Quantum PS2

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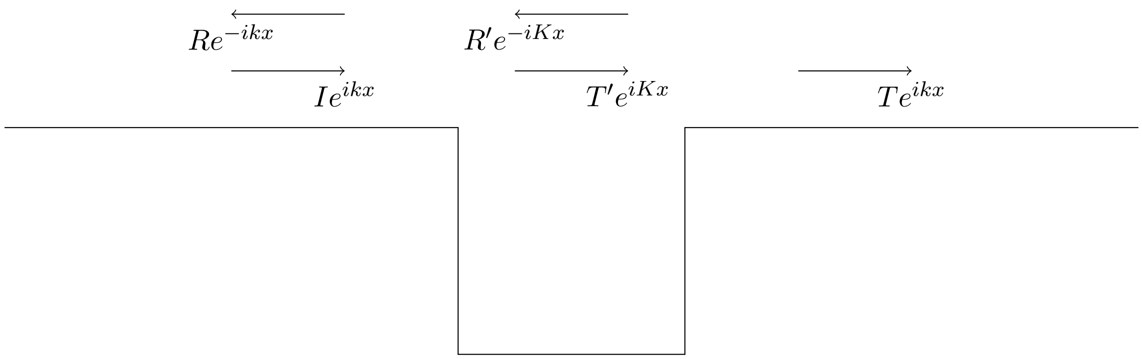
1 1.6) Well Scattering

A free particle of energy E approaches a square, one-dimensional potential well of depth V_0 and width $2a$. Show that the probability of being reflected by the well vanishes when $Ka = \frac{n\pi}{2}$, where n is an integer and $K = \left(\frac{2m(E+V_0)}{\hbar^2}\right)^{\frac{1}{2}}$. Explain this phenomenon in physical terms. [7]

We can use what we learnt from previous problems to set this up quickly. It should be obvious what the wavefunctions in each region are.



The boundary conditions at each boundary are continuity of the wavefunction and its derivative. So at boundary one

$$Ie^{-ika} + Re^{ika} = T'e^{-iKa} + R'e^{iKa},$$

$$Ike^{-ika} - Rke^{ika} = T'Ke^{-iKa} - R'Ke^{iKa}$$

and at the second boundary,

$$T'e^{iKa} + R'e^{-iKa} = Te^{ika},$$

$$T'Ke^{iKa} - R'Ke^{-iKa} = Tke^{ika}.$$

We can formulate this as a matrix problem. We start by setting $R = 0$ and then consider that

$$\begin{pmatrix} Ie^{-ika} \\ Ike^{-ika} \end{pmatrix} = \begin{pmatrix} e^{-iKa} & e^{iKa} \\ Ke^{-iKa} & -Ke^{iKa} \end{pmatrix} \begin{pmatrix} T' \\ R' \end{pmatrix},$$

$$\begin{pmatrix} Te^{ika} \\ Tke^{ika} \end{pmatrix} = \begin{pmatrix} e^{iKa} & e^{-iKa} \\ Ke^{iKa} & -Ke^{-iKa} \end{pmatrix} \begin{pmatrix} T' \\ R' \end{pmatrix}.$$

It is remarkably simply to take the inverse of these matrices as the determinant is simply $-2K$ in both cases. Thus, introducing $x = e^{ika}$ and $y = e^{iKa}$,

$$\begin{pmatrix} T' \\ R' \end{pmatrix} = \frac{1}{2K} \begin{pmatrix} Ky & y \\ K/y & -1/y \end{pmatrix} \begin{pmatrix} I/x \\ Ik/x \end{pmatrix}$$

$$\begin{pmatrix} T' \\ R' \end{pmatrix} = \frac{1}{2K} \begin{pmatrix} K/y & 1/y \\ Ky & -y \end{pmatrix} \begin{pmatrix} Tx \\ Tkx \end{pmatrix}$$

and therefore

$$\begin{pmatrix} Ky & y \\ K/y & -1/y \end{pmatrix} \begin{pmatrix} I/x \\ Ik/x \end{pmatrix} = \begin{pmatrix} K/y & 1/y \\ Ky & -y \end{pmatrix} \begin{pmatrix} Tx \\ Tkx \end{pmatrix}$$

$$I \begin{pmatrix} Ky/x + ky/x \\ K/xy - k/xy \end{pmatrix} = T \begin{pmatrix} Kx/y + kx/y \\ Kxy - kxy \end{pmatrix}.$$

We now divide the equation by each other to find our consistency equation,

$$\frac{Ky/x + ky/x}{K/xy - k/xy} = \frac{Kx/y + kx/y}{Kxy - kxy}$$

$$(Ky)^2 - (ky)^2 = \left(\frac{K}{y}\right)^2 - \left(\frac{k}{y}\right)^2$$

$$2i(K^2 - k^2)\sin(2Ka) = 0$$

$$\implies Ka = \frac{n\pi}{2}$$

as required.

The physics for this result is the same as that for an anti-reflection coating on glass. As the wave enters, part of it gets reflected straight away. However, another contribution comes from the ray that enters the well, reflects off the other side and then comes all the way back. These two waves add to give the total final reflection. It must then be the case that when $Ka = \frac{n\pi}{2}$ these two waves interfere destructively and hence the total intensity becomes zero.

2 1.7) Peak Scattering

A particle of energy E approaches from $x < 0$ a barrier in which the potential energy is $V(x) = V_\delta \delta(x)$. Show that the probability of its passing the barrier is

$$P_{\text{tun}} = \frac{1}{1 + (K/2k)^2} \qquad \text{where} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad K = \frac{2mV_\delta}{\hbar^2}.$$

[4]

This is a fairly simple scattering problem. The key difference is that our wavefunction's gradient is now discontinuous at the origin. To see this integrate the TISE over the origin,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2m(V-E)}{\hbar^2}\psi$$

$$\left.\frac{\partial \psi}{\partial x}\right|_{\epsilon} - \left.\frac{\partial \psi}{\partial x}\right|_{-\epsilon} = \int_{-\epsilon}^{\epsilon} \frac{2m(V-E)}{\hbar^2}\psi.$$

E is just a constant so the integral over that is zero but $V(x) = V_\delta \delta(x)$, which has non-zero integral over this infinitesimal range,

$$\Delta \frac{\partial \psi}{\partial x}(0) = \frac{2mV_\delta}{\hbar^2}\psi(0).$$

Thus, consider waves in and waves out again and apply the boundary conditions.

$$I + R = T$$

$$(ikI - ikR) - ikT = KT.$$

Eliminating R,

$$2ikI - 2ikT = KT.$$

Given both sides are at the same height, and therefore the same speed, we simply need $\left|\frac{T}{I}\right|^2$ to give the tunelling amplitude,

$$\frac{T}{I} = \frac{2ik}{2ik + K} \qquad \Longrightarrow \qquad P_{tun} = \frac{1}{1 + (K/2k)^2}.$$

3 1.9) Expectations

Let $\psi(x,t)$ be the correctly normalised wavefunction of a particle of mass m and potential energy $V(x)$. Write down expressions for the expectation values of (a) $\hat{x}$; (b) $\hat{x}^2$; (c) the momentum $\hat{p}_x$; (d) $\hat{p}_x^2$; (e) the energy.
What is the probability that the particle will be found in the interval (x_1, x_2)? [4]

In bra-ket notation everything is obvious. The expectation of some operator, O, is

$$\langle O \rangle = \langle \psi | \hat{O} | \psi \rangle .$$

To convert these to integrals we simply insert the identity operator,

$$\langle O \rangle = \int \mathrm{d}x \, \langle \psi | x \rangle \, O(x) \, \langle x | \psi \rangle$$

where this integral is over the range of ψ.

Thus,

$$\langle x \rangle = \int \mathrm{d}x x \, |\psi(x,t)|^2 ,$$

$$\langle x^2 \rangle = \int \mathrm{d}x x^2 \, |\psi(x,t)|^2 ,$$

$$\langle p_x \rangle = \int \mathrm{d}x \bar{\psi}(x,t) \, (-i\hbar\partial_x) \, \psi(x,t),$$

$$\langle p_x^2 \rangle = \int \mathrm{d}x \bar{\psi}(x,t) \left(-\hbar^2\partial_x^2\right) \psi(x,t),$$

$$E = \int \mathrm{d}x \bar{\psi}(x,t) \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x) \right) \psi(x,t).$$

Finally, we want the probability that we are in a particular range. We know that $|\psi(x,t)|^2$ is just the probability density so

$$P(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x |\psi(x,t)|^2 .$$

4 2.1) Position Representation

How is a wavefunction $\psi(x)$ written in Dirac notation? What's the physical significance of the complex number $\psi(x)$ for a given x? [2]

It's clearer to answer this question in reverse. $\psi(x)$ describes the amplitude for our state $|\psi\rangle$ to be measured in the range x to $x + \mathrm{d}x$. The state of being in the range x to $x + \mathrm{d}x$ is $|x\rangle$. Thus, clearly

$$\psi(x) = \langle x|\psi\rangle \,.$$

5 2.2) Adjoint States

Given that $|\psi\rangle = e^{\frac{i\pi}{5}} |a\rangle + e^{\frac{i\pi}{4}} |b\rangle$, express $\langle\psi|$ as a linear combination of $|a\rangle$ and $|b\rangle$. [1]

To turn a bra into a ket we take the complex conjugate of the coefficients, so

$$\langle\psi| = e^{-\frac{i\pi}{5}} \langle a| + e^{-\frac{i\pi}{4}} \langle b| \,.$$

This way of defining bras ensures that our norms, $\langle\psi|\psi\rangle$, are always real and non-negative.

6 2.3) Tunnelling

An electron can be in one of two potential wells that are so close that it can 'tunnel' from one to the other. Its state vector can be written

$$|\psi\rangle = a\,|A\rangle + b\,|B\rangle\,,$$

where $|A\rangle$ is the state of being in the first well and $|B\rangle$ is the state of being in the second well and all kets are correctly normalised. What is the probability of finding the particle in the first well given that: (a) $a = \frac{i}{2}$; (b) $b = e^{i\pi}$; (c) $b = \frac{1}{3} + \frac{i}{\sqrt{2}}$? [2]

Our state is normalised, which means

$$\langle\psi|\psi\rangle = |a|^2 + |b|^2 = 1.$$

Now, the probability of being in the first well is

$$|\langle A|\psi\rangle|^2 = |a|^2.$$

This is equivalent to $1 - |b|^2$ due to the normalisation. As such,

$$P_a = \frac{1}{4},$$

$$P_b = 1 - 1 = 0,$$

$$P_c = 1 - \left(\frac{1}{9} + \frac{1}{2}\right) = \frac{7}{18}.$$

7 2.4) Operators

Let $\hat{Q}$ be the operator of an observable and let $|\psi\rangle$ be the state of our system.
(a) What are the physical interpretations of $\langle\psi|\hat{Q}|\psi\rangle$ and $|\langle q_n|\psi\rangle|^2$, where $|q_n\rangle$ is the n^{th} eigenket of the observable Q and q_n is the corresponding eigenvalue?
(b) What is the operator $\sum_n |q_n\rangle\langle q_n|$, where the sum is over all eigenkets of $\hat{Q}$? What is the operator $\sum_n q_n |q_n\rangle\langle q_n|$?
(c) If $u_n(x)$ is the wavefunction of the state $|q_n\rangle$, write down an integral that evaluates to $\langle q_n|\psi\rangle$.
[5]

(a) When we sandwich the operator in between two states we get the expectation value of Q in the state $|\psi\rangle$,

$$\langle Q\rangle = \langle\psi|\hat{Q}|\psi\rangle \,.$$

The overlap of $|q_n\rangle$ with ψ then gives us the amplitude to measure the system in the individual state $|q_n\rangle$. Mod squaring gives the probability,

$$P(\text{system measured in state } q_n) = |\langle q_n|\psi\rangle|^2 \,.$$

(b) For these operators it is easiest to see how they act on some general state,

$$|\psi\rangle = \sum_n a_n |q_n\rangle$$

where a_n is the amplitude to measure our system in the q_n state. Thus,

$$\left(\sum_m |q_m\rangle\langle q_m|\right)\sum_n a_n |q_n\rangle = \sum_{n,m} a_n |q_m\rangle\langle q_m|q_n\rangle$$

but these $|q_n\rangle$ are orthonormal so $\langle q_m|q_n\rangle = \delta_{n,m}$ and

$$\left(\sum_m |q_m\rangle\langle q_m|\right)\sum_n a_n |q_n\rangle = \sum_n a_n |q_n\rangle \,.$$

This operator is the identity.

For the second operator consider the action simply on one of these eigenkets,

$$\left(\sum_n q_n |q_n\rangle\langle q_n|\right)|q_k\rangle = \sum_n q_n |q_n\rangle \delta_{n,k} = q_k |q_k\rangle \,.$$

Thus, this operator is simply $\hat{Q}$, as it's action on any eigenket returns the eigenvalue.

(c) We are told that

$$\langle x|q_n\rangle = u_n(x).$$

Thus,

$$\langle q_n|\psi\rangle = \int \mathrm{d}x \,\langle q_n|x\rangle\langle x|\psi\rangle$$

where we have inserted the identity in the x-basis (note the similarity to the identity in the q_n-basis, but x is continuous so we need an integral instead of a sum). Thus,

$$\langle q_n|\psi\rangle = \int \mathrm{d}x u_n^*(x)\psi(x).$$

8 2.5) Schrödinger Equations

Write down the time-independent (TISE) and the time-dependent (TDSE) Schrödinger equations. Is it necessary for the wavefunction of a system to satisfy the TDSE? Under what circumstances does the wavefunction of a system satisfy the TISE? [2]

The TISE is

$$H|\psi\rangle = E|\psi\rangle$$

and the TDSE is

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle .$$

All wavefunctions must satisfy the TDSE but the TISE is only satisfied by *stationary* states. These are states whose form does not change in time except for an overall (and unimportant) phase factor, $e^{-\frac{it}{\hbar}E}$.

9 2.6) Order of the TDSE

Why is the TDSE first-order in time, rather than second-order like Newton's equations of motion? [2]

Our wavefunction, $|\psi\rangle$, contains a complete set of information about our physical system, including all the initial conditions. Therefore, with only some initial state, all time-evolution should be computable without any additional information. If the TDSE were second order like Newton's equations of motion then we'd also need to know $\partial_t |\psi\rangle$ at t_0, which would suggest that $|\psi\rangle$ were not a complete set of information about the state of the system.

So can we do the same for Newton's laws? Yes, if we work in phase space,

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{F} \qquad\qquad m\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{p}.$$

Therefore, defining $\boldsymbol{Y} = (\boldsymbol{p}, \boldsymbol{x})$ as our phase space variable we have

$$\frac{\mathrm{d}\boldsymbol{Y}}{\mathrm{d}t} = \begin{pmatrix} \boldsymbol{F} \\ \frac{\boldsymbol{p}}{m} \end{pmatrix}.$$