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Problems set # 8	**Physics 400**	April 4, 2019

1. A particle of mass m moving in one dimension is confined to a space $0 < x < L$ by an infinite well potential. In addition, the particle experiences a delta function potential of strength λ given by $\lambda\delta(x - L/2)$ located at the center of the well. Find a transcendental equation for the energy eigenvalues E in terms of the mass m, the potential strength λ, and the size of the well L.

2. A repulsive short-range potential with a strongly attractive core can be approximated by a square barrier with a delta function at its center, namely,

$$V(x) = V_0\Theta(|x| - a) - \frac{\hbar g^2}{2m}\delta(x)$$

(i) Show that there is a negative energy eigenstate (the ground-state). *(ii)* If E_0 is the ground-state energy of the delta-function potential in the absence of the positive potential barrier, then the ground-state energy of the present system satisfies the relation $E \geq E_0 + V_0$. What is the particular value of V_0 for which we have the limiting case of a ground-state with zero energy.

3. Consider a one-dimensional potential with a step-function component and an attractive delta function component just at the edge of the step, namely,

$$V(x) = V\Theta(x) - \frac{\hbar^2 g}{2m}\delta(x)$$

(i) For $E > V$, compute the reflection coefficient for particle incident from the left. How does this result differ from that of the step barrier alone at high energy? *(ii)* For $E < 0$ determine the energy eigenvalues and eigenfunctions of any bound-state solutions.

4. A particle of mass m is confined to a space $0 < x < a$ in one dimension by infinitely high walls at $x = 0$ and $x = a$. At $t = 0$ the particle is initially in the left half of the well with a wave function given by

$$\Psi(x,0) = \begin{cases} \sqrt{2/a} & 0 < x < a/2 \\ 0 & a/2 < x < a \end{cases}$$

(i) Find the time-dependent wave function $\Psi(x,t)$. *(ii)* What is the probability that the particle is in the n-th eigenstate of the well at time t? *(iii)* Derive an expression for average value of particle energy. What is the physical meaning of your result?

5. An electron moves in one dimension and is confined to the right half-space ($x > 0$) where it has potential energy

$$V(x) = -\frac{e^2}{4x}$$

where e is the electron charge. The corresponding Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{e^2}{4x}\psi = E\psi = -|E|\psi\,,$$

since $E < 0$ for a bound state. *(i)* What is the solution of the Schrödinger equation at large x? *(ii)* What is the boundary condition at $x = 0$? *(iii)* Use the results of *(i)* and *(ii)* to guess the ground state solution of the equation. Remember the ground state wave function has no zeros except at the boundaries. *(iv)* Find the ground state energy. *(v)* Find the expectation value $\langle \hat{x} \rangle$ in the ground state.

SOLUTIONS

1.

We have two regions to consider:

Region I: $0 \le x \le L/2$ The solution is

$$\psi_I(x) = A_1 \sin kx$$

which already incorporates the boundary condition $\psi_I(x=0) = 0$.

Region II: $L/2 \le x \le L$ The solution is

$$\psi_{II}(x) = A_2 \sin k(x-L)$$

which already incorporates the boundary condition $\psi_{II}(x=L) = 0$.

At $x = L/2$, we have

$$\psi_I(x = L/2) = \psi_{II}(x = L/2) \rightarrow A_1 = A_2$$

The first derivative is discontinuous at $x = L/2$ and we have

$$\psi'_{II}(x = L/2) - \psi'_I(x = L/2) = \frac{2m\lambda}{\hbar^2}\psi_I(x = L/2)$$

or

$$-A_1 k \cos\frac{kL}{2} - A_1 k \cos\frac{kL}{2} = \frac{2m\lambda}{\hbar^2}\sin\frac{kL}{2} \rightarrow \tan\frac{kL}{2} = -\frac{\hbar^2}{m\lambda}k$$

Therefore, we have a transcendental equation for

$$k \rightarrow E = \frac{\hbar^2 k^2}{2m}$$

2. Let us define

$$\kappa^2 = \frac{2m\,|E|}{\hbar^2} \quad , \quad q^2 = \frac{2m(|E| + V_0)}{\hbar^2} \quad , \quad \beta^2 = \frac{2mV_0}{\hbar^2}$$

The Schrodinger equation is

$$\begin{array}{ll} \psi'' = \kappa^2 \psi & |x| > a \\ \psi'' = q^2 \psi & |x| < a \end{array}$$

The discontinuity at the origin gives

$$\psi'(0+) - \psi'(0-) = -g^2 \psi(0)$$

Odd parity solutions do not see the attractive delta function (they must be zero at the origin) and thus cannot exist for $E < 0$. Even parity solutions of the above equations have the form

$$\psi(x) = \begin{cases} Ae^{-\kappa|x|} & |x| > a \\ Be^{q|x|} + Ce^{-q|x|} & |x| < a \end{cases}$$

Continuity at $x = a$ and $x = 0$ leads to the condition (eigenvalue equation)

$$e^{2qa} \left(\frac{1 - g^2/2q}{1 + g^2/2q} \right) = \frac{q - \kappa}{q + \kappa}$$

In the case of vanishing V_0, we recover the equation

$$E_0 = -\frac{\hbar^2}{2m} \left(\frac{g^2}{2} \right)^2$$

appropriate to a delta function well.

Since the RHS of the eigenvalue equation is always positive, we necessarily have

$$1 - g^2/2q > 0 \Rightarrow \frac{2m}{\hbar^2}(-E + V_0) \geq \frac{g^4}{4}$$

or

$$E \leq V_0 - \frac{\hbar^2}{2m} \left(\frac{g^2}{2} \right)^2 = V + E_0$$

One can see graphically that the above eigenvalue equation has only one solution, by defining

$$\xi = qa \quad , \quad \lambda = \frac{g^2 a}{2} \quad , \quad b = \beta a$$

Then, we have

$$e^{2\xi}\left(\frac{\xi-\lambda}{\xi+\lambda}\right)=\frac{\xi-\sqrt{\xi^2-b^2}}{\xi+\sqrt{\xi^2-b^2}}$$

The solution exists provided that $\lambda \geq b$. In the limiting case, $\lambda = b$, or, equivalently,

$$\beta^2=\frac{2mV_0}{\hbar^2}=\frac{g^4}{4}$$

we get a vanishing ground state energy.

3. *(i)* The wave function will be of the form

$$\psi(x)=\begin{cases} e^{ikx}+Be^{-ikx} & x<0 \\ Ce^{ikx} & x>0 \end{cases}$$

with

$$k=\sqrt{\frac{2mE}{\hbar}} \quad , \quad q=\sqrt{\frac{2m(E-V)}{\hbar}}$$

Continuity of the wave function at $x=0$ gives

$$1+B=C$$

Integrating the Schrodinger equation over the infinitesimal interval around the origin gives

$$\begin{array}{l} -\frac{\hbar^2}{2m}\left(\psi'(0+)-\psi'(0-)\right)=\frac{\hbar^2 g}{2m}\psi(0) \\ 1-B=-\frac{i}{k}(g+iq)C \end{array}$$

From the two relationships between B and C we obtain

$$\begin{array}{l} C=\frac{2}{1+q/k-ig/k} \\ B=\frac{1-q/k+ig/k}{1+q/k-ig/k} \end{array}$$

The reflection coefficient is

$$\Re=\left|\frac{j_r}{j_l}\right|=\frac{(\hbar k/m)\left|B\right|^2}{\hbar k/m}=\left|\frac{1-q/k+ig/k}{1+q/k-ig/k}\right|^2=\frac{(1-q/k)^2+g^2/k^2}{(1+q/k)^2+g^2/k^2}$$

In the high energy limit we have

$$\Re = \frac{g\hbar^2}{8mE}$$

For the pure step barrier we have (in the same limit)

$$\Re = \frac{V^2}{8E^2}$$

which drops off faster with energy.

(ii) In order to study the case of negative energy, $E < 0$, it is convenient to introduce the notation

$$\kappa_- = \sqrt{\frac{2m\,|E|}{\hbar^2}} \quad , \quad \kappa_+ = \sqrt{\frac{2m(V+|E|)}{\hbar^2}}$$

Then we can write the bound-state wave function as

$$\psi(x) = \begin{cases} Ae^{\kappa_- x} & x < 0 \\ Ae^{-\kappa_+ x} & x > 0 \end{cases}$$

The discontinuity at the origin implies that

$$-\tfrac{\hbar^2}{2m}(-A\kappa_+ - A\kappa_-) = \tfrac{\hbar^2 g}{2m}A$$
$$\kappa_+ + \kappa_- = g$$

This then gives

$$E = -\frac{m}{2\hbar^2 g^2}\left(\frac{\hbar^2 g^2}{2m} - V\right)^2$$

and

$$\kappa_\pm^2 = \frac{m^2}{\hbar^4 g^2}\left(\frac{\hbar^2 g^2}{2m} \pm V\right)^2$$

and

$$A = \sqrt{\frac{2\kappa_+\kappa_-}{g}}$$

4. *(i)* The eigenfunctions and eigenvalues of $\hat{H}$ for this system are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad , \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \; n = 1, 2, 3, \ldots\ldots$$

We then have

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-iE_n t/\hbar}$$

We evaluate the a_n coefficients using the initial wavefunction

$$\psi(x,0) = \sum_{n=1}^{\infty} a_n \psi_n(x)$$

$$\int_0^a \psi(x,0)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \int_0^a \psi_n(x)\psi_k(x)dx = \sum_{n=1}^{\infty} a_n \delta_{nk} = a_k$$

so that

$$a_k = \int_0^a \psi(x,0)\psi_k(x)dx = \frac{2}{a}\int_0^{a/2} \sin\frac{k\pi x}{a} dx = \frac{2}{k\pi}\left(1 - \cos\frac{k\pi}{2}\right)$$

Therefore,

$$\psi(x,t) = \frac{2}{\pi}\sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} \frac{1}{n}\left(1 - \cos\frac{n\pi}{2}\right) \sin\frac{n\pi x}{a} e^{-i\frac{n^2\pi^2\hbar}{2ma^2}t}$$

(ii) The probability of being in the n^{th} eigenstate is

$$P_n = |a_n|^2 = \frac{4}{n^2\pi^2}\left(1 - \cos\frac{n\pi}{2}\right)^2$$

(iii) We have

$$\langle E\rangle = \langle\psi|\,\hat{H}\,|\psi\rangle = \sum_n E_n P_n = \sum_n E_n\,|a_n|^2 = \frac{2\hbar^2}{ma^2}\sum_n\left(1-\cos\frac{n\pi}{2}\right)^2$$

which does not converge! It takes an infinite amount of energy to form the initial wavefunction because of the sharp edges!

5. *(i)* For $x \to \infty$ this equation becomes

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \quad , \quad \frac{\hbar^2\alpha^2}{2m} = |E|$$

which has the solution

$$\psi(x\to\infty) = e^{-\alpha x}$$

(ii) The boundary condition at $x = 0$ is $\psi(0) = 0$.

(iii) We try the solution

$$\psi(x) = f(x)e^{-\alpha x}$$

which satisfies all boundary conditions if $f(0)=0$ and $\lim_{x\to\infty} f(x_e^{-ax} \to$ 0. Substituting into the Schrodinger equation we get

$$\left(f''(x)-2\alpha f'(x)+\frac{me^2}{2h^2x}f(x)\right)e^{-\alpha x}=0 \to f''(x)-2\alpha f'(x)+\frac{me^2}{2h^2x}f(x)=0$$

The solution to this equation is unique so that we only need to guess an expression for $f(x)$ that satisfies the equation and the boundary conditions. We find

$$f(x)=x \text{ with } \alpha=\frac{me^2}{4h^2}=\frac{1}{4a_0}$$

The full solution is then

$$\psi(x)=Axe^{-\alpha x}$$

where A is the normalization constant.

This is the solution for the ground sate since it has zeroes only at the boundaries ($x=0$ and $x\to\infty$). We find A by

$$1=A^2\int_0^\infty|\psi(x)|^2dx=A^2\int_0^\infty x^2e^{-2\alpha x}dx=\frac{A^2}{8\alpha^3}\int_0^\infty y^2e^{-y}dy=\frac{A^2}{8\alpha^3}\Gamma(3)=\frac{A^2}{4\alpha^3}\to A=2\alpha^{3/2}$$

(iv)

$$E_0=-\frac{\hbar^2\alpha^2}{2m}=-\frac{me^4}{32\hbar^2}=-\frac{e^2}{8a_0}=\frac{1}{4}E_{hydrogen}^{ground-state}$$

(v) We then have

$$\langle\psi|\,\hat{x}\,|\psi\rangle = \int_0^\infty\int_0^\infty \langle\psi \mid x'\rangle\,\langle x'|\,\hat{x}\,|x\rangle\,\langle x \mid \psi\rangle\,dxdx' = \int_0^\infty\int_0^\infty \langle\psi \mid x'\rangle x\delta(x-x')\,\langle x \mid \psi\rangle\,dxdx'$$

$$= \int_0^\infty \langle\psi \mid x\rangle\,x\,\langle x \mid \psi\rangle\,dx = \int_0^\infty x\,|\psi(x)|^2\,dx = A^2\int_0^\infty x^3 e^{-2\alpha x}dx$$

$$= \frac{4\alpha^3}{(2\alpha)^4}\Gamma(4) = \frac{3}{2\alpha} = 6a_0$$