Solutions to Assignment 1.

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

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

(1)

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

$$\tau|\vec{k}\rangle = \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} \tau_{\vec{a}}|\vec{r}\rangle
= \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}}|\vec{r} + \vec{a}\rangle
= \sum_{\vec{r}} e^{-i\vec{k}\cdot(\vec{r} - \vec{a})}|\vec{r}\rangle
= e^{i\vec{k}\cdot\vec{a}}|\vec{k}\rangle.$$

(2)

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

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

(3)

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

$$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.$$

(4)

where

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

(5)

is the corresponding energy eigenstate.

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

$$[\tau_{\vec{a}}, \tau_{\vec{b}}] = [e^{-i\vec{p}\cdot\vec{a}/\hbar}, e^{-i\vec{p}\cdot\vec{b}/\hbar}] = 0$$

(6)

Translation operators commute.

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

$$[D(\vec{n}, \phi), D(\vec{n}', \phi') \neq 0$$

(7)
(c) The inversion operator reverses the direction of all translation, so that
\[ \pi \tau_{-\vec{d}} = \tau_{-\vec{d}} \]  
(8)
Consequently, the inversion operator does not commute with the translation operator.
\[ [\pi, \tau_{\vec{d}}] \neq 0. \]  
(9)
(d) Under the inversion operation, angular momentum operators are invariant, \( \pi \vec{J} = \vec{J} \) 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.
\[ [\pi, D(R)] = 0. \]  
(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,
\[
\langle p | \Theta | \alpha \rangle = \langle p | \Theta \left( \int d^D p' |p'\rangle \phi(p') \right)
= \langle p | \int d^D p' \Theta |p'\rangle \phi^*(p')
= \langle p | \int d^D p' |p'\rangle \phi^*(p')
= \int d^D p' \langle p | -p' \rangle \phi^*(p') = \phi^*(-p)
\]  
(11)
4. Sakurai problem 12. We can rewrite the matrix as
\[ H = AS_z^2 + \frac{B}{2} [S_x^2 + S_y^2] \]  
(12)
where \( S_{\pm} = S_x \pm iS_y \). Written out explicitly for \( S = 1 \) we have
\[ H \equiv \begin{bmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{bmatrix} \]  
(13)
where I have taken \( \hbar = 1 \). Taking \( \det[E \mathbb{1} - H] = E((E - A)^2 - B^2) \) we see that the energy eigenvalues are
\[ E = A \pm B, 0 \]  
(14)
The corresponding eigenkets are
\[ |\pm\rangle = \frac{|+\rangle \pm |-_\rangle}{\sqrt{2}}, \quad (E = A \pm B) \]  
(15)
and for \( E = 0, |0\rangle = |m_s = 0\rangle \).
The Hamiltonian is invariant under time-reversal, since \( \Theta \tilde{S} \Theta^{-1} = \tilde{S} \) is unchanged by time-reversal. Since \( \Theta |m_J\rangle = (i)^{2m_J} |m_J\rangle \), we have
\[ \Theta |\pm\rangle = \mp |\pm\rangle, \quad \Theta |0\rangle = |0\rangle, \]  
(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

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

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

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

These states are now orthogonal and normalized.

We shall now approximate the complete wavefunction in the form

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

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

$$H_{ab} = \frac{\langle \tilde{\psi}_R | H | \tilde{\psi}_R \rangle \langle \tilde{\psi}_L | H | \tilde{\psi}_L \rangle}{\langle \tilde{\psi}_L | H | \tilde{\psi}_R \rangle \langle \tilde{\psi}_L | H | \tilde{\psi}_L \rangle}.$$ 

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

$$H = H_R + V_L = H_L + V_R$$

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

$$\begin{align*}
V_R &= -V_o[\theta(x - a) - \theta(x - a - b)] \\
V_L &= -V_o[\theta(x + a + b) - \theta(x + a)]
\end{align*}$$

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
\[
\langle \tilde{\psi}_R | H | \tilde{\psi}_L \rangle = E_o \langle \tilde{\psi}_L | \tilde{\psi}_R \rangle \approx \langle \tilde{\psi}_R | V_R | \tilde{\psi}_L \rangle \sqrt{1 - |\langle \psi_L | \psi_R \rangle|^2}.
\]
(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
\[
\pm \Delta = \pm |\langle \psi_L | V_R | \psi_L \rangle| \approx -V_o \left( \frac{2}{m} \frac{\hbar^2}{b^2} e^{-2\kappa a} \right) \approx \frac{2 \kappa b}{\hbar} \bar{\hbar}^2 \pi m b^2 e^{-2\kappa a}
\]
(27)

To leading exponential accuracy, this gives
\[
A = \sqrt{\frac{2}{b}}, \quad k = \frac{\pi}{b} \left[ 1 + \frac{1}{b\kappa} \right], \quad B = \sqrt{\frac{2 \pi}{b^2} e^{-\kappa a}}
\]
(26)

Carrying out the integral, we then obtain
\[
\langle \psi_R | V_R | \psi_L \rangle = -V_o \int_a^{a+b} dx \sqrt{\frac{2}{b} \sin[k(a + b - x)]} e^{-\kappa x}
\]
\[
= -V_o \left( \frac{2}{b} \right) \left( \frac{k_o}{\kappa} e^{-\kappa(2a+b)} \right) \int_0^b dx \sin[kx] e^{\kappa x}
\]
\[
= -V_o \left( \frac{2}{b} \right) \left( \frac{k_o}{\kappa} e^{-\kappa(2a+b)} \right) \int_0^b dx Im e^{(\kappa+ik)x}
\]
\[
\approx -V_o \left( \frac{2}{b} \right) \left( \frac{k_o}{\kappa} e^{-\kappa(2a)} \right) Im \left[ e^{ikb} \right] e^{-2\kappa a}
\]
(27)

The splitting between the two levels is then
\[
\Delta E = 2\Delta = \frac{\hbar^2}{m b^3} e^{-2\kappa a}
\]
(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.