Problem Set 3, Physics 622 (Fall 2001)
Solutions

1 (a) Let ψ_1, ψ_2 and ψ_3 be the wavefunctions in the three regions: $x < -a$, $-a \leq x < a$ and $x \geq a$ respectively, and they satisfy the time-independent Schrödinger equation,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (E > 0)$$

with solutions,

$$\psi_i(x) = a_i e^{ika} + b_i e^{-ika} \qquad (k^2 = \frac{2mE}{\hbar^2}).$$

Note that $b_3 = 0$ and at the boundaries $x = -a$ and $x = a$, the wavefunction is continuous and its derivative satisfies

$$\psi'(\pm a + \delta) - \psi'(\pm a - \delta) = \frac{2mA}{\hbar^2}\psi(\pm a) \qquad (\delta \to 0)$$

Note that the derivative is not continuous because the potential is not finite at the boundaries.

<u>$x = -a$</u>

$$\begin{aligned} a_2 e^{-ika} + b_2 e^{ika} &= a_1 e^{-ika} + b_1 e^{ika} \\ ik(a_2 e^{-ika} - b_2 e^{ika}) - ik(a_1 e^{-ika} - b_1 e^{ika}) &= \frac{2mA}{\hbar^2}(a_2 e^{-ika} + b_2 e^{ika}) \end{aligned}$$

<u>$x = a$</u>

$$\begin{aligned} a_2 e^{ika} + b_2 e^{-ika} &= a_3 e^{ika} \\ ika_3 e^{ika} - ik(a_2 e^{ika} - b_2 e^{-ika}) &= \frac{2mA}{\hbar^2} a_3 e^{ika} \end{aligned}$$

Putting in matrix form and let $\beta = \frac{mA}{\hbar^2 k}$, we have

$$\begin{aligned} \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} &= \begin{bmatrix} 1 + i\beta & i\beta e^{i2ka} \\ -i\beta e^{-i2ka} & 1 - i\beta \end{bmatrix} \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} \\ \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} &= \begin{bmatrix} 1 + i\beta \\ -i\beta e^{i2ka} \end{bmatrix} a_3 \\ \Rightarrow \begin{bmatrix} a_1 \\ b_1 \end{bmatrix} &= \begin{bmatrix} 1 - 2\beta^2 \sin^2\theta + i\beta(2 + \beta\sin^2\theta) \\ -2i\beta(\beta\sin\theta + \cos\theta) \end{bmatrix} a_3 \qquad (\theta = 2ka) \end{aligned}$$

The transmission and reflection coefficients are given by,

$$\begin{aligned} T = \frac{|a_3|^2}{|a_1|^2} &= \frac{1}{(1 - 2\beta^2\sin^2\theta)^2 + \beta^2(2 + \beta\sin 2\theta)^2} \qquad \blacksquare \\ R = \frac{|b_1|^2}{|a_1|^2} &= \frac{4\beta^2(\beta\sin\theta + \cos\theta)^2}{(1 - 2\beta^2\sin^2\theta)^2 + \beta^2(2 + \beta\sin 2\theta)^2} \qquad \blacksquare \end{aligned}$$

(b) For $A < 0$ and $E > 0$, we only need to make the substitution $\beta \to -\beta$ in the expressions for T and R in (a), thus

$$\begin{aligned} T &= \frac{1}{(1-2\beta^2\sin^2\theta)^2 + \beta^2(2-\beta\sin 2\theta)^2} \quad \blacksquare \\ R &= \frac{4\beta^2(-\beta\sin\theta + \cos\theta)^2}{(1-2\beta^2\sin^2\theta)^2 + \beta^2(2-\beta\sin 2\theta)^2} \quad \blacksquare \end{aligned}$$

For $E < 0$, the wavefunction is of the form

$$\psi(x) = \begin{cases} a_1 e^{\kappa x} & x < -a \\ a_2 e^{\kappa x} + b_2 e^{-\kappa x} & -a \leq x < a \\ b_3 e^{-\kappa x} & x \geq a \end{cases} \quad \text{where } \kappa^2 = \frac{2m|E|}{\hbar^2}$$

Following a similar procedures, the following two transcendental equations that determined the energy eigenvalues can be obtained. The algebra can be simplified by noticing that the symmetry of the potential implies the eigenfunctions will have definite parity. For even parity, $a_1 = a_3$ and $a_2 = b_2$, for odd parity, $a_1 = -a_3$ and $a_2 = -b_2$,

$$\begin{aligned} \frac{2m|A|}{\kappa\hbar^2} &= 1 + \tanh(\kappa a) \qquad \text{(even)} \\ \frac{2m|A|}{\kappa\hbar^2} &= 1 + \coth(\kappa a) \qquad \text{(odd)}\ . \end{aligned}$$

2 (a) Periodic boundary conditions can be used. $\blacksquare$

(b) For a periodic potential of period a, $\psi(x)$ must satisfy

$$\psi(x + na) = e^{inKa}\psi(x) \qquad \text{(Bloch condition)}$$

where K is a real number and $\frac{-\pi}{a} < K \leq \frac{\pi}{a}$. Because of the periodicity, we can consider $0 < x \leq a$ only, where

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

Matching boundary conditions at $x = a$,

$$\begin{aligned} \psi(a) &= e^{iKa}\psi(0) \\ e^{iKa}\psi'(0) - \psi'(a) &= \frac{2mV_\circ}{\hbar^2}\psi(a) \end{aligned}$$

which gives

$$\begin{aligned} [1 - e^{i(k-K)a}]A + [1 - e^{-i(k+K)a}]B &= 0 \\ [1 - (1 - i\beta)e^{i(k-K)a}]A + [1 - (1 + i\beta)e^{-i(k+K)a}]B &= 0 \end{aligned}$$

For the above system of homogeneous equations to have non-trivial solution, we must have,

$$\begin{vmatrix} 1-e^{i(k-K)a} & 1-e^{-i(k+K)a} \\ 1-(1-i\beta)e^{i(k-K)a} & 1-(1+i\beta)e^{-i(k+K)a} \end{vmatrix} = 0$$

$$\Rightarrow F(k) = \cos ka + \frac{mV_\circ}{\hbar^2 k}\sin ka = \cos Ka \qquad (k>0)$$

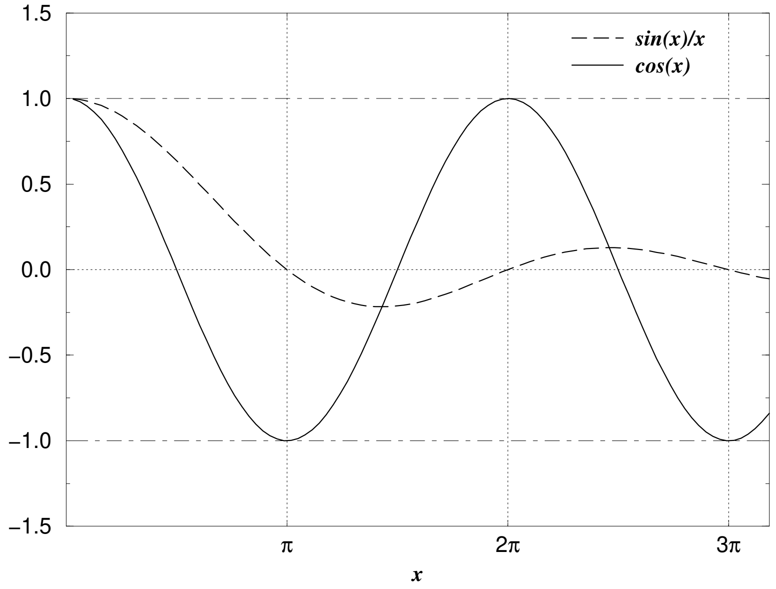
$$\therefore |F(k)| \leq 1$$

Note that $F(0) = 1 + \dfrac{mV_\circ}{\hbar^2} > 1$, so $k_\circ$ is given by

$$\cos k_\circ a + \frac{mV_\circ}{\hbar^2 k_\circ}\sin k_\circ a = 1 \quad \blacksquare$$

(c) From the graphs of $\cos(x)$ and $\sin(x)/x$, we can deduce that $F(k)$ will first drop below -1 when $ka=\pi$, hence the first gap begins at

$$E = \frac{\hbar^2\pi^2}{2ma^2} \quad \blacksquare$$



3 The Schrödinger equation for the given $V(x)$ is

$$\begin{aligned} \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + mgx\psi &= E\psi \\ \frac{d^2\psi}{dx^2} - \frac{2m^2 g}{\hbar^2}(x - \frac{E}{mg})\psi &= 0 \end{aligned}$$

Let $y = \left(\frac{2m^2 g}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{mg}\right)$,

$$\frac{d^2\psi}{dy^2} - y\psi = 0$$
$$\psi(y) = C_1\,Ai(y) + C_2\,Bi(y)$$

$$\begin{aligned}
\psi(x=\infty) = 0 \qquad &\Rightarrow \qquad C_2 = 0 \quad (\because\ Bi(y) \to \infty \text{ as } y \to \infty) \\
\psi(x=0) = 0 \qquad &\Rightarrow \qquad Ai\left[y = -E\left(\frac{2}{\hbar^2 m g^2}\right)^{\frac{1}{3}}\right] = 0 \\
& \qquad\qquad -E\left(\frac{2}{\hbar^2 m g^2}\right)^{\frac{1}{3}} = z_0, z_1, z_2, \ldots
\end{aligned}$$

where $Ai(z_i) = 0$ and $|z_0| < |z_1| < |z_2| < \ldots$, note that all z_i's are negative. Therefore,

$$E_\circ = \left(\frac{\hbar^2 m g^2}{2}\right)^{\frac{1}{3}} |z_0| \qquad z_0 \approx -2.3381 \quad \blacksquare$$

4(2.3) (a) It is given that

$$\hat{n} = \sin\beta\,\hat{i} + \cos\beta\,\hat{k}$$
$$\vec{S}\cdot\hat{n}|\psi(0)\rangle = \frac{\hbar}{2}|\psi(0)\rangle$$

Recall that $S_x = \frac{\hbar}{2}(\,|+\rangle\langle-| + |-\rangle\langle+|\,)$ and $S_z = \frac{\hbar}{2}(\,|+\rangle\langle+| - |-\rangle\langle-|\,)$, and let $|\psi(0)\rangle = a|+\rangle + b|-\rangle$, we have

$$\begin{aligned}
a(\cos\beta - 1) + b\sin\beta &= 0 \\
a\sin\beta - b(1+\cos\beta) &= 0.
\end{aligned}$$

$$\Rightarrow \qquad \begin{bmatrix} a \\ b \end{bmatrix} = \sqrt{\frac{1+\cos\beta}{2}} \begin{bmatrix} 1 \\ \frac{\sin\beta}{1+\cos\beta} \end{bmatrix}$$

Then from Eq.(2.1.56) in Sakurai, with $\omega = \frac{|e|B}{2m_e c}$,

$$|\psi(t)\rangle = \begin{bmatrix} a e^{-i\omega t} \\ b e^{i\omega t} \end{bmatrix}$$

Using Eq(1.4.17a) in Sakurai and the fact that $a^2 + b^2 = 1$, the required probability is,

$$\begin{aligned}
\left|\langle s_x = \tfrac{\hbar}{2}|\psi(t)\rangle\right|^2 &= \left|\frac{1}{\sqrt{2}}(a e^{-i\omega t} + b e^{i\omega t})\right|^2 \\
&= \frac{1}{2}(1 + \sin\beta\cos 2\omega t) \quad \blacksquare
\end{aligned}$$

(b)

$$\begin{aligned}\langle S_x\rangle &= \langle\psi(t)|S_x|\psi(t)\rangle\\ &= \begin{bmatrix} ae^{i\omega t} & be^{-i\omega t}\end{bmatrix}\frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}ae^{-i\omega t}\\ be^{-i\omega t}\end{bmatrix}\\ &= \frac{\hbar}{2}\sin\beta\cos 2\omega t \quad \blacksquare\end{aligned}$$

(c) For $\beta = 0$, $\hat{n}$ is along the z-axis, therefore there is equal probability that the electron is in $|s_x = \hbar/2\rangle$ and $|s_x = -\hbar/2\rangle$ and hence $\langle S_x\rangle$ is zero which is exactly what we get in (a) and (b). For $\beta = \pi/2$, $\langle S_x\rangle = \frac{\hbar}{2}\cos 2\omega t$. $\blacksquare$

5(2.8) (a) The Hamiltonian is $H = \delta\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$ whose eigenvalues are δ and $-\delta$, the corresponding eigenvectors are $|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix}$ and $|2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix}$ respectively. $\blacksquare$

(b)

$$\begin{aligned}|\psi(0)\rangle &= \begin{bmatrix}1\\ 0\end{bmatrix} = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)\\ |\psi(t)\rangle &= e^{-\frac{iHt}{\hbar}}|\psi(0)\rangle\\ &= \frac{1}{\sqrt{2}}e^{-\frac{iHt}{\hbar}}(|1\rangle + |2\rangle)\\ &= \frac{1}{\sqrt{2}}(e^{-\frac{i\delta t}{\hbar}}|1\rangle + e^{\frac{i\delta t}{\hbar}}|2\rangle)\\ &= \frac{1}{2}\begin{bmatrix}e^{-\frac{i\delta t}{\hbar}} + e^{\frac{i\delta t}{\hbar}}\\ e^{-\frac{i\delta t}{\hbar}} - e^{\frac{i\delta t}{\hbar}}\end{bmatrix}\\ &= \begin{bmatrix}\cos\frac{\delta t}{\hbar}\\ -i\sin\frac{\delta t}{\hbar}\end{bmatrix} \quad \blacksquare\end{aligned}$$

(c) The required probability is given by $|\langle a''|\psi(t)\rangle|^2$ which is equal to $\sin^2\frac{\delta}{\hbar}t$. $\blacksquare$

(d) This problem corresponds to a spin-$\frac{1}{2}$ system with Hamiltonian H proprotional to S_x and $|\psi(t)\rangle$ describes the time evolution of a spinor for a given initial conditions. $\blacksquare$

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