

Quantum Mechanics I

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1 Mathematical Introduction

1.1 Linear Vector Spaces: Basics

A linear vector space, V , is a collection of objects $|1\rangle, |2\rangle, \dots, |V\rangle, |W\rangle, \dots$, called vectors for which there exists

1. Definite rule for a vector sum, denoted $|V\rangle + |W\rangle$.
2. A definite rule for multiplication by scalars a, b , denoted $a|V\rangle$ with the following features:
 - Closure: $|V\rangle + |W\rangle \in V$
 - Scalar multiplication is distributive in the vectors: $a(|V\rangle + |W\rangle) = a|V\rangle + a|W\rangle$
 - Scalar multiplication is distributive in the scalars: $(a + b)|V\rangle = a|V\rangle + b|V\rangle$
 - Scalar multiplication is associative: $a(b|V\rangle) = ab|V\rangle$
 - Addition is commutative: $|V\rangle + |W\rangle = |W\rangle + |V\rangle$
 - Addition is associative: $|V\rangle + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle$
 - There exists a *null vector*: $|V\rangle + |0\rangle = |V\rangle$.
 - For every vector, there exists an inverse under addition such that: $|V\rangle + |-V\rangle = |0\rangle$.

Other important rules/definitions:

- Linear Independence: If in the relation $\sum a_i |i\rangle = |0\rangle$ all a_i 's must be zero for the relation to be satisfied.
- V has dimension n if it can accommodate a maximum of n linearly independent vectors.
- Any vector in V can be written as a linear combination of n linearly independent vectors.
- Basis: A set of n linearly independent vectors in an n -dimensional space.

1.2 Inner Product Spaces

- $\vec{A} \cdot \vec{B} = |A||B|\cos(\theta)$
- $\langle V|W \rangle = \langle W|V \rangle^*$
- $\langle V|(a|W\rangle + b|Z\rangle) = a\langle V|W\rangle + b\langle V|Z\rangle$
- $\langle aW + bZ|V \rangle = a^*\langle W|V \rangle + b^*\langle Z|V \rangle$
- Two vectors are *orthogonal* if their inner product vanishes.
- Gram-Schmidt Theorem: Let $|I\rangle, |II\rangle, |III\rangle$ be a linearly independent basis. The vectors of the orthonormal basis will be...
 1. $|1\rangle = \frac{|I\rangle}{|I|}$
 2. $|2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$ (normalize to get $|2\rangle$)
 3. $|3'\rangle = |III\rangle - |1\rangle\langle 1|III\rangle - |2\rangle\langle 2|III\rangle$ (normalize to get $|3\rangle$)

1.3 Dual Spaces and the Dirac Notation

- Expand vector in a basis: $|V\rangle = \sum |i\rangle\langle i|V\rangle = \sum v_i |i\rangle$
- Adjoint = $a|V\rangle \rightarrow \langle V|a^*$
 - Replace every bra by its ket and complex conjugate all of the coefficients.
- Schwarz Inequality: $|\langle V|W \rangle| \leq |V||W|$
- Triangle Inequality: $|V + W| \leq |V| + |W|$

1.4 Linear Operators

- $[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega$
- Commutator Identities
 - $[\Omega, \Lambda\theta] = \Lambda[\Omega, \theta] + [\Omega, \Lambda]\theta$
 - $[\Lambda\Omega, \theta] = \Lambda[\Omega, \theta] + [\Lambda, \theta]\Omega$
- $\Omega\Omega^{-1} = \Omega^{-1}\Omega = I$
- $(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1}$

1.5 Matrix Elements of Linear Operators

- *Matrix Elements*: The nxn matrix which represents a linear operator in a basis.
- action of a linear operator is fully specified by its action on the basis vectors.
- Projection Operator: $P_i = |i\rangle\langle i|$
- Adjoint of an Operator: $\Omega_{ij}^\dagger = \Omega_{ji}^*$
- $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger$

- Hermetian operator: $\Omega^\dagger = \Omega$
 - Eigenvalues of a hermetian operator are real. Represent observables.
 - To every hermetian operator, there exists (at least) a basis consisting of its orthonormal eigenvectors. It is diagonal in this eigenbasis and has its eigenvalues as the diagonal entries.
- Anti-Hermetian Operator: $\Omega^\dagger = -\Omega$
- Unitary Operator: $UU^\dagger = I$
 - Rows/Columns of unitary matrices are orthonormal.
 - Generalization of rotation operators.

Additionally worth noting is that the trace and determinant of an operator is unaffected by a unitary change in basis.

1.6 Active and Passive Transformations

- Active Transformation: Change the state, not the operator. $\langle V' | \Omega | V \rangle \rightarrow \langle UV' | \Omega | UV \rangle$
- Passive Transformation: Subject operators to the change, not the state: $\Omega \rightarrow U^\dagger \Omega U$

1.7 The Eigenvalue Problem

- $\Omega |V\rangle = \omega |V\rangle$
- $|V\rangle$ is the eigenket of Ω with an eigenvalue of ω .
- $(\Omega - \omega I) |V\rangle = |0\rangle$
- $\det(\Omega - \omega I) = 0$
- If Ω and Λ are two commuting Hamiltonian Operators, there exists (at least) a basis that diagonalizes them both. If one of the matrices is degenerate, take the non-degenerate one first and diagonalize that. This gives you the proper basis. $U^\dagger \Omega U$ to diagonalize. Note that the determinant of this diagonal matrix is the product of the eigenvalues and the trace is the sum of the eigenvalues.
- The Propogator: $|x(t)\rangle = U |x(0)\rangle$

1.8 Generalize to Infinite Dimensions

- $\langle f | g \rangle = \int_a^b f^*(x) g(x) dx$
- $\langle x | f \rangle = \int_a^b \langle x | x' \rangle \langle x' | f \rangle dx'$
- $\int_{x-\epsilon}^{x+\epsilon} \delta(x, x') dx' = 1$
- $\langle x | x' \rangle = \delta(x - x')$
- $\delta'(x - x') = \frac{d}{dx} \delta(x - x') = -\frac{d}{dx} \delta(x' - x)$
- $D |f\rangle = \left| \frac{df}{dx} \right\rangle$
- $K = -iD$
- in the x-basis $K = -i \frac{d}{dx}$

2 Review of Classical Mechanics

- Hamilton's Equations

1. $H(q_i, p_i) = \sum p_i \dot{q}_i - L(q, \dot{q})$

2. $\dot{q}_i = \frac{\partial H}{\partial p_i}$

3. $\dot{p}_i = -\frac{\partial H}{\partial q_i}$

- Cyclic Coordinate: when $\dot{p}_i = 0$

- Poisson Bracket : $\left\{ \omega, \lambda \right\} = \sum \left(\frac{\partial \omega}{\partial q_i} \frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i} \frac{\partial \lambda}{\partial q_i} \right)$

- $\dot{\omega} = \left\{ \omega, H \right\}$

- For canonical transformations, must have

1. $\left\{ \bar{q}_j, \bar{q}_k \right\} = 0 = \left\{ \bar{p}_j, \bar{p}_k \right\}$

2. $\left\{ \bar{q}_j, \bar{p}_k \right\} = \delta_{jk}$

2.1 Symmetries and their Consequences

- If H is invariant under an infinitesimal rotation, then the generator of the transformation $g(q,p)$ is conserved. $\dot{g} = \left\{ g, H \right\} = 0$
- If H is invariant under a canonical transformation, then the transformed trajectory is also a solution to the equations of motion.

3 All is not well with Classical Mechanics

3.1 Double Slit Experiment

- Send light at a double slit. Start with a slit open and cut down the intensity. The energy now arrives discontinuously as a particle's energy would. These bundles of energy are called photons and have the following properties.

1. $E^2 = p^2 c^2 + m^2 c^4$

2. photons have zero mass

3. $E = \hbar \omega, p = \hbar k$

3.2 Matter Waves (de Broglie Waves)

- $\lambda = \frac{h}{p}$

3.3 Conclusions

Wave function allows wave-particle duality to occur.

4 The Postulates, A General Discussion

4.1 Postulates in Classical Mechanics

1. The state of a particle at any given time t is specified by $x(t)$ and $p(t)$, a point in 2D phase space.
2. Every dynamical variable ω is a function of x and p such that $\omega(x, p)$.
3. If the particle is in the state x, p measurement of the variable ω will yield a value $\omega(x, p)$. The state will remain unaffected.
4. The state variables change with time according to Hamilton's equations.

4.2 Postulates in Quantum Mechanics

1. The state of the particle is represented by a vector in a Hilbert space. $|\psi(t)\rangle$
2. Classical variables x, p are now represented by the operators X and P . The operators corresponding to dependent variables $\omega(x, p)$ are given Hermetian operators $\Omega(X, P) = \omega(x \rightarrow X, p \rightarrow P)$
3. If the particle is in a state $|\psi\rangle$, measurement of the variable corresponding to Ω will yield one of the eigenvalues ω with probability $P(\omega) \propto |\langle\omega|\psi\rangle|^2$. The state of the system will change from $|\psi\rangle$ to $|\omega\rangle$ as a result of the measurement.
4. The state vector $|\psi(t)\rangle$ obeys the Schroedinger equation.

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

4.3 Discussion of the Postulates

Improper Vectors are those normalizable only to the Dirac delta functions whereas **proper vectors** are normalizable to 1. The *principle of superposition* states that if $|\psi\rangle$ and $|\psi'\rangle$ represent possible states, so does $\alpha|\psi\rangle + \beta|\psi'\rangle$.

- The probability of the system having a certain eigenvalue ω : $P(\omega_i) = |\langle\omega_i|\psi'\rangle|^2$ when $|\psi\rangle$ is normalized.
- When we want information about a variable, $P(\lambda) = |\langle\omega_i|\psi'\rangle|^2$
- If the eigenvalue spectrum is continuous, then one can expand $|\psi\rangle$ as $|\psi\rangle = \int |\omega\rangle \langle\omega|\psi\rangle$

4.4 Expectation Values and Uncertainties

The expectation value for a given operator Ω is given as

$$\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle \quad (1)$$

whereas the standard deviation is given by

$$\Delta\Omega = \langle(\Omega - \langle\Omega\rangle)^2\rangle^{\frac{1}{2}}. \quad (2)$$

The commutation of two operators is given by

$$[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega. \quad (3)$$

If two operators commute, we know that a complete basis of simultaneous eigenkets can be found. Each element of $|\omega\lambda\rangle$ of this basis has well-defined values for Ω and Λ . The most famous example of non-commuting operators, $[\Omega, \Lambda] \neq 0$, are position and momentum operators which obey $[X, P] = i\hbar$. Our probability calculation must now be slightly altered as the measurement of one variable followed by the other doesn't alter the eigenvalue obtained in the first measurement and we have in the end a state with a well-defined value for both observables.

$$P(\omega, \lambda) = |\langle \omega\lambda | \psi \rangle|^2 = P(\lambda, \omega) \quad (4)$$

Perhaps the most famous relation in all of quantum mechanics is the *Heisenberg Uncertainty Principle* $\Delta X \Delta P \geq \frac{\hbar}{2}$. Another important relation to know that the propagator for the SE is given by

$$U(t) = \sum |E\rangle \langle E| e^{\frac{-iEt}{\hbar}} \quad (5)$$

or alternatively

$$U(t) = e^{\frac{-iHt}{\hbar}} \quad (6)$$

5 Simple Problems in One Dimension

In general, have an i when $E > V$. You want this to be a plane wave.

5.1 The Free Particle

Free particle, no potential so the Hamiltonian is given by $H = \frac{p^2}{2m}$. Therefore, the SE becomes

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (7)$$

which can be written in a form that is easy to solve as

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad (8)$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. We will write the solutions in the exponential form

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (9)$$

However, this situation is a little more complicated, as there are no boundary conditions (it's a free particle so not really constrained by anything). So instead we tack on a time-dependent term.

$$\Psi(x, t) = Ae^{ik(x - \frac{\hbar k}{2m}t)} + Be^{-ik(x + \frac{\hbar k}{2m}t)} \quad (10)$$

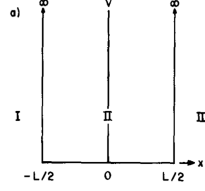
5.2 Particle in a Box

In this example the potential is given as follows where $V(x) = 0$ when $|x| < \frac{L}{2}$ and $V(x) = \infty$ when $|x| \geq \frac{L}{2}$. In general, this SE is given as

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad (11)$$

which simplifies to

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \quad (12)$$



We will now consider each of the regions separately, first consider region III. Even though V is infinite in this region, call it some V_0 which is greater than E . So in this region the SE becomes

$$\frac{d^2\psi_{III}}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_{III} = 0 \quad (13)$$

Solve this by

$$\psi_{III} = Ae^{-\kappa x} + Be^{\kappa x} = Ae^{-\kappa x} \quad (14)$$

where $\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$. But we see that we need to set $B = 0$ on physical grounds as this blows up as $x \rightarrow \infty$. Similarly in region I we have

$$\psi_I = Ae^{-\kappa x} + Be^{\kappa x} = Be^{\kappa x} \quad (15)$$

In region II, the SE takes the exact form of the free particle as $V = 0$. Therefore, the solution in this region is the same solution as that of the free particle, however, we will write this in a different form

$$\psi(x)_{II} = Ae^{ikx} + Be^{-ikx} \quad (16)$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. Now we must consider the boundary conditions for this case, which are that ψ must be continuous at the boundaries of the regions. We cannot say anything about ψ' as V jumps to infinity there, so it doesn't really make sense to require that this is continuous. From these conditions, we get the following two equations.

$$\psi_I\left(\frac{-L}{2}\right) = \psi_{II}\left(\frac{-L}{2}\right) = 0 \quad (17)$$

$$\psi_{III}\left(\frac{L}{2}\right) = \psi_{II}\left(\frac{L}{2}\right) = 0 \quad (18)$$

This requires

$$0 = Ae^{-ik\frac{L}{2}} + Be^{ik\frac{L}{2}} \quad (19)$$

$$0 = Ae^{ik\frac{L}{2}} + Be^{-ik\frac{L}{2}} \quad (20)$$

We can write this system of equations in matrix form as this will be easier to visualize.

$$\begin{bmatrix} e^{-ik\frac{L}{2}} & e^{ik\frac{L}{2}} \\ e^{ik\frac{L}{2}} & e^{-ik\frac{L}{2}} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

There is only a nontrivial solution when the determinant vanishes.

$$e^{-ikL} - e^{ikL} = -2i\sin(kL) = 0 \quad (21)$$

so we see $k = \frac{n\pi}{L}$ where $n = 0, \pm 1, \dots$. We see also that this depends on how we solved the equation, therefore the overall normalized solutions go as

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (22)$$

when n is even and

$$\psi_n(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) \quad (23)$$

Using our values of k and equation for energy, we see that the energy can be written as

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad (24)$$

5.3 Delta Potential

Here the potential is a delta function so it goes as $V = -\alpha\delta(x)$. Hence the SE becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \quad (25)$$

This will yield both bound and scattering states. In general, think of bound and scattering states in the classical sense. In general $E < 0$ represents a bound state and $E > 0$ represents a scattering state when $E \rightarrow 0$ as x goes to ∞ . Intuitively, we know that we should get exponential decays as our bound states and plane waves as our scattering states by their definition. Consider each example separately.

5.3.1 Bound States

In the region where $x < 0$, $V(x) = 0$ so the SE becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E)\psi = 0 = \frac{d^2\psi}{dx^2} + \kappa^2\psi \quad (26)$$

where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$. The general solution to this is given as

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \quad (27)$$

In the region where $x < 0$ this is

$$\psi(x) = Be^{\kappa x} \quad (28)$$

as we cannot physically have terms which blow up so we set $A = 0$. Similarly, for $x > 0$ we have

$$\psi(x) = Fe^{-\kappa x} \quad (29)$$

Now, we must consider the boundary condition at $x = 0$. we will integrate the SE from $+\epsilon$ to $-\epsilon$ to get the additional condition that

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0) \quad (30)$$

this yields that

$$\kappa = \frac{m\alpha}{\hbar^2} \quad (31)$$

Resulting in

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{\frac{-m\alpha|x|}{\hbar^2}}; E = \frac{-m\alpha^2}{2\hbar^2} \quad (32)$$

Note that there are also scattering states which will be produced when E has a different sign. We will consider these next.

5.3.2 Scattering States

We will now do the scattering states where $E > 0$. We will still divide this into two regions, where $x < 0$ and $x > 0$. For $x < 0$, the SE reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

Simplifying this becomes

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} E\psi = -k^2\psi$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. In general the solution for this is

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

Similarly, the solution for $x > 0$ will be no different (but with different constants of course)

$$\psi_{II}(x) = Fe^{ikx} + Ge^{-ikx}$$

Consider a wave incident from the left, therefore $G = 0$ as it makes no sense to have an incoming wave from the right if the wave is incident from the left. Hence, this becomes

$$\psi_{II}(x) = Fe^{ikx}$$

From continuity at $x = 0$ we have

$$A + B = F$$

Continuity in the derivative for the delta function is a little more complicated. The main idea is to integrate the SE from $-\epsilon$ to $+\epsilon$ and then take the limit as ϵ goes to zero.

$$\frac{-\hbar^2}{2m} \int_{-\epsilon}^{+\epsilon} \frac{d^2\psi}{dx^2} dx + \int_{-\epsilon}^{+\epsilon} V(x)\psi(x)dx = E \int_{-\epsilon}^{+\epsilon} \psi(x)dx$$

Simplifying this we see

$$\Delta \frac{d\psi}{dx} = \frac{2m}{\hbar^2} \lim(\epsilon \rightarrow 0) \int_{-\epsilon}^{+\epsilon} V(x)\psi(x)dx$$

since $V(x)$ is a delta potential, we know this will become

$$\Delta \frac{d\psi}{dx} = -\frac{2m\alpha}{\hbar^2} \psi(0)$$

which we used above. Now find the continuity in the derivative

$$\frac{d\psi}{dx} + = ik(F)$$

$$\frac{d\psi}{dx} - = ik(A - B)$$

Plugging into our above formula, note that $\psi(0) = A + B$.

$$ik(F - (A - B)) = ik(F - A + B) = -\frac{2m\alpha}{\hbar^2} (A + B)$$

Solving for B and F in terms of A we find

$$B = \frac{i\beta}{1 - i\beta} A$$

$$F = \frac{1}{1 - i\beta} A$$

where $\beta = \frac{m\alpha}{\hbar^2 k}$. We see that the reflection and transmission coefficients are given by

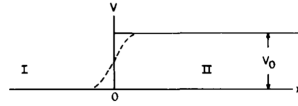
$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}$$

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}$$

which satisfies $R + T = 1$.

5.4 Single-Step Potential

The step potential has the form of $V(x) = 0$ when $x < 0$ and $V(x) = V_0$ when $x > 0$. In region I,



the solution is a familiar one for when $V = 0$.

$$\psi(x)_E = Ae^{ik_1 x} + Be^{-ik_1 x} \quad (33)$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$. In region II, we can simply replace E with $E - V_0$. Also there will not be an incoming wave from the left, so we set $D = 0$.

$$\psi(x)_E = Ce^{ik_2 x} + De^{-ik_2 x} = Ce^{ik_2 x} \quad (34)$$

where $k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$. Requiring that these maintain the continuity of ψ and its derivative across the step we get

$$A + B = C \quad (35)$$

$$ik_1(A - B) = ik_2 C \quad (36)$$

With this we basically find B and C in terms of k_1 , k_2 , and A .

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A \quad (37)$$

$$C = \left(\frac{2k_1}{k_1 + k_2} \right) A \quad (38)$$

We will now discuss this mostly in terms of reflection and transmission coefficients R and T . This such that

$$R + T = 1 \quad (39)$$

These are expressed in terms of the probability current density, j , which is written as

$$j = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*) \quad (40)$$

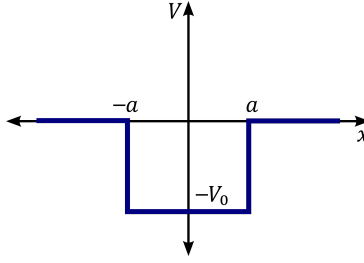


Figure 1: The finite square well potential

5.5 The Finite Square Well

Consider a finite square well potential so that $V(x) = -V_0$ for $-a < x < a$ and $V(x) = 0$ elsewhere. This also has bound and scattering states. We will consider the bound states. The SE gives

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

or simplifying this

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ is real and positive (remember $E < 0$ for bound states). The general solution for $x < -a$ is

$$\psi_I(x) = Be^{\kappa x}$$

as we set $A = 0$ to prevent that term from blowing up. For $x > a$ the solution is similarly

$$\psi_{III}(x) = Fe^{-\kappa x}$$

The region in the middle will be

$$\psi_{II}(x) = C\sin(lx) + D\cos(lx)$$

where $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$. The key to this problem is realizing that the potential is even, so the solutions are either even or odd. We will do both of these cases separately.

Even Solutions: Take $\psi_{II} = D\cos(lx)$ as Cosine is an even function. Continuity of $\psi(x)$ at $x = a$ says

$$Fe^{-\kappa x} = D\cos(la)$$

The continuity of $\frac{d\psi}{dx}$ at $x = a$ says

$$-\kappa e^{-\kappa x} = -lD\sin(la)$$

dividing the two equations we see that

$$\kappa = l\tan(la)$$

Note that the full solution would involve plotting this *transcendental equation* to see where it intersects. This is not practical for an exam, so we will end this explanation here.

Odd Solutions: Take $\psi_{II} = C\sin(lx)$ as Sine is an odd function. Continuity at $\psi(x)$ at $x = a$ says

$$Fe^{-\kappa x} = C\sin(la)$$

The continuity of $\frac{d\psi}{dx}$ at $x = a$ says

$$-\kappa e^{-\kappa x} = lC\cos(la)$$

Dividing these two equations we see

$$-\kappa = l\cot(la)$$

which gives us the odd solutions. We would also find a transcendental equation for this solution.

5.6 The Continuity Equation for Probability

Using the probability current density, as defined above, we can derive the continuity equation for probability by the following.

1. Start with the SE.
2. Take its complex conjugate to form a system of two equations.
3. Multiply each equation by ψ or ψ^* , whichever variable is not currently in the equation.
4. Take the difference of these equations.
5. Use $\psi^*\psi = P$ to simplify.

We get the result

$$\frac{\partial P}{\partial t} = -\nabla \cdot j$$

6 The Classical Limit

A useful relation to determine how the expectation value of an operator changes with time is *Ehrenfest's Theorem*. This is given as

$$\frac{d}{dt}\langle\Omega\rangle = \frac{-i}{\hbar}\langle[\Omega, H]\rangle \quad (41)$$

This is important as it allows us to determine the classical limit of quantum mechanics. Consider that $\langle\dot{X}\rangle = \frac{\langle P\rangle}{m}$. Given that $\frac{P}{m} = \frac{\partial H}{\partial P}$, this results in

$$\langle\dot{X}\rangle = \left\langle\frac{\partial H}{\partial P}\right\rangle \quad (42)$$

which in the classical limit looks a lot like Hamilton's equations. A similar equation can be derived for $\dot{P}$. This represents the classical limit of quantum mechanics.

7 The Harmonic Oscillator

The Harmonic Oscillator is the only system which can be exactly solved in both classical and Quantum theory. It is also incredibly relevant as any physical system which fluctuates by small amounts near a configuration of stable equilibrium may be described by an oscillator or by a collection of decoupled harmonic oscillators. The Hamiltonian for the harmonic oscillator is

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \quad (43)$$

where $\omega^2 = \frac{k}{m}$ is the classical frequency of oscillation. The Hamiltonian for a coupled harmonic oscillator is given as

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2[x_1^2 + x_2^2 + (x_1 - x_2)^2] = H_1 + H_2 + \frac{1}{2}m\omega^2(x_1 - x_2)^2 \quad (44)$$

7.1 Quantization of the Oscillator (Coordinate Basis)

The SE for the harmonic oscillator can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - \frac{1}{2}m\omega^2x^2)\psi = 0 \quad (45)$$

The first step is to write this in terms of dimensionless variables. We will choose $x = by$ where $b = (\frac{\hbar}{m\omega})^{1/2}$. The SE then becomes

$$\frac{d^2\psi}{dy^2} + \frac{2mEb^2}{\hbar^2}\psi - \frac{m^2\omega^2b^4}{\hbar^2}y^2\psi = 0 \quad (46)$$

We will also define a dimensionless variable ϵ corresponding to energy:

$$\epsilon = \frac{mEb^2}{\hbar^2} = \frac{E}{\hbar\omega} \quad (47)$$

This allows our SE to be written a lot more simply as

$$\psi'' + (2\epsilon - y^2)\psi = 0 \quad (48)$$

which in the limit of $y \rightarrow \infty$ becomes

$$\psi'' - y^2\psi = 0 \quad (49)$$

The solution of this is

$$\psi = Ay^m e^{\pm \frac{y^2}{2}} \quad (50)$$

Now we will consider the limit where $y \rightarrow 0$. We now have

$$\psi'' + 2\epsilon\psi = 0 \quad (51)$$

which has the solution

$$\psi = A\cos[\sqrt{2\epsilon}y] + B\sin[\sqrt{2\epsilon}y] \quad (52)$$

We therefore infer that ψ is in the form

$$\psi(y) = u(y)e^{-\frac{y^2}{2}}. \quad (53)$$

To determine $u(y)$ completely we have

$$u'' - 2yu' + (2\epsilon - 1)u = 0 \quad (54)$$

This indicates that a power series solution is possible. Let's assume this is true and see what happens. Consider the generic case where

$$u(y) = \sum C_n y^n \quad (55)$$

but we know that as $y \rightarrow 0$, $u(y) \rightarrow A + cy + O(y^2)$ we will plug these in for the general coefficients we get

$$\sum C_n [n(n-1)y^{(n-2)} - 2ny^n + (2\epsilon - 1)y^n] = 0 \quad (56)$$

consider the first term in the series where

$$\sum C_n n(n-1)y^{(n-2)} \quad (57)$$

substitute $m = n-2$

$$\sum C_{m+2}(m+2)(m+1)y^m \quad (58)$$

M is a dummy variable, we can switch this out for n and plug back into the equation that we had before.

$$\sum y^n [C_{n+2}(n+2)(n+1) + C_n(2\epsilon - 1 - 2n)] = 0 \quad (59)$$

Therefore the term inside the brackets must be zero, therefore we have

$$C_{n+2} = C_n \frac{2n+1-2\epsilon}{(n+2)(n+1)} \quad (60)$$

However, we have to find a way to kill the even and or odd coefficients. We see that when $\epsilon = n + \frac{1}{2}$ then the coefficients C_{n+2} vanish. If we choose $C_1 = 0$ when n is even or $C_0 = 0$ when n is odd, we have.

$$\psi(y) = [C_0 + C_2 y^2 + \dots + C_n y^n] e^{-\frac{y^2}{2}} \quad (61)$$

or

$$\psi(y) = [C_1 + C_3 y^3 + \dots + C_n y^n] e^{-\frac{y^2}{2}} \quad (62)$$

All of these point to the fact that energy is quantized (think about our ϵ).

$$E_n = (n + \frac{1}{2}) \hbar \omega \quad (63)$$

We see that we actually know how to find the polynomials in from of the $e^{-\frac{y^2}{2}}$. Mathematicians have figured this out to be a specific kind of polynomial, called the *Hermite Polynomials*.

- $H_0(y) = 1$
- $H_1(y) = 2y$
- $H_2(y) = -2(1 - 2y^2)$
- $H_3(y) = -12(y - \frac{2}{3}y^3)$

The normalized solutions are then given as

$$\psi_E(x) = (\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2})^{\frac{1}{4}} \exp(-\frac{m\omega x^2}{2\hbar}) H_n[(\frac{m\omega}{\hbar})^{1/2} x] \quad (64)$$

The following recursion relations among Hermite polynomials are useful

$$H'_n(y) = 2nH_{n-1} \quad (65)$$

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1} \quad (66)$$

The main features of the eigenvalues and eigenfunctions of the oscillator.

1. The energy is quantized. (Note that this is true for the classical oscillator as well, but the spacing is so small we don't observe this.)
2. The levels are spaced uniformly.
3. The lowest possible energy is $\frac{\hbar\omega}{2}$ and not zero.
4. The solutions $\psi_n(x)$ contain only even or odd powers of x, depending on whether n is even or odd. If n is even $\psi_n(-x) = \psi_n(x)$. If n is odd $\psi_n(-x) = -\psi_n(x)$.
5. The wave function does not vanish beyond the classical turning points, but dies out exponentially as $x \rightarrow \infty$.
6. $P(x) = |\psi(x)|^2$

7.2 The Oscillator in the Energy Basis

In order to do the operator in the Energy Basis we will introduce two operators $a, a^\dagger$.

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \quad (67)$$

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P \quad (68)$$

These satisfy the commutation relation $[a, a^\dagger] = 1$. We have the hamiltonian written as follows

$$H = \left(a^\dagger a + \frac{1}{2}\right)\hbar\omega \quad (69)$$

We will now derive the Energy etc. for the harmonic oscillator in the energy basis. We will begin by defining a new operator $\hat{H}$.

$$\hat{H} = \frac{H}{\hbar\omega} = \left(a^\dagger a + \frac{1}{2}\right) \quad (70)$$

The eigenvalue equation for $\hat{H}$ is given as

$$\hat{H} |\epsilon\rangle = \epsilon |\epsilon\rangle \quad (71)$$

$$a^\dagger a |\epsilon_0\rangle = 0$$

$$\left(\hat{H} - \frac{1}{2}\right) |\epsilon_0\rangle = 0$$

so $\epsilon_0 = \frac{1}{2}$. Resulting in $\epsilon_0 = n + \frac{1}{2}$ which results in $E_n = (n + \frac{1}{2})\hbar\omega$. These are ladder operators obeying the following relations

1. $a |n\rangle = \sqrt{n} |n-1\rangle$
2. $a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$

8 The Heisenberg Uncertainty Relations

We can derive general uncertainty relations. For example, consider Ω, Λ which are two Hermetian operators with a commutator $[\Omega, \Lambda] = i\Gamma$. Consider the uncertainty product

$$(\Delta\Omega)^2(\Delta\Lambda)^2 = \langle\psi|\hat{\Omega}^2|\psi\rangle\langle\psi|\hat{\Lambda}^2|\psi\rangle \quad (72)$$

where

$$\hat{\Omega} = \Omega - \langle\Omega\rangle$$

$$\hat{\Lambda} = \Lambda - \langle\Lambda\rangle$$

Applying the Schwarz inequality we see that

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\psi|\hat{\Omega}\hat{\Lambda}|\psi\rangle|^2 \quad (73)$$

Simplifying this using the anticommutator

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\psi|\frac{1}{2}[\hat{\Omega}, \hat{\Lambda}]_+ + \frac{1}{2}[\hat{\Omega}, \hat{\Lambda}]|\psi\rangle|^2$$

where the anti-commutator is expressed as

$$[\Omega, \Lambda]_+ = \Omega\Lambda + \Lambda\Omega$$

Plugging in the commutation relation from before

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq \frac{1}{4}(\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle^2 + \langle\psi|\Gamma|\psi\rangle^2)$$

For the case of X and P we have

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq \frac{1}{4}(\langle\psi|[\hat{\Omega}, \hat{\Lambda}]_+|\psi\rangle^2 + \hbar^2)$$

so then the uncertainty relation

$$\Delta X \Delta P \geq \frac{\hbar^2}{2}$$

8.1 Minimizing the Mean energy of the System $\langle H \rangle$

Here are the steps:

1. Lowest energy, set $\langle P_i \rangle = 0$. This means that we can substitute ΔP_i^2 for $\langle P_i^2 \rangle$.
2. Argue that $\langle (X^2 + Y^2 + Z^2)^{\frac{1}{2}} \rangle \approx (\langle X^2 \rangle + \langle Y^2 \rangle + \langle Z^2 \rangle)^{\frac{1}{2}}$
3. Assume $\langle X \rangle = 0$ (and Y and Z) as we are looking for the lowest energy state.
4. Reduce it to a 1D problem as the lowest energy state with spherical symmetry will have $(\Delta X)^2 = (\Delta Y)^2 = (\Delta Z)^2$
5. Do the same for ΔP_i .
6. Now use Heisenberg's uncertainty principle to plug in for ΔP . This makes it an equation of just X.
7. Take the derivative with respect to ΔX and set this equal to zero.
8. Solve for ΔX and plug back into your Hamiltonian. Then you have your minimum energy!

9 Systems with N Degrees of Freedom

9.1 Two Particle Hilbert Space

If we are considering two classical particles with position and momenta (x_1, p_1) and (x_2, p_2) , we by postulate 2 promote them to quantum operators (X_1, P_1) , (X_2, P_2) which will obey the canonical commutation relations.

1. $[X_i, P_j] = i\hbar\delta_{ij}$
2. $[X_i, X_j] = 0$
3. $[P_i, P_j] = 0$

These have simultaneous eigenkets which obey $X_1 |x_1 x_2\rangle = x_1 |x_1 x_2\rangle$. The probability for this may also become $P(x_1, x_2) = |\langle x_1 x_2 | \psi \rangle|^2$ where these are normalized to unity. Note that now we are in a two particle Hilbert Space called $V_{1 \otimes 2}$.

We can also arrive at this space by building it out of two one-particle spaces $|x_1\rangle \otimes |x_2\rangle$. Where $\otimes$ is called the *direct product* representing the multiplication of two vectors from different spaces

(this is a linear operation). Note that transferring operators to these new spaces can be a little tricky. We have the following relations which control how this works.

$$X_1^{1\otimes 2} |x_1\rangle \otimes |x_2\rangle = x_1 |x_1\rangle \otimes |x_2\rangle$$

$$X_1^{1\otimes 2} = X_1^{(1)} \otimes I^{(2)}$$

$$P_2^{1\otimes 2} = I^{(1)} \otimes P_2^{(2)}$$

In matrix form this is given as

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix}$$

For example if B was a 2x2 matrix this will result in a 4 x 4 matrix.

9.2 Evolution of the Two-Particle State Vector

These divide up into two types of problems depending on the Hamiltonian.

1. H is separable, $H = H_1 + H_2$
2. H is not separable $H \neq H_1 + H_2$

With class 1, it is easy to show that this can be separated such that $E = E_1 + E_2$. When you perform the separation of variables, one can show that $\psi_E(x_1, x_2) = \psi_{E_1}(x_1)\psi_{E_2}(x_2)$. For the second class, let's just say the potential is dependent on the distance between particles $V(x_1, x_2) = V(x_1 - x_2)$. We can write this in terms of two fictitious particles, one which is the CM which is free from the potential and has $M = m_1 + m_2$ and momentum P_{CM} and a second particle which has a reduced mass of $\mu = \frac{m_1 m_2}{m_1 + m_2}$ and momentum $p = \mu \dot{x}$ and feels the influence of the potential. The Hamiltonian then becomes

$$H = \frac{P_{CM}^2}{2M} + \frac{p^2}{2\mu} + V(x) \quad (74)$$

One can also think of two particles in one dimension as mathematically equivalent to one particle in two dimensions.

9.3 Identical Particles

In classical mechanics possible to distinguish two identical particles based on their trajectories, in quantum mechanics this is not possible. Therefore, the states under exchange become more complicated. We see that we can either have *symmetric* or *anti-symmetric* cases.

$$|ab, S\rangle = |ab\rangle + |ba\rangle \quad (75)$$

$$|ab, A\rangle = |ab\rangle - |ba\rangle \quad (76)$$

A given species of particles must choose between Symmetric and Anti-Symmetric(they will always follow the same rules). We see this divides up into bosons and fermions.

1. Bosons: Symmetric (Pion, photon, graviton)
2. Fermions: Anti-Symmetric (Electron, proton, neutron)
 - Pauli-Exclusion Principle: Two fermions cannot be in the same state.

We find though that there is an additional difficulty in writing the normalized state vector, this will result in an extra factor of 2. To integrate over the usual area, write the normalized state vector as

$$|\omega_1\omega_2, S\rangle = \frac{1}{\sqrt{2}}[|x_1x_2\rangle + |x_2x_1\rangle] \quad (77)$$

The corresponding wave function (note only asymmetric is also written in the form

$$\psi_A(x_1, x_2) = 2^{-1/2}[\psi_3(x_1)\psi_4(x_2) - \psi_4(x_1)\psi_3(x_2)] = 2^{-1/2} \begin{vmatrix} \psi_3(x_1) & \psi_4(x_1) \\ \psi_3(x_2) & \psi_4(x_2) \end{vmatrix} \quad (78)$$

10 Symmetries and Their Consequences

10.1 Translational Invariance in Quantum Theory

The translation operator is given $T(\epsilon)$. The Operators are modified as

$$T^\dagger(\epsilon)XT(\epsilon) = X + \epsilon I$$

$$T^\dagger(\epsilon)PT(\epsilon) = P$$

The impact on a ket of definite position $|x\rangle$ is the following

$$T(\epsilon)|x\rangle = |x + \epsilon\rangle \quad (79)$$

$$\langle x|T(\epsilon)|\psi\rangle = \psi(x - \epsilon) \quad (80)$$

This translation operator is defined as follows

$$T(\epsilon) = I - \frac{i\epsilon}{\hbar}P$$

Also interesting is that any $\Omega(x, p)$ which can be expanded in a power series, for any unitary operator U we have.

$$U^\dagger\omega(x, p)U = \Omega(U^\dagger XU, U^\dagger PU)$$

Applying this to the case $U = T(\epsilon)$ we see

$$\Omega(x, p) \rightarrow \Omega(T^\dagger XT, T^\dagger PT)$$

so we get the more important definition of translation invariance

$$H(X + \epsilon I, P) = H(X, P)$$

We can also see that there is a unique correspondence between an infinitesimal canonical transformation generated by $g(x, p)$ and a unitary transformation generated by $G(X, P)$.

10.2 Time translation

The Hamiltonian is the generator of translations in time. Therefore the Time-translation operator goes as

$$T(\epsilon_t) = [I - \frac{i\epsilon}{\hbar}H]$$

10.3 Parity Invariance

Classically the parity operation refers to the action of reflecting the particle through the origin.

$$x \rightarrow -x$$

$$p \rightarrow -p$$

However, there is no conservation law associated with parity invariance in classical mechanics as this is a discrete operation. In quantum theory, we similarly define this as the following.

$$\hat{\Pi} |x\rangle = |-x\rangle$$

$$\hat{\Pi} |p\rangle = |-p\rangle$$

We see the action of this operator on a state $|\psi\rangle$ is

$$\langle x | \hat{\Pi} |\psi\rangle = \psi(-x)$$

Here are some other properties of the parity operator

1. $\hat{\Pi}^2 = I$
2. $\hat{\Pi} = \hat{\Pi}^{-1}$
3. The eigenvalues of $\hat{\Pi}$ at ± 1 .
4. $\hat{\Pi}$ is hermetian and unitary.
5. Or $\hat{\Pi}^{-1} = \hat{\Pi}^\dagger = \hat{\Pi}$

We also say that $H(x,p)$ is parity invariant if $[\hat{\Pi}, H] = 0$.

The big difference between parity and other types of symmetries is that if a certain phenomena can happen, its translated or rotated versions can also happen, but if the phenomena involves weak interactions, than its mirrored version cannot happen.

10.4 Time-Reversal Symmetry

We define a time reversed state as one where the position is the same, but the momentum is reversed $x_r(t) = x(t)$ and $p_r(t) = -p(t)$. We can think of this in the context of a real planet in orbit. We can then take the following two videos

1. Can take a video of the real planet's orbit and run it in reverse.
2. Can take a planet which follows the opposite trajectory.

The question is whether or not we can tell the difference between these two videos. Time reversal symmetry is broken if you can tell the difference between these two movies.

Magnetic fields do not have time reversal invariance, even in classical mechanics.