H_R = \frac{P_R^2}{2\mu_R} + \frac{1}{2}\mu_R \omega_R^2 \Big[X_R - \frac{2a}{1+4\lambda}\Big]^2 \tag{79}$$

where $\mu_G = 2m$, $\mu_R = m/2$, $\omega_G = \omega$, and $\omega_R = \omega\sqrt{1+4\lambda}$. From these we can derive $a_G^\dagger$ and $a_R^\dagger$ which act on states $|\psi_{n,p}\rangle = |\psi_n^G\rangle\,|\psi_p^R\rangle$ just as a normal harmonic oscillator wood. I will skip the derivations, as they are quite long, but the energies are described as

$$E_{n,p} = \Big(n + \frac{1}{2}\Big)\hbar\omega_G + \Big(p + \frac{1}{2}\Big)\hbar\omega_R + m\omega^2 a^2 \frac{4\lambda}{1+4\lambda} \tag{80}$$

which is equivalent to the energies of two uncoupled harmonic oscillators plus a constant.

5.4 Chain of coupled harmonic oscillators

Consider an infinite chain of identical one-dimensional harmonic oscillators denoted by positions X_q and momenta P_q. The Hamiltonian is represented by

$$H = V + \sum_q H_q, \qquad H_q = \frac{1}{2}m\omega^2 X_q^2 + \frac{1}{2m}P_q^2, \qquad V = \frac{1}{2}m\omega_1^2 \sum_q (X_q - X_{q+1})^2 \tag{81}$$

We'll introduce the operators $\Xi(k)$ and $\Pi(k)$

$$\Xi(k) = \sum_q X_q e^{-iqkl}, \qquad \Pi(k) = \sum_q P_q e^{-iqkl} \tag{82}$$

where l is the distance between successive oscillators.

$$\Xi(-k) = \Xi^\dagger(k), \qquad \Pi(-k) = \Pi^\dagger(k), \qquad [\Xi(k), \Pi^\dagger(k')] = i\hbar\frac{2\pi}{l}\delta(k-k') \tag{83}$$

We can then derive ladder operators

$$a^\dagger(k) = \frac{1}{\sqrt{2}}\Big[\beta(k)\Xi^\dagger(k) - \frac{i}{\hbar\beta(k)}\Pi^\dagger(k)\Big], \qquad \beta(k) = \sqrt{\frac{m\Omega(k)}{\hbar}} \tag{84}$$

where $\Omega(k)$ is the dispersion relation. This quantity determines the phase and group velocity of waves in the chain.

$$\Omega(k) = \sqrt{\omega^2 + 4\omega_1^2 \sin^2\Big(\frac{kl}{2}\Big)}, \qquad v_\phi(k) = \frac{\Omega(k)}{k}, \qquad v_G(k) = \frac{d\Omega(k)}{dk} \tag{85}$$

Lastly, we can derive a Hamiltonian

$$H = \frac{l}{2\pi}\int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} dk\ H'(k), \qquad H'(k) = \frac{1}{2}\hbar\Omega(k)[a(k)a^\dagger(k) + a^\dagger(k)a(k)] \tag{86}$$

Stationary states in the presence of coupling are difficult to derive (even by CT standards).

Normal modes in a crystal are called phonons. We choose $\omega = 0$ because the atoms are not elastically bound to their equilibrium positions. For a phonon in the Debye model,

$$E(k_j) = \hbar\Omega(k_j), \qquad k_j = \frac{2\pi j}{Nl}, \qquad -\frac{N}{2} + 1 \leq j \leq \frac{N}{2} \tag{87}$$

5.5 One dimensional harmonic oscillator in thermodynamic equilibrium

The density operator for a statistical mixture of stationary states in thermodynamic equilibrium at temperature T is

$$\rho = Z^{-1} e^{-\frac{H}{kT}}, \qquad Z = Tr\ e^{-\frac{H}{kT}} \tag{88}$$

For a harmonic oscillator, $E_n = (n + 1/2)\hbar\omega$.

$$Z = \sum_{n=0}^{\infty} e^{-(n+1/2)\frac{\hbar\omega}{kT}} = \frac{e^{-\frac{\hbar\omega}{2kT}}}{1 - e^{-\frac{\hbar\omega}{kT}}} \tag{89}$$

$$\langle H \rangle = Tr(H\rho) = kT^2 \frac{1}{Z}\frac{dZ}{dT} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1} \tag{90}$$

For a solid composed of N independently vibrating atoms with the same angular frequency ω_E

$$U = 3N \langle H \rangle, \qquad c_V = \frac{dU}{dT} = 3N\frac{d}{dT}\langle H \rangle \tag{91}$$

6 General properties of angular momentum in QM

[CT 641-771]

6.1 General angular momentum J

We'll define a general angular momentum $\mathbf{J}$ as any set of three observables J_x, J_y, J_z which satisfies.

$$[J_x, J_y] = i\hbar J_z, \qquad [J_y, J_z] = i\hbar J_x, \qquad [J_z, J_x] = i\hbar J_y, \qquad [J_i, J_j] = i\hbar\epsilon_{ijk}J_k \tag{92}$$

Then we'll introduce $\mathbf{J}^2$

$$\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2, \qquad [\mathbf{J}^2, \mathbf{J}] = 0 \tag{93}$$

We'll therefore seek a system of eigenvectors common to $\mathbf{J}^2$ and J_z. We'll introduce J_+ and J_- which act analogous to operators a and $a^\dagger$ from the harmonic oscillator.

$$J_+ = J_x + iJ_y, \qquad J_- = J_x - iJ_y, \qquad [J_z, J_\pm] = \pm\hbar J_\pm, \qquad [J_+, J_-] = 2\hbar J_z \tag{94}$$

$$\mathbf{J^2} = \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2, \qquad [\mathbf{J}^2, J_\pm] = [\mathbf{J}^2, J_z] = 0 \tag{95}$$

[CT 647-655] proves eigenvalue relationships for the eigenvectors $|k, j, m\rangle$.

$$\mathbf{J}^2 |k, j, m\rangle = j(j+1)\hbar^2 |k, j, m\rangle, \qquad J_z |k, j, m\rangle = m\hbar |k, j, m\rangle \tag{96}$$

where $j \geq 0$ by convention. $-j \leq m \leq j$. Lastly, k is an index we'll ignore for now, but is necessary to form a C.S.C.O.

$$J_\pm \left|k,j,m\right\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\left|k,j,m\pm 1\right\rangle, \qquad J_- \left|k,j,-j\right\rangle = 0, \qquad J_+ \left|k,j,j\right\rangle = 0 \tag{97}$$

We can write matrices representing the angular momentum operators in the standard way $A_{ij} = \langle\psi_i| A |\psi_j\rangle$. For $j = 1/2$,

$$(J_z)^{(1/2)} = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad (J_x)^{(1/2)} = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad (J_y)^{(1/2)} = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{98}$$

$J_\pm$ and $\mathbf{J}^2$ can be derived from these and the definitions above.

6.2 Orbital angular momentum L

The orbital angular momentum $\mathbf{L}$ is defined as

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}, \qquad [L_x, L_y] = i\hbar L_z, \qquad [L_y, L_z] = i\hbar L_x, \qquad [L_z, L_x] = i\hbar L_y \tag{99}$$

In the $\{|\mathbf{r}\rangle\}$ representation, the observables $\mathbf{R}$ and $\mathbf{P}$ correspond to $\mathbf{r}$ and $\frac{\hbar}{i}\nabla$, respectively.

$$L_x = \frac{\hbar}{i}\Big(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\Big), \qquad L_y = \frac{\hbar}{i}\Big(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\Big), \qquad L_z = \frac{\hbar}{i}\Big(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\Big) \tag{100}$$

In spherical coordinates, these are

$$L_x = i\hbar\Big(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\Big), \qquad L_y = i\hbar\Big(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\Big), \qquad L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \tag{101}$$

These yield

$$\mathbf{L}^2 = -\hbar^2\Big(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big), \qquad L_\pm = \hbar\, e^{\pm i\phi}\Big(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\Big) \tag{102}$$

The eigenstates of $\mathbf{L}^2$ and L_z are the angle-dependent spherical harmonics $Y_l^m(\theta,\phi)$.

$$\mathbf{L}^2\ Y_l^m(\theta,\phi) = l(l+1)\hbar^2\ Y_l^m(\theta,\phi), \qquad L_z\ Y_l^m(\theta,\phi) = m\hbar\ Y_l^m(\theta,\phi) \tag{103}$$

The full equation for spherical harmonics include radial functions $\psi(\mathbf{r}) = R_{k,l}(r)Y_l^m(\theta,\phi)$. Both behave as orthonormal functions.

$$\int_0^\infty r^2\ dr\ R_{k,l}^*(r)\ R_{k',l}(r) = \delta_{kk'}, \qquad \int_\Omega d\Omega\ Y_l^{m*}(\theta,\phi)\ Y_{l'}^{m'}(\theta,\phi) = \delta_{ll'}\delta_{mm'} \tag{104}$$

We can write any arbitrary wave function in terms of these eigenfunctions.

$$\psi(\mathbf{r}) = \sum_{l,m} a_{l,m}(r)Y_l^m(\theta,\phi), \qquad a_{l,m}(r) = \sum_k c_{k,l,m}R_{k,l}(r) \tag{105}$$

We can describe wavefunctions in terms of r-dependent coefficients, $a_{l,m}(r)$, or constant coefficients, $c_{k,l,m}$. These are calculated by

$$c_{k,l,m} = \int d^3r\ \psi^*_{k,l,m}(\mathbf{r})\ \psi(\mathbf{r}), \qquad a_{l,m}(r) = \int d\Omega\ Y_l^{m*}(\theta,\phi)\ \psi(r,\theta,\phi) \tag{106}$$

We can calculate probabilities of measuring eigenvalues.

$$P_{\mathbf{L}^2,L_z}(l,m) = \sum_k |c_{k,l,m}|^2 = \int_0^\infty r^2\ dr\ |a_{l,m}(r)|^2 \tag{107}$$

6.3 Spherical Harmonics

The general formula for spherical harmonics is

$$Y_l^m(\theta,\phi) = \frac{(-1)^{l+m}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}(\sin\theta)^m\frac{d^{l+m}}{d(\cos\theta)^{l+m}}(\sin\theta)^{2l} \tag{108}$$

The first couple are

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \qquad Y_1^{\pm1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\ e^{\pm i\phi}, \qquad Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{109}$$

Spherical harmonics satisfy parity such that they are symmetrical with respect to the origin of the reference frame. Also, they are complex-valued functions.

$$\psi_{k,l,m}(\mathbf{r}) = \psi_{k,l,m}(-\mathbf{r}), \qquad [Y_l^m(\theta,\phi)]^* = (-1)^m Y_l^{-m}(\theta,\phi) \tag{110}$$

6.4 Angular momentum and rotations

Rotations are one-to-one transformations of three-dimensional space which conserves distances and angles as well as handedness of reference frames. Rotation operators in state space, R, are linear, unitary, and form a complete representation across the rotation group. Infinitesimal rotation operators can be represented simply as

$$R_{\hat{\mathbf{z}}}(d\alpha) = 1 - \frac{i}{\hbar}\ d\alpha\ L_z, \qquad R_{\mathbf{u}}(d\alpha) = 1 - \frac{i}{\hbar}\ d\alpha\ \mathbf{L}\cdot\mathbf{u} \tag{111}$$

where $\mathbf{u}$ is an arbitrary rotation axis and $d\alpha$ is an infinitesimal rotation angle. Finite rotation operators are represented by exponentials, which can be expanded in a power series.

$$R_{\hat{\mathbf{z}}}(\alpha) = e^{-\frac{i}{\hbar}\alpha\ L_z}, \qquad R_{\mathbf{u}}(\alpha) = e^{-\frac{i}{\hbar}\alpha\ \mathbf{L}\cdot\mathbf{u}} \tag{112}$$

The general transformation law for observables is $A' = RAR^\dagger$.

In the special cases of an infinitesimal rotation,

$$A' = A - \frac{i}{\hbar}\ d\alpha\ [\mathbf{J}\cdot\mathbf{u}, A] \tag{113}$$

An observable A is said to be scalar if

$$A' = A, \qquad [A, \mathbf{J}] = \mathbf{0} \tag{114}$$

A vector operator $\mathbf{W}$ is one which satisfies

$$[W_i, J_j] = i\hbar\ \epsilon_{ijk} W_k \tag{115}$$

where ϵ_{ijk} is the 3d Levi-Civita symbol. For reference, the cross product of two vector operators is given as

$$(\mathbf{A} \times \mathbf{B})_k = \epsilon_{ijk}\ A_i B_j \tag{116}$$

A key consequence of these relations is that the Hamiltonian of an isolated physical system is a scalar observable, $[H, \mathbf{J}] = 0$.

6.5 Angular momentum of stationary states of a two-dimensional harmonic oscillator

We'll define a two-dimensional harmonic oscillator in the standard way,

$$H_{xy} = H_x + H_y, \qquad H_x = \frac{P_x^2}{2\mu} + \frac{1}{2}\mu\omega^2 X^2 \tag{117}$$

where μ is the reduced mass of the object(s) in question.

It'll prove convenient to use the operators a_x and a_y,

$$a_x = \frac{1}{\sqrt{2}}\Big(\beta X + i\frac{P_x}{\beta\hbar}\Big), \qquad a_y = \frac{1}{\sqrt{2}}\Big(\beta Y + i\frac{P_y}{\beta\hbar}\Big), \qquad \beta = \sqrt{\frac{\mu\omega}{\hbar}} \tag{118}$$

This enables us to write H_{xy} in the form

$$H_{xy} = H_x + H_y = (N_x + N_y + 1)\hbar\omega, \qquad N_x = a_x^\dagger a_x, \qquad N_y = a_y^\dagger a_y \tag{119}$$

However, this poses a problem: **$\mathbf{H_{xy}}$ does not constitute a C.S.C.O.**

$$E_{xy} = (n_x + n_y + 1)\hbar\omega = (n+1)\hbar\omega, \qquad n = n_x + n_y \tag{120}$$

Instead, we introduce the L_z component of the angular momentum to eliminate this degeneracy.

$$L_z = XP_y - YP_x, \qquad [H_{xy}, L_z] = 0 \tag{121}$$

In order to more easily describe a basis of eigenvectors common to H_{xy} and L_z, we introduce the right and left circular quanta operators a_d and a_g,

$$a_d = \frac{1}{\sqrt{2}}(a_x - ia_y), \qquad a_g = \frac{1}{\sqrt{2}}(a_x + ia_y) \tag{122}$$

These operate as standard ladder operators in independent spaces, $[a_d, a_g] = 0$, $[a_d, a_d^\dagger] = 1$, and so on. These allow us to write

$$H_{xy} = (N_d + N_g + 1)\hbar\omega, \qquad L_z = \hbar(N_d - N_g), \qquad N_d = a_d^\dagger a_d, \qquad N_g = a_g^\dagger a_g \tag{123}$$

H_{xy} and L_z form a C.S.C.O

$$H_{xy} = (n+1)\hbar\omega, \qquad L_z = \hbar m, \qquad n = n_d + n_g, \qquad m = n_d - n_g \tag{124}$$

The first couple wave functions in position space are given as χ_{n_d,n_g},

$$\chi_{0,0}(\rho) = \frac{\beta}{\sqrt{\pi}} e^{-\beta^2\rho^2/2}, \qquad \chi_{1,0} = \frac{\beta}{\sqrt{\pi}} \beta\rho e^{-\beta^2\rho^2/2} e^{i\phi}, \qquad \chi_{0,1} = \frac{\beta}{\sqrt{\pi}} \beta\rho e^{-\beta^2\rho^2/2} e^{-i\phi} \tag{125}$$

7 Particle in a Central Potential: The Hydrogen Atom

[CT 773-871]

7.1 Stationary states in a central potential

For a radially-dependent potential, $V(r)$, we can put the Hamiltonian in the form

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{2\mu r^2}\mathbf{L}^2 + V(r), \qquad [H, \mathbf{L}] = [H, \mathbf{L}^2] = 0 \tag{126}$$

These are solved by $\phi_{k,l,m}$ and have the following eigenvalues.

$$\phi_{k,l,m}(\mathbf{r}) = R_{k,l}(r) Y_l^m(\theta, \phi), \qquad \mathbf{L}^2\phi(\mathbf{r}) = l(l+1)\hbar^2\phi(\mathbf{r}), \qquad L_z\phi(\mathbf{r}) = m\hbar\phi(\mathbf{r}) \tag{127}$$

H, $\mathbf{L}^2$, and L_z make up a C.S.C.O.

7.2 Motion of the center of mass for a system of two interacting particles

The Hamiltonian of two particles, $\mathbf{R_1}$ and $\mathbf{R_2}$, under a potential $V(\mathbf{R_1} - \mathbf{R_2})$ can be treated like a relative particle.

$$M = m_1 + m_2, \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} \tag{128}$$

$$\mathbf{R}_G = \frac{m_1\mathbf{R}_1 + m_2\mathbf{R}_2}{m_1 + m_2}, \qquad \mathbf{R} = \mathbf{R_1} - \mathbf{R_2}, \qquad \mathbf{P}_G = \mathbf{P}_1 + \mathbf{P}_2, \qquad \mathbf{P} = \frac{m_2\mathbf{P}_1 - m_1\mathbf{P}_2}{m_1 + m_2} \tag{129}$$

We can then write the Hamiltonian as

$$H = \frac{\mathbf{P}_G^2}{2M} + \frac{\mathbf{P}^2}{2\mu} + V(\mathbf{R}) \tag{130}$$

Total angular momentum parallels nicely too.

$$\mathbf{J} = \mathbf{L}_G + \mathbf{L}, \qquad \mathbf{L}_G = \mathbf{R}_G \times \mathbf{P}_G, \qquad \mathbf{L} = \mathbf{R} \times \mathbf{P} \tag{131}$$

7.3 The Hydrogen Atom

The hydrogen atom consists of a proton m_p and electron m_e ($m_e \ll m_p$) interacting under electric potential.

$$V(r) = -\frac{q^2}{4\pi\epsilon_0}\frac{1}{r} = -\frac{e^2}{r}, \qquad \mu = \frac{m_e m_p}{m_e + m_p} \simeq m_e\Big(1 - \frac{m_e}{m_p}\Big) \tag{132}$$

This leads to a Hamiltonian as a function of r, the distance between the proton and electron.

$$\Big[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{r}\Big]u_{k,l}(r) = E_{k,l}u_{k,l}(r), \qquad \phi_{k,l,m}(\mathbf{r}) = \frac{1}{r}u_{k,l}(r)Y_l^m(\theta,\phi) \tag{133}$$

where $k > |l|$. This gives energies of

$$E_{k,l} = -\frac{E_I}{n^2}, \qquad n = k + l \qquad E_I = \frac{\mu e^4}{2\hbar^2}, \qquad g_n = n^2 \tag{134}$$

where g_n is the degeneracy of each energy level. The first energy level has $g_1 = 1$ degeneracy and is given by

$$\phi_{1,0,0} = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}, \qquad a_0 = \frac{\hbar^2}{\mu e^2} \tag{135}$$

7.4 The isotropic three-dimensional harmonic oscillator

The three-dimensional harmonic oscillator is an extension of the two-dimensional case with

$$V(r) = \frac{1}{2}\mu\omega^2(x^2+y^2+z^2) = \frac{1}{2}\mu\omega^2 r^2, \qquad E_{k,l} = \hbar\omega(n+\frac{3}{2}), \qquad n = k+l, \qquad g_n = \frac{1}{2}(n+1)(n+2) \tag{136}$$

We can define the Hamiltonian H using the ladder operators from the two-dimensional harmonic oscillator.

$$N_d = a_d^\dagger a_d, \qquad N_g = a_g^\dagger a_g, \qquad N_z = a_z^\dagger a_z, \qquad H = \hbar\omega(N_d + N_g + N_z + \frac{3}{2}) \tag{137}$$

$$L_z = \hbar(N_d - N_g), \qquad L_+ = \hbar\sqrt{2}(a_z^\dagger a_g - a_d^\dagger a_z), \qquad L_- = \hbar\sqrt{2}(a_g^\dagger a_z - a_z^\dagger a_d) \tag{138}$$

7.5 Probability currents

The general equation for probability current of a charged particle in a magnetic field is

$$\mathbf{J}(\mathbf{r},t) = \frac{1}{2m}\Big[\psi^*\Big(\frac{\hbar}{i}\nabla - q\mathbf{A}\Big)\psi + \psi\Big(-\frac{\hbar}{i}\nabla - q\mathbf{A}\Big)\psi^*\Big] \tag{139}$$

Under the conditions $\mathbf{A}(\mathbf{r}) = \frac{1}{2}(\mathbf{r}\times\mathbf{B})$ and $l = 0$,

$$\mathbf{J}(\mathbf{r}) = \frac{\omega_c}{2}\rho(\mathbf{r})\hat{\mathbf{r}}\times\mathbf{r}, \qquad \omega_c = -\frac{qB}{\mu} \tag{140}$$

7.6 Hydrogen atom in a uniform magnetic field

We can write the Hamiltonian of a spinless particle subjected to a scalar central potential and constant magnetic field

$$H = H_0 + H_1 + H_2, \qquad H_0 = \frac{\mathbf{P}^2}{2m_e} + V(\mathbf{R}), \qquad H_1 = -\frac{\mu_B}{\hbar}\mathbf{L}\cdot\mathbf{B}, \qquad H_2 = \frac{q^2\mathbf{B}^2}{8\mu}{\mathbf{R}_\perp}^2 \tag{141}$$

$$\mu_B = \frac{q\hbar}{2\mu}, \qquad \mathbf{R}_\perp^2 = \mathbf{R}^2 - \frac{(\mathbf{R}\cdot\mathbf{B})^2}{\mathbf{B}^2} \tag{142}$$

If $\mathbf{B} = B_0\hat{\mathbf{z}}$,

$$H_1 = -\frac{\mu_B B_0}{\hbar} L_z, \qquad H_2 = \frac{q^2 B_0^2}{8\mu}(X^2 + Y^2) \tag{143}$$

μ_B is called the Bohr magneton. H_1 is the paramagnetic term while H_2 is the diamagnetic term. Typically, $H_1 \gg H_2$, but $H_1 = 0$ if $l = 0$ so the diamagnetic term is more prominent in states with zero angular momentum.