GRADUATE QUANTUM MECHANICS: 502 Spring 2002

Solutions to Assignment 1.

1. (a) To construct an eigenket of $\tau_{\vec{a}}$, we take the combination

$$|\vec{k}\rangle = \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}|\vec{r}\rangle, \tag{1}$$

where $\vec{k} = (k_x, k_y, k_z)$. Now

$$\begin{aligned} \tau|\vec{k}\rangle &= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}\tau_{\vec{a}}|\vec{r}\rangle \\ &= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}|\vec{r}+\vec{a}\rangle \\ &= \sum_{\vec{r}'} e^{-i\vec{k}\cdot(\vec{r}'-\vec{a})}|\vec{r}\rangle \\ &= e^{i\vec{k}\cdot a}|\vec{k}\rangle. \end{aligned} \tag{2}$$

(b) The action of H on the state $|r\rangle$ is

$$H|r\rangle = E_o|\vec{r}\rangle - \Delta \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} [|\vec{r}-\vec{a}\rangle + |\vec{r}+\vec{a}\rangle] \tag{3}$$

so that the action of H on $|\vec{k}\rangle$ is

$$\begin{aligned} H|\vec{k}\rangle &= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}H|\vec{r}\rangle \\ &= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}\left(E_o|\vec{r}\rangle - \Delta \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})}[|\vec{r}-\vec{a}\rangle\right) \\ &= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}\left(E_o - \Delta \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})}(e^{i\vec{k}\cdot\vec{a}} + e^{-i\vec{k}\cdot\vec{a}})\right)|\vec{r}\rangle \\ &= E(\vec{k})|\vec{k}\rangle. \end{aligned} \tag{4}$$

where

$$\begin{aligned} E(\vec{k}) &= E_o - 2\Delta \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} \cos(\vec{k}\cdot a) \\ &= E_o - 2\Delta(\cos k_x + \cos k_y + \cos k_z) \end{aligned} \tag{5}$$

is the corresponding energy eigenstate.

2. (a) Since momentum operators always commute, any function of these operators also commutes, so that

$$[\tau_{\vec{d}}, \tau_{\vec{d}'}] = [e^{-i\vec{P}\cdot\vec{d}/\hbar}, e^{-i\vec{P}\cdot\vec{d}'/\hbar}] = 0 \tag{6}$$

Translation operators commute.

(b) Rotations about different axes do not commute, so that

$$[D(\hat{n}, \phi), D(\hat{n}', \phi')] \neq 0 \tag{7}$$

(c) The inverstion operator reverses the direction of all translation, so that

$$\pi \tau_{\vec{d}} \pi^{-1} = \tau_{-\vec{d}} \tag{8}$$

Consequently, the inversion operator does not commute with the translation operator.

$$[\pi, \tau_{\vec{d}}] \neq 0. \tag{9}$$

(d) Under the inversion operation, angular momentum operators are invariant, $\pi \vec{J} \pi^{-1} = \vec{J}$ so that $[\pi, \vec{J}] = 0$. Consequently, the inversion operation commutes with functions of the angular momentum operator, and thus commutes with the rotation operator.

$$[\pi, D(R)] = 0. \tag{10}$$

3. Sakurai problem 9. When we time reverse a momentum eigenstate, we reverse the sign of the momentum, in addition to complex conjugating the state. We therefore expect that the time reversal of $\phi(p)$ is $\phi(-p)^*$. To show this explicitly,

$$\begin{aligned}
\langle p|\Theta|\alpha\rangle &= \langle p|\Theta \left(\int d^D p' |p'\rangle \phi(p') \right) \\
&= \langle p| \int d^D p' \Theta |p'\rangle \phi^*(p') \\
&= \langle p| \int d^D p' |-p'\rangle \phi^*(p') \\
&= \int d^D p' \, \overbrace{\langle p|-p'\rangle}^{\delta^{(D)}(p+p')} \, \phi^*(p') = \phi^*(-p)
\end{aligned} \tag{11}$$

4. Sakurai problem 12. We can rewrite the matrix as

$$H = AS_z^2 + \frac{B}{2}[S_+^2 + S_-^2] \tag{12}$$

where $S_\pm = S_x \pm iS_y$. Written out explicitly for $S = 1$ we have

$$H \equiv \begin{bmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{bmatrix} \tag{13}$$

where I have taken $\hbar = 1$. Taking $\det[E\underline{1} - H] = E((E-A)^2 - B^2)$ we see that the energy eigenvalues are

$$E = A \pm B, 0 \tag{14}$$

The corresponding eigenkets are

$$|\pm\rangle = \frac{|+1\rangle \pm |-1\rangle}{\sqrt{2}}, \qquad (E = A \pm B) \tag{15}$$

and for $E = 0$, $|0\rangle = |m_s = 0\rangle$.

The Hamiltonian is invariant under time-reversal, since $\Theta \vec{S} \Theta^{-1} = \vec{S}$ is unchanged by time-reversal. Since $\Theta|m_J\rangle = (i)^{2m_J}|-m_J\rangle$, we have

$$\Theta|\pm\rangle = \mp|\pm\rangle, \qquad \Theta|0\rangle = |0\rangle, \tag{16}$$

i.e the lower and upper eigenstates are odd-parity under time reversal, whereas the central state is even-parity under time-reversal.

5. Sakurai, chapter 4, Q 6. This is a tricky problem. There are two ways you could do it: (i) solving the complete problem but to exponential accuracy or (ii) by directly calculating the matrix elements between the states on the left, and right hand side. I shall illustrate method (ii). To begin, let us consider the problem when the length a is infinitely large. In this case, the wavefunction for the left, and right hand ground-states are

$$\begin{aligned} \psi_R(x) &= \langle x|\psi_R\rangle = \begin{cases} 0 & (x > a+b) \\ A\sin[k(a+b-x)] & (a < x < b) \\ Be^{\kappa x} & (x < a) \end{cases} \\ \psi_L(x) &= \langle x|\psi_L\rangle = \begin{cases} 0 & (x < -a-b) \\ A\sin[k(a+b+x)] & (-b < x < -a) \\ Be^{-\kappa x} & (x > -a) \end{cases} \end{aligned} \tag{17}$$

where $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_o + E)} \approx \sqrt{\frac{2m}{\hbar^2}V_o}$.

Now the tricky bit is that we need to construct orthogonalized wavefunctions. To do this, we construct

$$\begin{aligned} |\tilde{\psi}_R\rangle &= \frac{1}{[1 - |\langle\psi_L|\psi_R\rangle|^2]^{\frac{1}{2}}}[|\psi_R\rangle - |\psi_L\rangle\langle\psi_L|\psi_R\rangle] \\ |\tilde{\psi}_L\rangle &= |\psi_L\rangle \end{aligned} \tag{18}$$

These states are now orthogonal and normalized.

We shall now approximate the complete wavefunction in the form

$$|\psi\rangle = \alpha_R|\tilde{\psi}_R\rangle + \alpha_L|\tilde{\psi}_L\rangle \tag{19}$$

Applying the Hamiltonian to this expression, and demanding that $H|\psi\rangle = E|\psi\rangle$, we obtain the eigenvalue equation $H_{ab}\alpha_b = E\alpha_b$, $(a, b \in \{R, L\})$, where

$$H_{ab} \equiv \begin{bmatrix} \langle\tilde{\psi}_R|H|\tilde{\psi}_R\rangle & \langle\tilde{\psi}_R|H|\tilde{\psi}_L\rangle \\ \langle\tilde{\psi}_L|H|\tilde{\psi}_R\rangle & \langle\tilde{\psi}_L|H|\tilde{\psi}_L\rangle \end{bmatrix}. \tag{20}$$

To evaluate this matrix, it is helpful to realize that the complete Hamiltonian can be written

$$H = H_R + V_L = H_L + V_R \tag{21}$$

where H_L is the Hamiltonian for the left-hand well and H_R is the Hamiltonian for the right-hand well and

$$\begin{aligned} V_R &= -V_o[\theta(x-a) - \theta(x-a-b)], \\ V_L &= -V_o[\theta(x+a+b) - \theta(x+a)], \end{aligned} \tag{22}$$

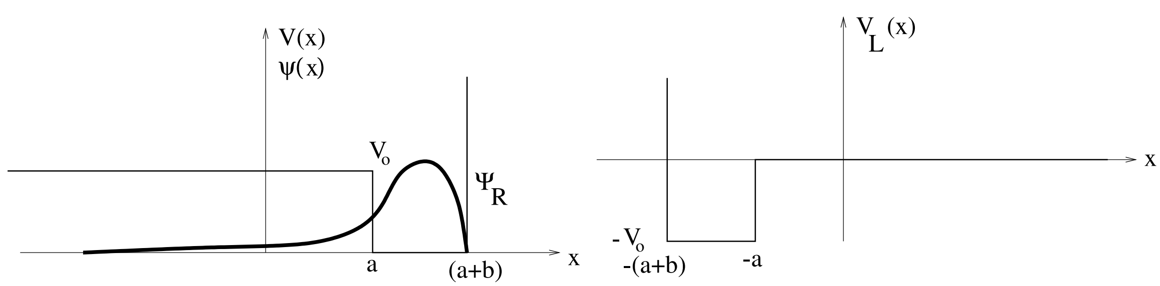

Fig. 1.: Showing $\psi_R(x)$ and the potential $V_L(x)$.

With this set-up, we note that $H_{L,R}|\psi_{L,R}\rangle = E_o|\psi_{L,R}\rangle$, where E_o is the energy of an isolated well. If you now compute the matrix element $\langle\tilde{\psi}_R|H|\tilde{\psi}_L\rangle$, you obtain

$$\begin{aligned}
\langle\tilde{\psi}_R|H|\tilde{\psi}_L\rangle &= E\langle\tilde{\psi}_R|\tilde{\psi}_L\rangle + \frac{\langle\tilde{\psi}_R|V_R|\psi_L\rangle}{\sqrt{1-|\langle\psi_L|\psi_R\rangle|^2}} \\
&= \frac{\langle\tilde{\psi}_R|V_R|\psi_L\rangle}{\sqrt{1-|\langle\psi_L|\psi_R\rangle|^2}} \\
&\approx \langle\psi_R|V_R|\psi_L\rangle.
\end{aligned} \tag{23}$$

In the last step, we have noted that $|\langle\psi_L|\psi_R\rangle|$ is exponentially smaller than unity, so that terms containing this quantity have been dropped. The splitting between the two states is then going to be simply

$$\pm\Delta = \pm|\langle\psi_R|V_R|\psi_L\rangle| \tag{24}$$

Now to calculate this, we need to compute the exponential tail in ψ_L. Applying continuity of the wavefunction and continuity of the logarithmic derivative, we obtain

$$A\sin kb = Be^{\kappa a}, \qquad k\tan(kb) = -\kappa \tag{25}$$

To leading exponential accuracy, this gives

$$\begin{aligned}
A &= \sqrt{\frac{2}{b}}, \\
k &= \frac{\pi}{b}\left[1+\frac{1}{\kappa b}\right], \\
B &= \sqrt{\frac{2}{b}}\frac{\pi}{\kappa b}e^{-\kappa a}
\end{aligned} \tag{26}$$

Carrying out the integral, we then obtain

$$\begin{aligned}
\langle\psi_R|V_R|\psi_L\rangle &= -V_o\int_a^{a+b} dx\sqrt{\frac{2}{b}}\sin[k(a+b-x)]Be^{-\kappa x} \\
&= -V_o\left(\frac{2}{b}\right)\left(\frac{k_o}{\kappa}e^{-\kappa(2a+b)}\right)\int_0^b dx\sin[kx]e^{\kappa x} \\
&= -V_o\left(\frac{2}{b}\right)\left(\frac{k_o}{\kappa}e^{-\kappa(2a+b)}\right)\int_0^b dx Im e^{(\kappa+ik)x} \\
&\approx -V_o\left(\frac{2}{b}\right)\left(\frac{k_o}{\kappa}e^{-\kappa(2a)}\right)Im\overbrace{\left[\frac{e^{ikb}}{\kappa+ik}\right]}^{\approx 2k_o/\kappa} \\
&\approx -V_o\left(\frac{4k_o^2}{b\kappa^3}\right)e^{-\kappa 2a} \\
&= \frac{2}{\kappa b}\left(\frac{\hbar^2\pi^2}{mb^2}\right)e^{-2\kappa a}
\end{aligned} \tag{27}$$

The splitting between the two levels is then

$$\Delta E = 2\Delta = \frac{h^2}{m\kappa b^3}e^{-2\kappa a} \tag{28}$$

where $\kappa = \sqrt{\frac{2m}{\hbar^2}V_o}$ for large V_o.

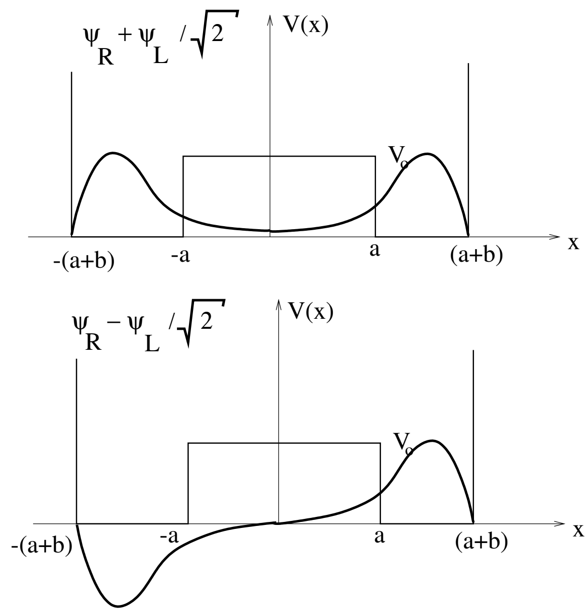

Fig. 2.: Showing the even and odd wavefunctions for the symmetric potential well.