Quantum Physics Key Formulae

Postulates - Coordinate Space

1. The quantum state for a system of N particles is given by a wavefunction, which determines everything that can be known about the system. The wavefunction must be:
    - A solution to the Schrodinger equation
    - Normalizable
    - Continuous in x and have a continuous derivative

2. The time evolution of the wavefunction is given by the Schrodinger equation:
$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\right]\Psi(x,t)$$

3. The wavefunction represents the probability amplitude for finding a particle at a given point in space at a given time:
$$\int_{-\infty}^{\infty}\Psi^*(x)\Psi(x)\,dx = \int_{-\infty}^{\infty}|\Psi(x)|^2\,dx = 1$$

4. With every physical observable q there is a Hermitian operator $\hat{Q}$, of which the wavefunctions are eigenfunctions and definite values are eigenvalues:
$$\hat{Q}\psi_i = q_i\psi_i$$

5. Thus the expected value of q is given by:
$$\langle q\rangle = \int \Psi^*\hat{Q}\Psi\,dr$$

6. The eigenfunctions of any Hermitian operator form a complete basis for the space of all wavefunctions:
$$\Psi(r,t) = \sum_n c_n(t)\psi_n(r) + \int c_A(t)\psi_A(r)\,dA$$

Postulates - State Vector

1. Each physical system is associated with a complex Hilbert space. States of that system are represented by one-dimensional abstract vectors of length one:
$$\int \left||\psi\rangle\right|^2 dx = 1$$

2. The Schrödinger equation is now written:
$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

3. Physical observables are represented by Hermitian matrices which act on these states:
$$H|\psi\rangle = E|\psi\rangle$$

4. The expectation value of the observable A is given by:
$$\langle A\rangle = \langle\psi|A|\psi\rangle$$

Delta Function

Some important delta function relations:

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1$$
$$\int_{-\infty}^{\infty} f(t)\delta(t-T)\, dt = f(T)$$

Operators

- Hermitian property: $\langle\Psi|\hat{Q}\Psi\rangle = \langle\hat{Q}\Psi|\Psi\rangle$
- Position: $\hat{x} = x$
- Momentum: $\hat{p}_x = -i\hbar\frac{\partial}{\partial x} = -i\hbar\nabla$
- Total energy: $\hat{E} = i\hbar\frac{\partial}{\partial t}$
- Hamiltonian: $\hat{H} = \frac{\hat{p}^2}{2m} + V = \hat{T} + \hat{V}$
- Kinetic energy: $\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = -\frac{\hbar^2}{2m}\nabla^2$
- Time evolution: $\Psi_n(r,t) = e^{-\frac{iHt}{\hbar}}\Psi_n(r,0) = e^{-\frac{iE_n t}{\hbar}}\psi_n(r)$
- Angular momentum: $\hat{L}_x = yp_z - zp_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$
- Angular momentum: $\hat{L}_y = zp_x - xp_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$
- Angular momentum: $\hat{L}_z = xp_y - yp_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

Basic Wavefunction Equations

Wavefunctions:

$$\Psi(x) = \sum c_n\psi_n(x)$$
$$\Psi(x,t) = \sum c_n\psi_n(x)e^{-\frac{iE_n t}{\hbar}}$$

Normalisation:

$$\int \psi_m^*(x)\psi_n(x)\, dx = \delta_{mn}$$
$$\sum|c_n|^2 = 1$$
$$c_n = \int \psi_n^*(x)\Psi(x)\, dx$$

Operators:

$$\langle\hat{H}\rangle = \int \Psi^*(x)\hat{H}\Psi(x)\, dx = \sum|c_n|^2 E_n$$

Bra-ket Notation

Basic properties:

$$\langle\psi_a,\psi_n\rangle = \langle a|b\rangle = \int \psi_a^*(r)\psi_b(r)\, dr$$
$$\langle\psi_a,\psi_n\rangle = \langle\psi_b,\psi_a\rangle^*$$
$$\langle\psi,\psi_a+\psi_b\rangle = \langle\psi,\psi_a\rangle + \langle\psi,\psi_b\rangle$$
$$\langle\psi_a,\alpha\psi_b\rangle = \alpha\langle\psi_a,\psi_b\rangle$$
$$\langle\psi_a,\psi_b\rangle = \delta_{ab}$$

Eigenvalues:

$$\psi_a(r) = \langle r|a\rangle = \langle a|r\rangle^*$$
$$\langle a|\hat{A}^\dagger|b\rangle = \langle b|\hat{A}|a\rangle^*$$
$$|a\rangle = \sum c_n|n\rangle$$
$$c_n = \langle\psi_n|\Psi\rangle$$
$$\langle m|a\rangle = \sum c_n\langle m|n\rangle$$
$$\langle A\rangle = \langle a|\hat{A}|a\rangle$$

Inserting a complete set of states:

$$\sum|n\rangle\langle n| = \int |A\rangle\langle A|\, dA = 1$$

$$\begin{aligned}\langle a|b\rangle &= \langle a|1|b\rangle \\ &= \langle a|\left(\int |r\rangle\langle r|\, d^3r\right)|b\rangle \\ &= \int \langle a|r\rangle\langle b|r\rangle\, d^3r\end{aligned}$$

$$\langle a|b\rangle = \int \psi_a(r)\psi_b(r)\, d^3r$$

Raising and lowering operators:

$$\hat{a}^\dagger\hat{a}|\lambda\rangle = \lambda|\lambda\rangle$$
$$[\hat{a}, \hat{a}^\dagger] = 1$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}mw^2\hat{x}^2 = \hbar w\left(\hat{a}^\dagger\hat{a} - \frac{1}{2}\right)$$
$$\hat{V} = \frac{1}{2}mw^2\hat{x}^2 = \frac{\hbar w}{4}\left(\hat{a} + \hat{a}^\dagger\right)^2$$

Commutators

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$
$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$[\hat{x}, \hat{p}_x] = i\hbar$$
$$[\hat{x}, \hat{y}] = 0$$
$$[\hat{p}_x, \hat{y}] = 0$$
$$[\hat{p}_x, \hat{p}_y] = 0$$
$$[\hat{L}_x, \hat{y}] = i\hbar z$$
$$[\hat{L}_x, \hat{p}_y] = i\hbar p_z$$
$$[\hat{L}_x, \hat{x}] = 0$$
$$[\hat{L}_x, \hat{p}_x] = 0$$

Angular Momentum

Eigenvalues:

$$L_z Y_l^m = m\hbar Y_l^m$$
$$L^2 Y_l^m = \hbar^2 l(l+1) Y_l^m$$

$$L_z|lm\rangle = \hbar m|lm\rangle$$
$$L^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle$$

Commutation relations:

$$[L_x, L_y] = i\hbar L_z$$
$$[L^2, L_z] = 0$$

Raising and lowering operators:

$$L_\pm = L_x \pm iL_y$$
$$[L^2, L_\pm] = 0$$
$$L_+ f_t = 0$$
$$L_- f_b = 0$$

Spin

Eigenvalues:

$$S_z|sm\rangle = \hbar m|sm\rangle$$
$$S^2|sm\rangle = \hbar^2 s(s+1)|sm\rangle$$

Commutation relations:

$$[S^2, S_z] = 0$$
$$[S_x, S_y] = i\hbar S_z$$

Pauli Matrices:

$$\bar{\sigma} = \sigma_1 \hat{x} + \sigma_2 \hat{y} + \sigma_3 \hat{z}$$
$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$
$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$S_x = \frac{\hbar}{2}\sigma_x$$
$$S_y = \frac{\hbar}{2}\sigma_y$$
$$S_z = \frac{\hbar}{2}\sigma_z$$

Spin 1/2:

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$
$$\chi(t) = a\chi_+ e^{-\frac{iE_+ t}{\hbar}} + b\chi_- e^{-\frac{iE_- t}{\hbar}}$$
$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$|a|^2 + |b|^2 = 1$$
$$\langle S_x \rangle = \chi^\dagger S_x \chi$$
$$c_n = \langle \psi_n | \Psi \rangle$$

Identical Particles

Given single particle wavefunctions $\psi_a(x), \psi_b(x)$, we consider the joint wavefunction.

For non-interacting bosons:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\big(\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)\big) = \frac{1}{\sqrt{2}}(|n_a\rangle|n_b\rangle + |n_b\rangle|n_a\rangle)$$
$$|\psi_{gs}\rangle = \psi_1(x_1)\psi_1(x_2) = |0\rangle_1|0\rangle_2$$

For non-interacting fermions:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\big(\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)\big) = \frac{1}{\sqrt{2}}(|n_a\rangle|n_b\rangle - |n_b\rangle|n_a\rangle)$$
$$|\psi_{gs}\rangle = \frac{1}{\sqrt{2}}\big(\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\big) = \frac{1}{\sqrt{2}}(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2)$$

A product state can be written:

$$\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$$

Fock states:

$$\Psi_i^1 = |K_i\rangle = |0,0, \dots, n_i = 1,0,0, \dots\rangle$$

Number operator:

$$N_i = a_i^\dagger a_i$$
$$[a_i, a_i^\dagger] = 1$$

Quantum Computing

Superposition of states:

$$|\psi\rangle = \left(\frac{1}{\sqrt{2}}\right)^N (|00 \dots 0\rangle + |10 \dots 0\rangle + \cdots + |11 \dots 1\rangle)$$

Hadamaard gate:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Flip gate:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Phase gate:

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Controlled not (flips target if control is 1):

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle)$$

Perturbation Theory

Used when we have a potential of the form:

$$H = H^0 + \lambda H'$$

Write ψ and E_n as power series:

$$\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \cdots$$
$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$$

Sub this into the eigenvalue equation:

$$H\psi_n = E_n\psi_n$$
$$H(\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \cdots) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots)\psi_n$$
$$(H^0 + \lambda H')(\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \cdots) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots)\psi_n$$
$$H^0\psi_n^0 + \lambda(H^0\psi_n^1 + H'\psi_n^0) + \lambda^2(H^0\psi_n^2 + H'\psi_n^1) + \cdots$$
$$= E_n^0\psi_n^0 + \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0) + \lambda^2(E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0) + \cdots$$

Taking first order λ and setting it equal to one:

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$$

Taking the inner product with ψ_n^0:

$$\langle\psi_n^0|H^0\psi_n^1\rangle + \langle\psi_n^0|H'\psi_n^0\rangle = \langle\psi_n^0|E_n^0\psi_n^1\rangle + \langle\psi_n^0|E_n^1\psi_n^0\rangle$$
$$\langle\psi_n^0|H^0\psi_n^1\rangle + \langle\psi_n^0|H'\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle$$

Because H^0 is Hermitian we have:

$$\langle\psi_n^0|H^0\psi_n^1\rangle = \langle H^0\psi_n^0|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle$$

Thus our equation becomes:

$$E_n^0\langle\psi_n^0|\psi_n^1\rangle + \langle\psi_n^0|H'\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle$$
$$\langle\psi_n^0|H'\psi_n^0\rangle = E_n^1$$

This yields the result:

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle$$

To get the wavefunction:

$$\lambda(H^0\psi_n^1 + H'\psi_n^0) = \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0)$$
$$H^0|\psi_n^1\rangle - E_n^0|\psi_n^1\rangle = E_n^1|\psi_n^0\rangle - H'|\psi_n^0\rangle$$
$$(H^0 - E_n^0)|\psi_n^1\rangle = (E_n^1 - H')|\psi_n^0\rangle$$
$$(H^0 - E_n^0)\sum c_m|\psi_m^0\rangle = (E_n^1 - H')|\psi_n^0\rangle$$
$$\sum c_m(H^0 - E_n^0)|\psi_m^0\rangle = (E_n^1 - H')|\psi_n^0\rangle$$
$$\sum c_m(E_m^0 - E_n^0)\langle\psi_l^0|\psi_m^0\rangle = \langle\psi_l^0|(E_n^1 - H')|\psi_n^0\rangle$$
$$\sum c_m(E_m^0 - E_n^0)\langle\psi_l^0|\psi_m^0\rangle = E_n^1\langle\psi_l^0|\psi_n^0\rangle - \langle\psi_l^0|H'|\psi_n^0\rangle$$

For $n \neq l$ this simplifies by orthogonality to:

$$c_l\left(E_l^0 - E_n^0\right) = -\langle\psi_l^0|H'|\psi_n^0\rangle$$

$$c_l = \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_l^0}$$

Since eigenfunctions form a complete basis we have:

$$\psi_n^1 = \sum c_m \psi_m^0$$
$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$$

Variational Principle

An inequality which states:

$$E_0 \leq \langle \psi_{trial} | H | \psi_{trial} \rangle$$

Using:

$$|\psi_{trial}\rangle = \sum c_n |\psi_n\rangle$$
$$\hat{H}|\psi_{trial}\rangle = E_n |\psi_{trial}\rangle$$
$$\langle \psi_{trial} | \psi_{trial} \rangle = 1$$

We have:

$$\sum c_{n'}^* \langle \psi_{n'} | \sum c_n | \psi_n \rangle = 1$$
$$\sum c_{n'}^* \sum c_n \langle \psi_{n'} | \psi_n \rangle = 1$$
$$\sum c_{n'}^* \sum c_n = 1$$

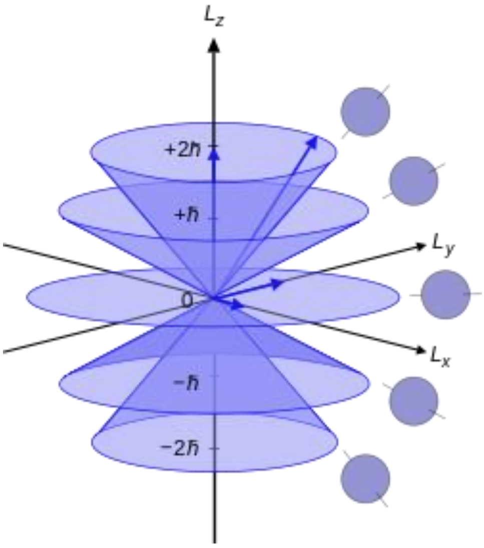
Similarly:

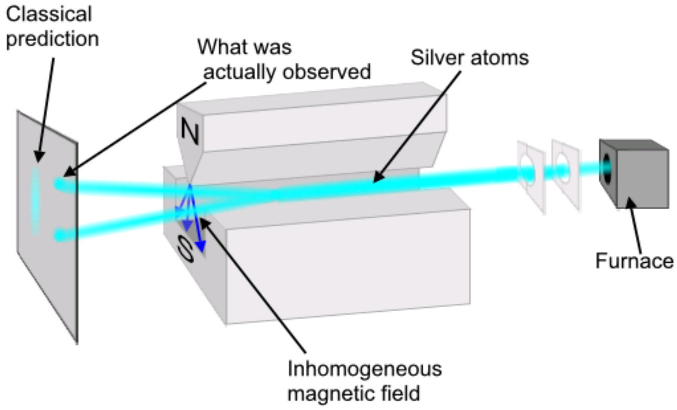
$$\begin{aligned}
\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle &= \sum c_{n'}^* \langle \psi_{n'} | \hat{H} | \psi_n \rangle \sum c_n \\
&= \sum c_{n'}^* \sum c_n \langle \psi_{n'} | \hat{H} | | \psi_n \rangle \\
&= \sum c_{n'}^* \sum c_n \langle \psi_{n'} | E_n \psi_n \rangle \\
&= \sum c_{n'}^* \sum c_n E_n \langle \psi_{n'} | \psi_n \rangle \\
&= \sum c_{n'}^* \sum c_n E_n \\
&= \sum |c_n|^2 E_n \\
&\geq E_0 \sum |c_n|^2 \\
\langle \psi_{trial} | \hat{H} | \psi_{trial} \rangle &\geq E_0
\end{aligned}$$

Other Stuff

- Fourier transform of integral
  - Substitute out wavefunctions for fourier transform (using x and x')
  - Pull the conjugate wavefunction by itself out the front
  - Apply the operator to the second wavefunction
  - Rewrite the remaining integral as a plain wavefunction using formula
- Degeneracy of orbitals
  - $\sum_{i=0}^{n} (2(i+1) - 1)$
- Product states are independent, not correlated/entangled. For a system $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$:
  - Entangled state: $|\psi\rangle_1 = \frac{1}{\sqrt{2}}(|0\rangle|0\rangle + |1\rangle|1\rangle)$
  - Product state: $|\psi\rangle_2 = \frac{1}{2}(|0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle)$

- Exchange force: exchange interaction is a quantum mechanical effect between identical particles which alters the expectation value of the distance when the wave functions of two or more indistinguishable particles overlap. It increases (for fermions) or decreases (for bosons) the expectation value of the distance between identical particles (as compared to distinguishable particles).
- $\psi_a(r)$ is a projection of $|a\rangle$ along $|r\rangle$
- Stern–Gerlach experiment
    - The Stern–Gerlach experiment involves sending a beam of particles through an inhomogeneous magnetic field and observing their deflection
    - If it moves through a homogeneous magnetic field, the forces exerted on opposite ends of the dipole cancel each other out and the trajectory of the particle is unaffected. However, if the magnetic field is inhomogeneous then the force on one end of the dipole will be slightly greater than the opposing force on the other end
    - If the particles were classical spinning objects, one would expect the distribution of their spin angular momentum vectors to be random and continuous. Instead, the particles passing through the Stern–Gerlach apparatus are deflected either up or down by a specific amount
    - This shows that particles possess an intrinsic angular momentum that is closely analogous to the angular momentum of a classically spinning object, but that takes only certain quantized values
    - Another important result is that only one component of a particle's spin can be measured at one time, meaning that the measurement of the spin along the z-axis destroys information about a particle's spin along the x and y axis.
- Orbital and extrinsic angular momentum
    - Dd
- Spin probabilities: the ratio of spin probabilities is given by the ratio of the normalization constants $\chi = \alpha\chi_+ + \beta\chi_-$, not by the components of $\chi = \binom{a}{b}$. These will only be the same when you measure exactly along the z-axis.
- For taking expected values of multi-particle states, one must integrate over both variables
- Commutation relations: sub in more complex operator and expand out
- Raising operator: Use $L_z(L_\pm f) = L_z(L_\pm f) - L_\pm(L_z f) + L_\pm(L_z f) = [L_z, L_\pm]f + L_\pm(L_z f)$
- Integer eigenvalues: note that angular momentum eigenvalues must be integers while spin eigenvalues can be half-integers. This asymmetry arises from the fact that the spherical harmonics must remain constant when rotated about by 360 degrees (i.e. $\psi(\phi + 2\pi) = \psi(\phi)$). Spin is not described by spatial coordinates so does not have the same restriction placed on it.
- Postulates: WaSP-HEB


L_z
$+2\hbar$
$+\hbar$
0
$-\hbar$
$-2\hbar$
L_y
L_x


Classical prediction
What was actually observed
Silver atoms
N
S
Furnace
Inhomogeneous magnetic field