Solutions to Problem Set 8
Physics 480 / Fall 1999
Professor Klaus Schulten / Prepared by Guochun Shi

Problem 1
(a)

$$\begin{pmatrix} E_0 & U \\ U & E_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\Longrightarrow \begin{pmatrix} E_0 - E & U \\ U & E0 - E \end{pmatrix} \Longrightarrow \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

$$\Longrightarrow \begin{vmatrix} E_0 - E & U \\ U & E0 - E \end{vmatrix} = 0$$

$$\Longrightarrow U^2 - (E_0 - E)^2 = 0$$

$$\Longrightarrow E = E_0 \pm U$$

$$E_1 = E_0 + U \Longrightarrow \alpha = \beta \Longrightarrow \phi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$E_2 = E_0 - U \Longrightarrow \alpha = -\beta \Longrightarrow \phi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Since the initial wavefunction is $\psi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2)$, then the wavefunction at time t is

$$\begin{aligned} \psi(t) &= \frac{1}{\sqrt{2}}(\phi_1 e^{\frac{-iE_1 t}{\hbar}} + \phi_2 e^{\frac{-iE_2 t}{\hbar}}) \\ &= \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}} \begin{pmatrix} e^{\frac{-it(E_0+U)}{\hbar}} \\ e^{\frac{-it(E_0+U)}{\hbar}} \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} e^{\frac{-it(E_0-U)}{\hbar}} \\ -e^{\frac{-it(E_0-U)}{\hbar}} \end{pmatrix}) \\ &= \frac{1}{2} \begin{pmatrix} 2cos(\frac{ut}{\hbar}) \\ -2isin(\frac{ut}{\hbar}) \end{pmatrix} e^{\frac{-iE_0 t}{\hbar}} \end{aligned}$$

(b)
Since

$$\psi(t) = \begin{pmatrix} cos(\frac{ut}{\hbar}) \\ -isin(\frac{ut}{\hbar}) \end{pmatrix} e^{\frac{-iE_0 t}{\hbar}}$$

the probability of finding the system in the state —2¿ at time t is $|-isin\frac{ut}{\hbar}|^2 = sin^2\frac{ut}{\hbar}$
(c) Since

$$H = \begin{pmatrix} 0 & 1 \\ 1 & \delta \end{pmatrix}$$

follow the same precedure in the previous part we can get

$$\begin{cases} E_1 = \frac{1}{2}\delta + \frac{1}{2}\sqrt{\delta^2+4} \\ \phi_1 = \begin{pmatrix} \frac{1}{2}\sqrt{\delta^2+4} - \frac{1}{2}\delta \\ 1 \end{pmatrix} \end{cases}$$

$$\begin{cases} E_2 = \frac{1}{2}\delta - \frac{1}{2}\sqrt{\delta^2+4} \\ \phi_2 = \begin{pmatrix} -\frac{1}{2}\sqrt{\delta^2+4} - \frac{1}{2}\delta \\ 1 \end{pmatrix} \end{cases}$$

note: ϕ_1 and ϕ_2 are not normalized.
We know

$$\psi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{\delta^2+4}}(\phi_1 - \phi_2)$$

then at time t

$$\begin{aligned} \psi(t) &= \frac{1}{\sqrt{\delta^2+4}} \begin{pmatrix} (\frac{1}{2}\sqrt{\delta^2+4} - \frac{1}{2}\delta)e^{\frac{-iE_1t}{\hbar}} + (\frac{1}{2}\sqrt{\delta^2+4} + \frac{1}{2}\delta)e^{\frac{-iE_2t}{\hbar}} \\ -2isin\frac{\frac{1}{2}t\sqrt{\delta^2+4}}{\hbar} \end{pmatrix} \\ &= \frac{1}{\sqrt{\delta^2+4}} e^{\frac{-i\delta t}{2\hbar}} \begin{pmatrix} \sqrt{\delta^2+4}cos(\frac{t\sqrt{\delta^2+4}}{2\hbar}) + i\delta sin(\frac{\sqrt{\delta^2+4}t}{2\hbar}) \\ -2isin(\frac{t\sqrt{\delta^2+4}}{2\hbar}) \end{pmatrix} \end{aligned}$$

the probability of finding the system in $|2>$ is

$$\frac{1}{\sqrt{\delta^2+4}} * 4 * sin^2(\frac{\sqrt{\delta^2+4}t}{2\hbar}) = \frac{4}{\sqrt{\delta^2+4}} sin^2(\frac{\sqrt{\delta^2+4}t}{2\hbar})$$

plug in $\delta = 0, 0.1, 1, 1, 10$, we can find the wavefunction and probability for each δ

Problem 2
(a)
We know(here I use μ for mass to avoid confusion)

$$H_0 = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 x^2$$

$$\begin{cases} a^+ = \sqrt{\frac{\mu\omega}{2\hbar}}x - \frac{i}{\sqrt{2\mu\hbar\omega}}p \\ a^- = \sqrt{\frac{\mu\omega}{2\hbar}}x + \frac{i}{\sqrt{2\mu\hbar\omega}}p \end{cases}$$

$$\Longrightarrow x = \sqrt{\frac{\hbar}{2\mu\omega}}(a^+ + a^-)$$

Then we have

$$\begin{aligned} H_a &= H_0 - \mu\omega^2 a x \\ &= H_0 - \mu\omega^2 a\sqrt{\frac{\hbar}{2\mu\omega}}(a^+ + a^-) \\ &= H_0 - A(a^+ + a^-) \end{aligned}$$

where$A \equiv \mu\omega^2 a\sqrt{\frac{\hbar}{2\mu\omega}} = \omega a\sqrt{\frac{\mu\hbar\omega}{2}}$ The matrix element of H_a is

$$\begin{aligned} < m|H_a|n > &= (\frac{1}{2} + n)\delta_{mn} - A < m|a^+|n > -A < m|a^-|n > \\ &= (\frac{1}{2} + n)\delta_{mn} - \sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1} \end{aligned}$$

note:we use $a^+|n >= \sqrt{n+1}|n >$ and $a^-|n >= \sqrt{n}|n-1 >$ in the derivation above.
Now we can write H_a down.

$$H_a = \begin{pmatrix} \frac{1}{2}\hbar\omega & -A & 0 & \cdots & 0 \\ -A & \frac{3}{2}\hbar\omega & -A\sqrt{2} & \cdots & 0 \\ 0 & -A\sqrt{2} & \frac{5}{2}\hbar\omega & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & -A\sqrt{n} \\ 0 & 0 & 0 & -A\sqrt{n} & (\frac{1}{2}+n)\hbar\omega \end{pmatrix}$$

where $n \to \infty$
(b)

$$\begin{aligned} H_a &= \frac{1}{2}\mu\omega^2 x^2 + \frac{p^2}{2\mu} - \mu\omega^2 a x \\ &= \frac{1}{2}\mu\omega^2(x^2 - 2ax) + \frac{p^2}{2\mu} \\ &= \frac{1}{2}\mu\omega^2(x-a)^2 + \frac{p^2}{2\mu} - \frac{1}{2}\mu\omega^2 a^2 \end{aligned}$$

It's similar to non-displaced oscillator if replace $x - a$ with x. It is easy to see te ground state energy is

$$E_{groundstate} = -\frac{1}{2}\mu\omega^2 a^2 + \frac{1}{2}\hbar\omega = \hbar\omega(\frac{1}{2} - \frac{\mu\omega}{2\hbar}a^2)$$

(c)
assume $|0>_a = \sum_{n=0}^{\infty} C_n|n>_0$, then

$$H_a|0>_a = H_a\sum_{n=0}^{\infty} C_n|n>_0$$

$$\Longrightarrow {}_0\!<m|H_a|0>_a = \sum_{n=0}^{\infty} C_n \; {}_0\!<m|H_a|0>_0 = \sum_{n=0}^{\infty} C_n H_{mn}$$

$$\begin{aligned} LHS &= {}_0\!<m|H_a|0>_a \\ &= E_{0a} \; {}_0\!< m|0>_a \\ &= \sum_{n=0}^{\infty} E_{0a} \; {}_0\!< m|C_n|n>_0 \\ &= \sum_{n=0}^{\infty} E_{0a} C_n \delta_{mn} \end{aligned}$$

$$\Longrightarrow \sum_{n=0}^{\infty} E_{0a} C_n \delta_{mn} = \sum_{n=0}^{\infty} C_n H_{mn}$$

$$\Longrightarrow \sum_{n=0}^{\infty} (H_n - E_{0a}\delta_{mn}) = 0$$

(d)
Here I use other method instead of the recursion equation of C_n
For undisplaced oscillator

$$\phi_n(x) = \frac{\alpha^{\frac{1}{2}}}{\sqrt{2_n n! \sqrt{\pi}}} e^{-\frac{\alpha^2 x^2}{2}} H_n x$$

For displaced oscillator (gound state)

$$\phi_{a0} = \alpha^{\frac{1}{2}} \pi^{-\frac{1}{4}} e^{-\frac{\alpha^2 (x-a)^2}{2}}$$

The following formula will be used in the derivation

$$\int_{-\infty}^{\infty} dx e^{-x^2} H_n(x) H_l(x) = 2^n n! \sqrt{\pi} \delta_{nl}$$

$$e^{2tx - t^2} = \sum_{l=0}^{\infty} \frac{H_l(x)}{l!} t^l$$

$$\int_{-\infty}^{\infty} dx e^{-x^2} = \sqrt{\pi}$$

assume $\phi_{a0} = C_n \sum_{n=0}^{\infty} \phi_n$

$$\Longrightarrow C_n = \int_{-\infty}^{\infty} dx \phi_{a0} \phi_n$$

$$
\begin{aligned}
&= \alpha^{\frac{1}{2}}\pi^{-\frac{1}{4}}\frac{\alpha^{\frac{1}{2}}}{\sqrt{2^n n!\sqrt{\pi}}}\int_{-\infty}^{\infty} dx\, e^{\frac{-\alpha^2(2x^2-2xa+a^2)}{2}} H_n(\alpha x) \\
&= \frac{\alpha}{\sqrt{2^n n!\sqrt{\pi}}}\int_{-\infty}^{\infty} dx\, e^{-(\alpha^2x^2-\alpha^2ax+\frac{\alpha^2a^2}{2})} H_n(\alpha x) \\
&\overset{y=\alpha x}{=} \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\int_{-\infty}^{\infty} dy\, e^{-(y^2-\alpha ay+\frac{\alpha^2a^2}{2})} H_n(y) \\
&= \frac{e^{-\frac{1}{4}a^2\alpha^2}}{\sqrt{2^n n!\sqrt{\pi}}}\int_{-\infty}^{\infty} dy\, e^{-y^2} e^{2(\frac{a\alpha}{2})y-(\frac{a\alpha}{2})^2} H_n(y) \\
&= \frac{e^{-\frac{1}{4}a^2\alpha^2}}{\sqrt{2^n n!\sqrt{\pi}}}\int_{-\infty}^{\infty} dy\, e^{-y^2} \sum_{l=0}^{\infty}\frac{H_l(y)}{l!}(\frac{a\alpha}{2})^l H_n(y) \\
&= \frac{e^{-\frac{1}{4}a^2\alpha^2}}{\sqrt{2^n n!\sqrt{\pi}}}\sum_{l=0}^{\infty}\frac{(\frac{a\alpha}{2})^l}{l!}2^l l!\sqrt{\pi}\delta_{mn} \\
&= \frac{e^{-\frac{1}{4}a^2\alpha^2}}{\sqrt{2^n n!\sqrt{\pi}}}\frac{(\frac{a\alpha}{2})^n}{n!}2^n n!\sqrt{\pi} \\
&= \frac{(a\alpha)^n}{\sqrt{2^n n!}}e^{-\frac{1}{4}a^2\alpha^2}
\end{aligned}
$$

Obviously

$$
C_0 = e^{-\frac{1}{4}a^2\alpha^2}
$$

$$
C_n = \frac{(a\alpha)^n}{\sqrt{2^n n!}}c_0
$$

It is easy to plot C_n^2 as function of n.
Problem 3
(a)

$$
H = \begin{pmatrix}
E_0 & -t & 0 & 0 & 0 & -t \\
-t & E_0 & -t & 0 & 0 & 0 \\
0 & -t & E_0 & -t & 0 & 0 \\
0 & 0 & -t & E_0 & -t & 0 \\
0 & 0 & 0 & -t & E_0 & -t \\
-t & 0 & 0 & 0 & -t & E_0
\end{pmatrix}
$$

$$
\begin{aligned}
(H\psi_n)_k &= -t\psi_{n,k-1} + E_0\psi_{n,k} - t\psi_{n,k+1} \\
&= -t(\psi_{n,k-1} + \psi_{n,k+1}) + E_0\psi_{n,k} \\
&= -tN_n(e^{i\frac{2n\pi}{6}(k-1)} + e^{i\frac{2n\pi}{6}(k+1)}) + E_0N_ne^{i\frac{2n\pi}{6}k} \\
&= N_ne^{i\frac{2n\pi}{6}k}(E_0 - 2tcos\frac{2n\pi}{6}) \\
&= E_n(\psi_n)_k
\end{aligned}
$$

$$\Longrightarrow E_n = E_0 - 2tcos\frac{2n\pi}{6}$$

Plot the energies(n=1,2,3,4,5,6) . The corresponding eigenstates are

$$\begin{pmatrix} \psi_{n1} \\ \psi_{n2} \\ \psi_{n3} \\ \psi_{n4} \\ \psi_{n5} \\ \psi_{n6} \end{pmatrix} (n = 1, 2, 3, 4, 5, 6)$$

(b)
For $2N$-dimensional Hamiltonian of the same type, follow the same procedure in part a):

$$\psi_n = \begin{pmatrix} \psi_{n1} \\ \psi_{n2} \\ \vdots \\ \psi_{n,2N} \end{pmatrix} \quad \psi_{nm} = A_n exp(i\frac{2mn\pi}{2N})$$

$$\begin{aligned} (H\psi_n)_k &= -t\psi_{n,k-1} + E_0\psi_{n,k} - t\psi_{n,k+1} \\ &= A_n e^{i\frac{2n\pi}{2N}k}(E_0 - 2tcos\frac{2n\pi}{2N}) \\ &= E_n(\psi_n)_k \end{aligned}$$

where

$$\begin{aligned} E_n &= E_0 - 2tcos(\frac{2n\pi}{2N}) \\ &= E_0 - 2tcos(\frac{n\pi}{N}) \end{aligned}$$

while $2N = 16$, $E_n = E_0 - 2tcos\frac{n\pi}{8}$. Plot the energies for $n = 1, 2, 3, \cdots, 16$

Problem 4
(a)

$$H = \begin{pmatrix} E_0 & -t & 0 & 0 & 0 & 0 \\ -t & E_0 & -t & 0 & 0 & 0 \\ 0 & -t & E_0 & -t & 0 & 0 \\ 0 & 0 & -t & E_0 & -t & 0 \\ 0 & 0 & 0 & -t & E_0 & -t \\ 0 & 0 & 0 & 0 & -t & E_0 \end{pmatrix}$$

assume

$$\psi_n = \begin{pmatrix} \psi_{n1} \\ \psi_{n2} \\ \psi_{n3} \\ \psi_{n4} \\ \psi_{n5} \\ \psi_{n6} \end{pmatrix}$$

where $\psi_{nm} = N_n sin\frac{2mn\pi}{7}$

$$\begin{aligned} (H\psi_n)_k &= -t(\psi_{n,k-1} + \psi_{n,k+1}) + E_0\psi_{nk} \\ &= -tN_n(sin\frac{2n\pi(k-1)}{7} + sin\frac{2n\pi(k+1)}{7}) + E_0 N_n sin\frac{2n\pi k}{7} \\ &= -tN_n 2sin\frac{2n\pi k}{7}cos\frac{2n\pi}{7} + E_0 N_n sin\frac{2n\pi k}{7} \\ &= (N_n sin\frac{2n\pi k}{7})(E_0 - 2tcos\frac{2n\pi}{7}) \\ &= E_n(\psi_n)_k \end{aligned}$$

where $E_n = E_0 - 2tcos\frac{2n\pi}{7}$ we need to prove $(H\psi_n)_k = E_n(\psi_n)_k$ are satisfied when k=1 or 6.

$$\begin{aligned} (H\psi_n)_1 &= -t\psi_{n2} + E_0\psi_{n1} \\ &= -tN_n sin\frac{2n\pi \cdot 2}{7} + E_0 N_n sin\frac{2n\pi}{7} \\ &= -tN_n\, 2sin\frac{2n\pi}{7}cos\frac{2n\pi}{7} + E_0 N_n sin\frac{2n\pi}{7} \\ &= (N_n sin\frac{2n\pi}{7})(E_0 - 2tcos\frac{2n\pi}{7}) \\ &= E_n\psi_{n1} \end{aligned}$$

$$\begin{aligned} (H\psi_n)_6 &= -t\psi_{n5} + E_0\psi_{n6} \\ &= -tN_n sin\frac{2n\pi \cdot 5}{7} + E_0 N_n sin\frac{2n\pi \cdot 6}{7} + E_n N_n sin\frac{2n\pi \cdot 7}{7} \\ & \quad (the\ last\ term\ above\ is\ equal\ 0) \\ &= -t \cdot N_n(sin\frac{2n\pi \cdot 5}{7} + sin\frac{2n\pi \cdot 7}{7}) + E_0 N_n sin\frac{2n\pi \cdot 6}{7} \\ &= -tN_n \cdot 2sin\frac{2n\pi \cdot 6}{7}cos\frac{2n\pi}{7} + E_0 N_n sin\frac{2n\pi \cdot 6}{7} \\ &= (N_n sin\frac{2n\pi \cdot 6}{7})(E_0 - 2tcos\frac{2n\pi}{7}) \\ &= E_n\psi_{n6} \end{aligned}$$

From above we know

$$E_n = E_0 - 2tcos\frac{2n\pi}{7} \quad (n = 1, 2, \cdots, 6)$$

(b)
For the case of 2N-dimension follow the same procedure, we can get

$$E_n = E_0 - 2tcos(\frac{2n\pi}{2N+1})$$

(c)
Plot eigenvalues for $N = 3, 11$.
Plot all eigenstates for $N = 3$.
Problem 5
(a)
the Hamiltonian is

$$H = \begin{pmatrix} E_0 & w & 0 & \cdots & w \\ w & E_0 & w & \cdots & 0 \\ 0 & w & E_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ w & 0 & 0 & \cdots & E_0 \end{pmatrix}$$

It is a 16*16 matrix
w is the potential due to interaction between molecules in the nearest neighbour. Obviously when we rotate the ring by $\frac{360^o}{16} = 22.5^o$,The ring is the same as it is before rotation and the Hamiltonian is not changed.

(b) $2N = 16$. Do the same as we did in problem 3, we can prove(8,9) are eigenstates with eigenvalues

$$E_n = E_0 - 2wcos\frac{2n\pi}{16} = 1.5 - 2wcos\frac{2n\pi}{16}$$

now we evaluate w:
assume θ is angle between the directions of two neighboring chlorophyl, obviously $\theta = 22.5^o$

$$w_{jk} = C\left(\frac{\vec{d_j}\cdot\vec{d_k}}{{r_{jk}}^3} - \frac{3(\vec{r}_{jk}\cdot\vec{d_j})\,(\vec{r}_{jk}\cdot\vec{d_k})}{{r_{jk}}^5}\right)$$

$$\vec{d_j}\cdot\vec{d_k} = cos\theta$$

$$r_{jk} = 2Rsin\frac{\theta}{2}$$

$$\vec{r_{jk}} \cdot \vec{d_j} = \vec{r_{jk}} \cdot \vec{d_k} = Rsin\frac{\theta}{2}$$
$$C = 100, R = 46$$
$$\Longrightarrow w = w_{jk} = \frac{C(cos\theta - 0.75)}{8R^3 sin^3\frac{\theta}{2}} = 0.003$$

$$\Longrightarrow E_n = 1.5 - 0.006 \cdot cos\frac{2n\pi}{16}$$

the lowest 5 energies are:

$$E_{16} = 1.494ev$$
$$E_{15} = E_1 = 1.49446ev$$
$$E_{14} = E_2 = 1.49675ev$$

(c)
the hamiltonian for 2 rings is :

$$H = \begin{pmatrix} E_0 & w & 0 & \cdots & w & 0 & 0 & 0 & \cdots & 0 \\ w & E_0 & w & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & w & E_0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ w & 0 & 0 & \cdots & E_0 & w_{rr} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & w_{rr} & E_0 & w & 0 & \cdots & w \\ 0 & 0 & 0 & \cdots & 0 & w & E_0 & w & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & w & E_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & w & 0 & 0 & \cdots & E_0 \end{pmatrix}$$

where w_{rr} is the interaction term between 2 rings.

$$w_{int} = C\left(\frac{\vec{d_1} \cdot \vec{d_2}}{{r_{12}}^3} - \frac{3(\vec{r}_{12} \cdot \vec{d_1})\ (\vec{r}_{12} \cdot \vec{d_2})}{{r_{12}}^5}\right)$$
$$\vec{d_1} \cdot \vec{d_2} = -1$$
$$r_{12} = 110 - 2 * 46 = 12$$
$$\vec{r_{12}} \cdot \vec{d_1} = \vec{r_{12}} \cdot \vec{d_2} = 0$$
$$w_{int} = -\frac{C}{r_{12}^3} = -\frac{100}{12^3} = -0.058$$

We use mathematica to solve eigenvalues and eigenvectors.
The probability of finding electronic excitation in ring 2 is also calculated in methematica notebook.