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Practice for Qualifying Exams

Problem Source: **CMU Qualification Exam Day 2 (August 2005)**

Consider a particle of mass m moving in a one-dimensional potential with infinitely high walls placed at $x = \pm a$. The potential vanishes between the walls.

(a) Write down the eigenenergies and the corresponding eigenstates of the system in the x basis.

The eigenstates, even and odd, are

$$\psi_n(x) = C_n e^{i\frac{n\pi}{2a}x} + C_{-n} e^{-i\frac{n\pi}{2a}x}$$

with the constants chosen to satisfy $\psi_n(a) = \psi_n(-a) = 0$. The particular constants are not relevant in this problem since both exponentials have the same energy eigenfunction,

The corresponding eigen-energies are given by:

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

For:

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2$$

(b) Suppose that at time t = 0, the particle is in a state that can be well approximated by the wave function

$\psi(x) = Ne^{-\frac{x^2}{\delta^2}}$**, where** $\delta << a$**.**

(i) Determine N and then determine the wave function at some later time t_0**.**

$$\int_{-\infty}^{\infty} \psi^2(x)dx = \int_{-\infty}^{\infty} e^{-\frac{2}{\delta^2}x^2} dx$$

$$\left[\int_{-\infty}^{\infty} \psi^2(x)dx\right]^2 = \int_{-\infty}^{\infty} e^{-\frac{2}{\delta^2}x^2} dx \int_{-\infty}^{\infty} e^{-\frac{2}{\delta^2}y^2} dy = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{2}{\delta^2}\left(x^2+y^2\right)} dxdy = \int_0^{2\pi}\int_0^{\infty} e^{-\frac{2}{\delta^2}r^2} rdrd\theta$$

$$= 2\pi\left[\frac{\delta^2}{2}\right]$$

$$\int_{-\infty}^{\infty} \psi^2(x)dx = \delta\sqrt{\pi} \qquad N = \frac{1}{\delta\sqrt{\pi}}$$

The wave function at a later time is given by

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$
$$\Psi(x,t) = \psi(x)\phi(t)$$
$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial}{\partial x}\left[\left[-\frac{4}{\delta^2}x\right]\psi(x)\right]\phi(t) = \frac{-\hbar^2}{2m}\left[\left[-\frac{4}{\delta^2}\right]+\left[\frac{16}{\delta^4}x^2\right]\right]\psi(x)\phi(t)$$
$$= \frac{-\hbar^2}{2m}\frac{4}{\delta^2}\left[\frac{4}{\delta^2}x^2 - 1\right]\psi(x)\phi(t)$$

Results of this form indicate that separation of variables is not possible in this case. I'll use another method. I assume in this integral that since $\delta << a$, and so coefficient on the n-th component of the wave function is:

$$\rho_n(t=0) = \int_{-\infty}^{\infty}\psi_n(x)e^{-\frac{x^2}{\delta^2}}dx$$
$$= C_n N\int_{-\infty}^{\infty}e^{i\frac{n\pi}{2a}x}e^{-\frac{x^2}{\delta^2}}dx + C_{-n}N\int_{-\infty}^{\infty}e^{-i\frac{n\pi}{2a}x}e^{-\frac{x^2}{\delta^2}}dx$$
$$= C_n N\int_{-\infty}^{\infty}e^{-\frac{1}{\delta^2}\left(-i\frac{n\pi}{2a}\delta^2 x + x^2\right)}dx + C_{-n}N\int_{-\infty}^{\infty}e^{-\frac{1}{\delta^2}\left(i\frac{n\pi}{2a}\delta^2 x + x^2\right)}dx$$
$$= C_n N\int_{-\infty}^{\infty}e^{\frac{1}{\delta^2}\left(i\frac{n\pi}{4a}\delta^2\right)^2}e^{-\frac{1}{\delta^2}\left(\left(i\frac{n\pi}{4a}\delta^2\right)^2 - i\frac{n\pi}{2a}\delta^2 x + x^2\right)}dx + C_{-n}N\int_{-\infty}^{\infty}e^{\frac{1}{\delta^2}\left(i\frac{n\pi}{4a}\delta^2\right)^2}e^{-\frac{1}{\delta^2}\left(\left(i\frac{n\pi}{4a}\delta^2\right)^2 + i\frac{n\pi}{2a}\delta^2 x + x^2\right)}dx$$
$$= C_n N e^{-\frac{1}{\delta^2}\left(\frac{n\pi}{4a}\delta^2\right)^2}\int_{-\infty}^{\infty}e^{-\frac{1}{\delta^2}\left(x - i\frac{n\pi}{4a}\delta^2\right)^2}dx + C_{-n}N e^{-\frac{1}{\delta^2}\left(\frac{n\pi}{4a}\delta^2\right)^2}\int_{-\infty}^{\infty}e^{-\frac{1}{\delta^2}\left(x + i\frac{n\pi}{4a}\delta^2\right)^2}dx$$
$$= C_n e^{-\left(\frac{n\pi}{4a}\delta\right)^2} + C_{-n}e^{-\left(\frac{n\pi}{4a}\delta\right)^2}$$

and since

$$1 = C_n^2\int_{-a}^{a}e^{i\frac{n\pi}{2a}x}e^{-i\frac{n\pi}{2a}x}dx + C_{-n}^2\int_{-a}^{a}e^{i\frac{n\pi}{2a}x}e^{-i\frac{n\pi}{2a}x}dx$$
$$C_n = \pm C_{-n} = \sqrt{\frac{1}{4a}}$$
$$where \quad + \to even \quad - \to odd$$

I have:

$$\rho_{n\ even}(t=0) = 2\sqrt{\frac{1}{4a}}e^{-\left(\frac{n\pi}{4a}\delta\right)^2}$$
$$\rho_{n\ odd}(t=0) = 0$$

Having broken this Gaussian down into its frequency components, now I may find the time-dependent portion:

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi_n(x,t) = i\hbar\frac{\partial}{\partial t}\Psi_n(x,t)$$
$$\Psi(x,t) = \psi(x)\phi(t)$$
$$\frac{-\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2\psi(x)\phi(t) = i\hbar\psi(x)\frac{\partial}{\partial t}\phi(t)$$
$$\frac{-\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2\phi(t) = i\hbar\frac{\partial}{\partial t}\phi(t)$$
$$\frac{i\hbar}{2m}\left(\frac{n\pi}{2a}\right)^2\phi(t) = \frac{\partial}{\partial t}\phi(t)$$
$$\phi_n(t) = B_n e^{\frac{i\hbar}{2m}\left(\frac{n\pi}{2a}\right)^2 t}$$
$$\phi_n(t)\phi^*{}_n(t) = 1 = B_n$$
Finally, then, I may decompose my Gaussian into the components
$$\Psi(x,t_0) = \sum_{n=1}^{\infty}\rho_n(t=0)\psi_n(x)\phi_n(t_0)$$
$$= \sum_{n=2,4,6,\ldots}^{\infty}\frac{1}{\sqrt{a}}e^{-\left(\frac{n\pi}{4a}\delta\right)^2}\left[\frac{1}{a}\right]\left(e^{i\frac{n\pi}{2a}x} + e^{-i\frac{n\pi}{2a}x}\right)e^{\frac{i\hbar}{2m}\left(\frac{n\pi}{2a}\right)^2 t_0}.$$
$$= \frac{1}{a^{\frac{3}{2}}}\sum_{n=2,4,6,\ldots}^{\infty}e^{-\left(\frac{n\pi}{4a}\delta\right)^2}\left(e^{i\frac{n\pi}{2a}x} + e^{-i\frac{n\pi}{2a}x}\right)e^{\frac{i\hbar}{2m}\left(\frac{n\pi}{2a}\right)^2 t_0}$$

(ii) What is the probability of finding the particle in the n-th energy state at some later time t_0?

Using the result above, the result is simply

$\int_{-a}^{a}|\rho_n(t=0)|^2\,dx$ since $\psi_n(x)$ is normal and non-degenerate, or

$$P_n(t_0) = \begin{cases} 0 & : \quad n \quad odd \\ 2e^{-2\left(\frac{n\pi}{4a}\delta\right)^2} & : \quad n \quad odd \end{cases}$$

Thanks to LC for pointing out mistakes in part (a) and (b).

(c) Suppose that the width of the well is now taken to be zero in such a way as the potential can be written

$$V(x) = -|V_0|\delta(x)$$

where V_0 is a constant. Does this system have a bound state? If so, what is the wave function and energy eigenvalue. If not, explain why not.

The time-independent Schrodinger equation gives

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x)$$

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0\delta(x)\right]\psi(x) = E\psi(x)$$

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0\psi(0)\right]\psi(x) = E\psi(x)$$

Now propose that the solution has the form $\psi(x) = Ne^{-a|x|}$. In this case, I have

$$\psi(0) = N$$

$$\frac{1}{N^2} = 2\int_0^\infty e^{-2ax}$$

$$\frac{\partial}{\partial x}|x| = -\theta(-x) + \theta(x)$$

$$\frac{\partial^2}{\partial x^2}|x| = 2\delta(x)$$

$$\frac{\partial^2}{\partial x^2}e^{-a|x|} = -a\frac{\partial}{\partial x}\left[\frac{\partial|x|}{\partial x}e^{-a|x|}\right] = -a\left[\frac{\partial^2|x|}{\partial x^2}e^{-a|x|} - a\left(\frac{\partial|x|}{\partial x}\right)^2 e^{-a|x|}\right]$$

$$= \left[2\delta(x)e^{-a|x|} - a(\theta(x) - \theta(-x))^2 e^{-a|x|}\right] = \left[-2a\delta(x)e^{-a|x|} + a^2(\theta(x) - \theta(-x))^2 e^{-a|x|}\right]$$

$$= \left[-2a\delta(x) + a^2\right]e^{-a|x|}$$

Thus,

$$-\frac{\hbar^2}{2m}[-2a] - V_0 = 0$$

$$a = \frac{mV_0}{\hbar^2}$$

Next, I have

$$\frac{1}{N^2} = 2\int_0^\infty e^{-2ax}dx = \frac{1}{a}$$

$$N = \sqrt{a}$$

$$\psi(x) = \sqrt{\frac{mV_0}{\hbar^2}}e^{-\frac{mV_0}{\hbar^2}|x|}$$

With energy eigenvalue given by

$$E = \frac{-\hbar^2}{2m}\left[a^2\right] = -\frac{\hbar^2}{2m}\left[\frac{m^2V_0^2}{\hbar^2}\right] = -\frac{mV_0^2}{2\hbar^2}$$

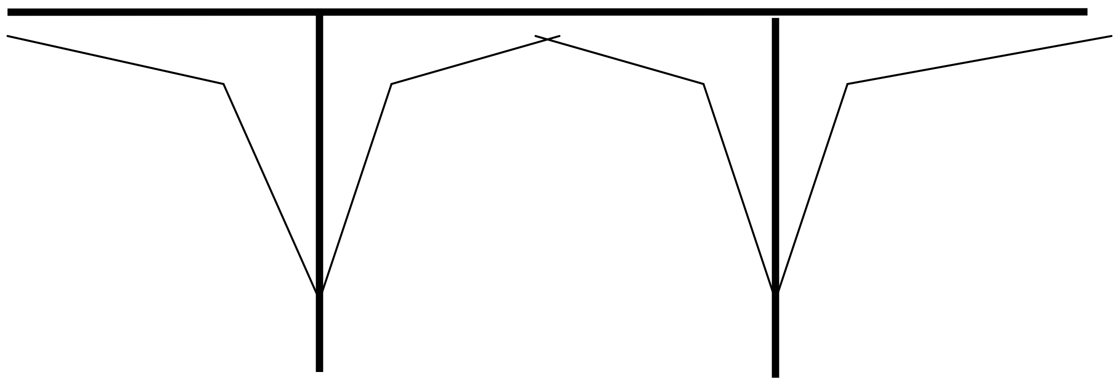
(d) Suppose now that we generalize the potential to look like:

$$V(x) = -|V_0|\delta(x-a) - |V_0|\delta(x+b).$$

Consider the case $a = b$. What operator commutes with the Hamiltonian that would not if $a \neq b$?

Due to symmetry, the parity operator would commute with the Hamiltonian, as opposed to the case where $a \neq b$.

(e) Draw the wave function in the x representation of the lowest energy eigenstate of the system. Do you expect the particle to be more strongly bound in the double well case or the single well case? Explain your answer.



Classically, I wouldn't expect the particle to be any more strongly bound with two wells of the same depth than with one. Quantum-mechanically, then, it certainly seems implausible that the binding could possibly get worse, however the binding might be slightly better.

(f) Now consider the case where $a \neq b$. Does the number of operators that commutes with the Hamiltonian change?

No. Regardless of the choice of a and b, by a suitable shift of the coordinate system I may find a system under which this case is identical to a case where $a = b$.