1.1

(a) $$\bar{X} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \qquad x = x_1 - x_2$$

$$\therefore \frac{\partial}{\partial x_1} = \frac{\partial \bar{X}}{\partial x_1}\frac{\partial}{\partial \bar{X}} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x} = \frac{m_1}{m_1+m_2}\frac{\partial}{\partial \bar{X}} + \frac{\partial}{\partial x}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial \bar{X}}{\partial x_2}\frac{\partial}{\partial \bar{X}} + \frac{\partial x}{\partial x_2}\frac{\partial}{\partial x} = \frac{m_2}{m_1+m_2}\frac{\partial}{\partial \bar{X}} - \frac{\partial}{\partial x}$$

The 2nd-order derivatives :

$$\frac{\partial^2}{\partial x_1^2} = \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_1} = \left(\frac{m_1}{m_1+m_2}\frac{\partial}{\partial \bar{X}} + \frac{\partial}{\partial x}\right)\left(\frac{m_1}{m_1+m_2}\frac{\partial}{\partial \bar{X}} + \frac{\partial}{\partial x}\right)$$

$$= \left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial \bar{X}^2} + \frac{\partial^2}{\partial x^2} + \frac{2m_1}{m_1+m_2}\frac{\partial}{\partial \bar{X}}\frac{\partial}{\partial x}$$

$$\frac{\partial^2}{\partial x_2^2} = \frac{\partial}{\partial x_2}\frac{\partial}{\partial x_2} = \left(\frac{m_2}{m_1+m_2}\frac{\partial}{\partial \bar{X}} - \frac{\partial}{\partial x}\right)\left(\frac{m_2}{m_1+m_2}\frac{\partial}{\partial \bar{X}} - \frac{\partial}{\partial x}\right)$$

$$= \left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial \bar{X}^2} + \frac{\partial^2}{\partial x^2} - \frac{2m_2}{m_1+m_2}\frac{\partial}{\partial \bar{X}}\frac{\partial}{\partial x}$$

The KE term :

$$-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2}$$

$$= -\frac{\hbar^2}{2}\left\{\frac{1}{m_1}\left[\left(\frac{m_1}{m_1+m_2}\right)^2\frac{\partial^2}{\partial \bar{X}^2} + \frac{\partial^2}{\partial x^2} + \frac{2m_1}{m_1+m_2}\frac{\partial}{\partial \bar{X}}\frac{\partial}{\partial x}\right]\right.$$

$$\left. + \frac{1}{m_2}\left[\left(\frac{m_2}{m_1+m_2}\right)^2\frac{\partial^2}{\partial \bar{X}^2} + \frac{\partial^2}{\partial x^2} - \frac{2m_2}{m_1+m_2}\frac{\partial}{\partial \bar{X}}\frac{\partial}{\partial x}\right]\right\}$$

$$= -\frac{\hbar^2}{2}\left[\frac{1}{m_1+m_2}\frac{\partial^2}{\partial \bar{X}^2} + \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{\partial^2}{\partial x^2}\right]$$

Total mass : $M = m_1 + m_2$

Reduced mass : $\mu = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)^{-1}$

$$= -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial \bar{X}^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}$$

1.1

(a)

The Hamiltonian :

$$\hat{H} = -\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + U(x_1 - x_2)$$

$$= -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + U(x)$$

(b)

Writing $\psi(x_1, x_2) = \Phi(X)\,\phi(x)$, the TISE is

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + U(x)\right]\Phi(X)\,\phi(x) = E\,\Phi(X)\,\phi(x)$$

$$-\frac{\hbar^2}{2M}\phi(x)\frac{\partial^2}{\partial X^2}\Phi(X) - \frac{\hbar^2}{2\mu}\Phi(X)\frac{\partial^2}{\partial x^2}\phi(x) + U(x)\,\Phi(X)\,\phi(x) = E\,\Phi(X)\,\phi(x)$$

$$-\frac{\hbar^2}{2M}\frac{1}{\Phi(X)}\frac{\partial^2}{\partial X^2}\Phi(X) - \frac{\hbar^2}{2\mu}\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + U(x) = E$$

$$\underbrace{-\frac{\hbar^2}{2M}\frac{1}{\Phi(X)}\frac{\partial^2}{\partial X^2}\Phi(X)}_{\text{Depend on } X \text{ only}} = \underbrace{-\left[-\frac{\hbar^2}{2\mu}\frac{1}{\phi(x)}\frac{\partial^2}{\partial x^2}\phi(x) + U(x) - E\right]}_{\text{Depend on } x \text{ only}}$$

Therefore, LHS and RHS of this equation equal to a constant ε simultaneously

$$\begin{cases} -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2}\Phi(X) = \varepsilon\,\Phi(X) & \cdots (1) \\ -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\phi(x) + U(x)\,\phi(x) = (E - \varepsilon)\,\phi(x) & \cdots (2) \end{cases}$$

Obviously $\Phi(X) = e^{iKX}$ is a solution of (1) and we have

$$-\frac{\hbar^2}{2M}(-K)^2 e^{iKX} = \varepsilon\, e^{iKX} \quad \Rightarrow \quad \varepsilon = \frac{\hbar^2 K^2}{2M}$$

$\therefore$ The center-of-mass motion is free with energy $\varepsilon = \frac{\hbar^2 K^2}{2M}$

1.2

(a)

$$\begin{vmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} \\ H_{21} - ES_{21} & H_{22} - ES_{22} \end{vmatrix} = 0$$

$$(H_{11} - ES_{11})(H_{22} - ES_{22}) - (H_{12} - ES_{12})(H_{21} - ES_{21}) = 0$$

$$(S_{11}S_{22} - S_{12}S_{21})E^2 + (H_{12}S_{21} + H_{21}S_{12} - H_{11}S_{22} - H_{22}S_{11})E + H_{11}H_{22} - H_{12}H_{21} = 0$$

Denote
$$A = S_{11}S_{22} - S_{12}S_{21}$$
$$B = H_{12}S_{21} + H_{21}S_{12} - H_{11}S_{22} - H_{22}S_{11}$$
$$C = H_{11}H_{22} - H_{12}H_{21}$$

$$E = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}$$

(b)

Now, $A = 1$

$$B = -E^{(0)} - H'_{11} - E^{(0)} - H'_{22} = -2E^{(0)} - H'_{11} - H'_{22}$$

$$C = (E^{(0)} + H'_{11})(E^{(0)} + H'_{22}) - |H'_{12}|^2$$
$$= E^{(0)2} + (H'_{11} + H'_{22})E^{(0)} + H'_{11}H'_{22} - |H'_{12}|^2$$

$$B^2 - 4AC = H'^2_{11} + H'^2_{22} - 2H'_{11}H'_{22} + 4|H'_{12}|^2$$
$$= (H'_{11} - H'_{22})^2 + 4|H'_{12}|^2$$

$$E = E^{(0)} + \frac{H'_{11} + H'_{22}}{2} \pm \frac{1}{2}\sqrt{(H'_{11} - H'_{22})^2 + 4|H'_{12}|^2}$$

1.3

(a) Eigenvalue : E_A

Corresponding eigenvector : $(1 \quad 0)^T$

Eigenvalue : E_B

Corresponding eigenvector : $(0 \quad 1)^T$

(b)

$$\begin{vmatrix} E_0 - E & \Delta \\ \Delta & E_0 - E \end{vmatrix} = 0$$

$$(E_0 - E)^2 - \Delta^2 = 0$$

$$(E_0 - E + \Delta)(E_0 - E - \Delta) = 0$$

$$E = E_0 + \Delta \text{ or } E_0 - \Delta$$

For $E = E_0 + \Delta$

$$\begin{cases} E_0 c_1 + \Delta c_2 = (E_0 + \Delta) c_1 \\ \Delta c_1 + E_0 c_2 = (E_0 + \Delta) c_2 \end{cases}$$

$$\Rightarrow \quad c_1 = c_2$$

Normalization : $c_1^2 + c_2^2 = 2c_1^2 = 1 \Rightarrow c_1 = c_2 = \frac{1}{\sqrt{2}}$

Normalized eigenvector : $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

1.3

(b) For $E = E_0 - \Delta$,

$$\begin{cases} E_0 c_1 + \Delta c_2 = (E_0 - \Delta) c_1 \\ \Delta c_1 + E_0 c_2 = (E_0 - \Delta) c_2 \end{cases}$$

One can also choose
$c_1 = -\frac{1}{\sqrt{2}} = -c_2$
These 2 choices correspond to the same state

$\Rightarrow \quad c_1 = -c_2$

Normalization : $c_1^2 + c_2^2 = 2c_1^2 = 1 \Rightarrow c_1 = \frac{1}{\sqrt{2}} = -c_2$

Normalized eigenvector : $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$\therefore$ Eigenstates : $\psi_\pm \sim \frac{1}{\sqrt{2}}\phi_1 \pm \frac{1}{\sqrt{2}}\phi_2$

Both eigenstates are EQUAL mixing of the original basis ϕ_1 and ϕ_2

(c)

$$\begin{vmatrix} E_A - E & \Delta \\ \Delta & E_B - E \end{vmatrix} = 0$$

$$(E_A - E)(E_B - E) - \Delta^2 = 0$$

$$E^2 - (E_A + E_B)E + (E_A E_B - \Delta^2) = 0$$

$$E = \frac{(E_A + E_B) \pm \sqrt{(E_A + E_B)^2 - 4E_A E_B + 4\Delta^2}}{2}$$

$$E = \frac{1}{2}\left[E_A + E_B \pm \sqrt{(E_A - E_B)^2 + 4\Delta^2} \right]$$

$$= \frac{1}{2}\left[E_A + E_B \pm (E_B - E_A)\sqrt{1 + \frac{4\Delta^2}{(E_B - E_A)^2}} \right] \quad (E_B > E_A)$$

1.3

(c) $$E_1 = \frac{1}{2}\left[E_A + E_B - \sqrt{(E_A - E_B)^2 + 4\Delta^2}\right]$$ → Eigenvalue closer to E_A

For $E = E_1$,

$$\begin{cases} E_A C_1 + \Delta C_2 = E C_1 \\ \Delta C_1 + E_B C_2 = E C_2 \end{cases}$$

$$\Rightarrow \quad C_2 = \frac{(E - E_A)}{\Delta} C_1$$

$$\text{Eigenvector} = C_1 \begin{pmatrix} 1 \\ \dfrac{E_B - E_A - \sqrt{(E_A - E_B)^2 + 4\Delta^2}}{2\Delta} \end{pmatrix}$$

One has the freedom to choose any non-zero complex number C_1 and they correspond to the same quantum state. However, the requirement of normalized eigenvector would fix the value of C_1.

$$E_2 = \frac{1}{2}\left[E_A + E_B + \sqrt{(E_A - E_B)^2 + 4\Delta^2}\right]$$ → Eigenvalue closer to E_B

For $E = E_2$,

$$\begin{cases} E_A C_1 + \Delta C_2 = E C_1 \\ \Delta C_1 + E_B C_2 = E C_2 \end{cases}$$

$$\Rightarrow \quad C_2 = \frac{(E - E_A)}{\Delta} C_1$$

$$\text{Eigenvectors} = C_1 \begin{pmatrix} 1 \\ \dfrac{E_B - E_A + \sqrt{(E_A - E_B)^2 + 4\Delta^2}}{2\Delta} \end{pmatrix}$$

1.3

(d)

$$E = \frac{1}{2}\left[E_A + E_B \pm \sqrt{(E_A - E_B)^2 + 4\Delta^2}\right]$$

$$= \frac{1}{2}\left[E_A + E_B \pm (E_B - E_A)\sqrt{1 + 4\Delta^2/(E_B - E_A)^2}\right] \qquad (E_B > E_A)$$

$$\approx \frac{1}{2}\left[E_A + E_B \pm (E_B - E_A)\left(1 + 2\Delta^2/(E_B - E_A)^2\right)\right]$$

(We assume $|\Delta| \ll |E_B - E_A|$ such that $\Delta^2/(E_B - E_A)^2 \ll 1$ and we can expand the square root as $\sqrt{1+x} \approx 1 + \frac{1}{2}x + \cdots$)

Two eigenvalues :

$$E_1 \approx \frac{1}{2}\left[E_A + E_B - (E_B - E_A) - 2\Delta^2/(E_B - E_A)\right]$$

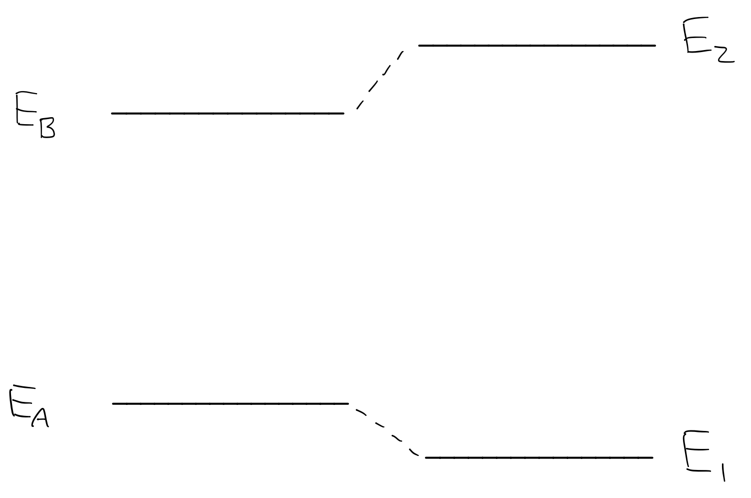
$$= E_A - \frac{\Delta^2}{E_B - E_A}$$

(close to and lower than E_A since $E_B - E_A > 0$)

$$E_2 \approx \frac{1}{2}\left[E_A + E_B + (E_B - E_A) + 2\Delta^2/(E_B - E_A)\right]$$

$$= E_B + \frac{\Delta^2}{E_B - E_A}$$

(close to and higher than E_B)



1.3

(d) Eigenvector of E_1 $\sim$ $\begin{pmatrix} 1 \\ \Delta/(E_A-E_B) \end{pmatrix}$

E_1 is close to E_A and its eigenvector has a larger proportion of ϕ_A as $\left|\frac{\Delta}{E_A-E_B}\right| \ll 1$

$(1\ 0)^T$

Eigenvector of E_2 $\sim$ $\begin{pmatrix} 1 \\ \frac{E_B-E_A}{\Delta} + \frac{\Delta}{E_B-E_A} \end{pmatrix}$

E_2 is close to E_B and its eigenvector has a larger proportion of $\phi_B = (0\ 1)^T$ as $\left|\frac{E_B-E_A}{\Delta}\right| \gg 1$

(e)

For $\Delta = 2$,

Exact eigenvalues : 12.4244, 2.5756

Approximation : 12.4444, 2.5556

Use $E_1 = E_A + \Delta^2/E_A - E_B$

$E_2 = E_B + \Delta^2/E_B - E_A$

and $E_A = 3$, $E_B = 12$

For $\Delta = 0.5$,

Exact eigenvalues : 12.02769, 2.97231

Approximation : 12.02778, 2.97222

1.4

(a) $\phi_{trial}(x) = A e^{-\lambda x^2}$

Normalization condition :

$$\int_{-\infty}^{\infty} |\phi_{trial}(x)|^2 dx = 1$$

$$A^2 \int_{-\infty}^{\infty} e^{-2\lambda x^2} dx = 1 \qquad \left(\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \right)$$

$$A^2 \sqrt{\frac{\pi}{2\lambda}} = 1$$

$$A = \left(\frac{2\lambda}{\pi}\right)^{1/4}$$

Expectation value of Hamiltonian :

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \phi_{trial}^*(x) \hat{H} \phi_{trial}(x) dx$$

$$= A^2 \int_{-\infty}^{\infty} e^{-\lambda x^2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right) e^{-\lambda x^2} dx$$

$$= A^2 \int_{-\infty}^{\infty} \left[e^{-\lambda x^2} \left(-\frac{\hbar^2}{2m}\right)\left(-2\lambda e^{-\lambda x^2} + 4\lambda^2 x^2 e^{-\lambda x^2}\right) + \frac{1}{2}m\omega^2 x^2 e^{-2\lambda x^2} \right] dx$$

$$= A^2 \left[\int_{-\infty}^{\infty} \frac{\hbar^2}{m}\lambda e^{-2\lambda x^2} dx - \int_{-\infty}^{\infty} \frac{2\hbar^2}{m}\lambda^2 x^2 e^{-2\lambda x^2} dx + \int_{-\infty}^{\infty} \frac{1}{2}m\omega^2 x^2 e^{-2\lambda x^2} dx \right]$$

Now, we use the identities

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \qquad \int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}\,\frac{(2n-1)(2n-3)\cdots 1}{(2a)^n}$$

1.4

(a)

$$\langle \hat{H} \rangle = A^2 \left(\frac{\hbar^2}{m} \lambda \sqrt{\frac{\pi}{2\lambda}} - \frac{2\hbar^2}{m} \lambda^2 \sqrt{\frac{\pi}{2\lambda}} \frac{1}{4\lambda} + \frac{1}{2} m\omega^2 \sqrt{\frac{\pi}{2\lambda}} \frac{1}{4\lambda} \right)$$

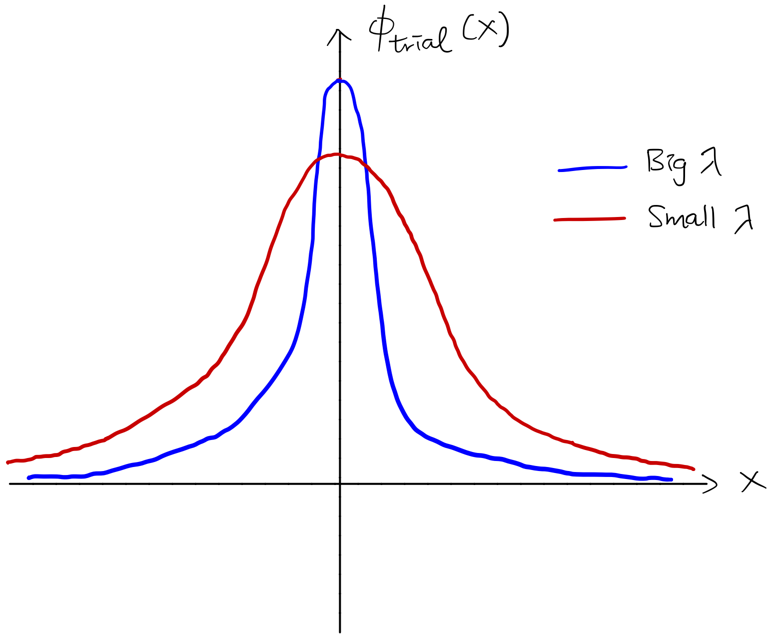
$$= \frac{\hbar^2}{m} \lambda - \frac{\hbar^2}{2m} \lambda + \frac{1}{8} m\omega^2 \frac{1}{\lambda} \qquad \left(A^2 = \sqrt{\frac{2\lambda}{\pi}} \right)$$

$$= \frac{\hbar^2}{2m} \lambda + \frac{1}{8} m\omega^2 \frac{1}{\lambda}$$

$$\therefore \quad \langle \hat{T} \rangle = \frac{\hbar^2}{2m} \lambda \qquad \langle \hat{V} \rangle = \frac{1}{8} m\omega^2 \frac{1}{\lambda}$$

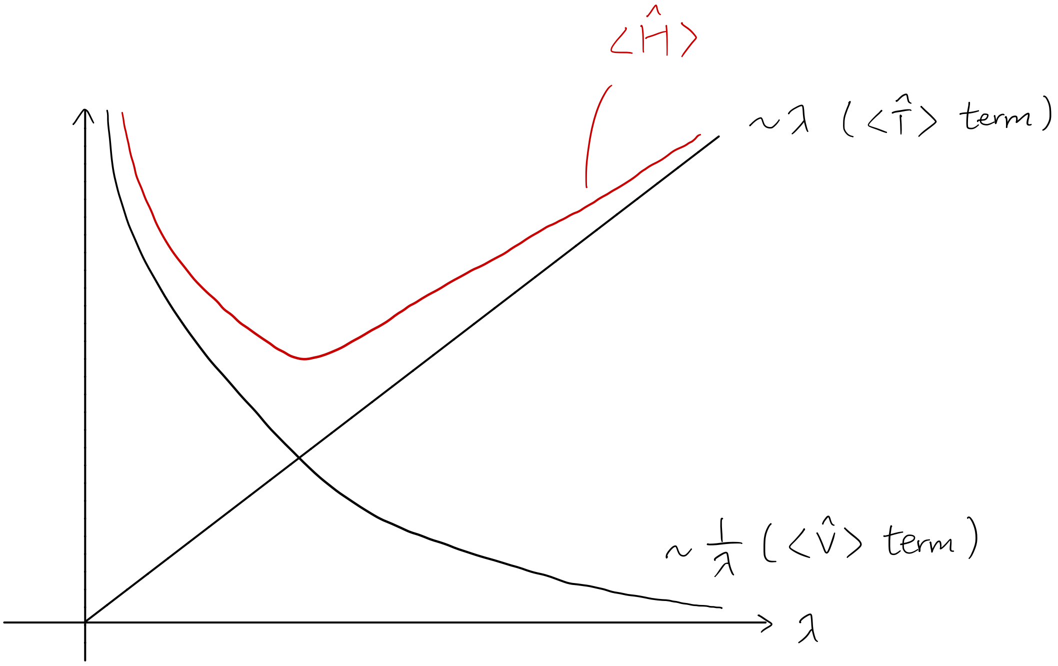
(b) $\frac{1}{\lambda}$ is the characteristic "width" of the wavefunction.

when λ goes from big to small, the width of $\phi_{trial}(x)$ increases.



1.4

(c)



As we see in the figure, $\langle \hat{T} \rangle$ term increases and $\langle \hat{V} \rangle$ term decreases when λ increases.

When λ is small, the wavefunction is very broad. Although the expectation value of KE is small because the wavefunction changes gradually in space ($\frac{-\hbar^2}{2m}\frac{d^2\phi}{dx^2}$ is small), the expectation value of PE is high because the probability density of the particle is not low at large x and the PE of harmonic oscillator increases quadratically with x as $\frac{1}{2}m\omega^2x^2$

when λ is large, the wavefunction is very narrow. Although the expectation value of PE is small because the probability density of the particle decays quickly with increasing x, the expectation value of KE is high because the wavefunction is more wriggling ($\frac{-\hbar^2}{2m}\frac{d^2\phi}{dx^2}$ is high)

Since $\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$, we cannot have too big or too small λ for the variational ground state wavefunction. From the above figure, it is clear that there is an optimal value of λ which compromises the effects of KE and PE to obtain the lowest total energy.

1.4

(d) Let λ_{min} be the optimal value of λ. To find the minimum of $\langle \hat{H} \rangle$,

$$\frac{\partial}{\partial \lambda} \langle \hat{H} \rangle \Big|_{\lambda = \lambda_{min}} = 0$$

$$\frac{\hbar^2}{2m} - \frac{1}{8} m \omega^2 \frac{1}{\lambda_{min}^2} = 0$$

$$\lambda_{min} = \frac{m\omega}{2\hbar}$$

The estimated ground state energy is

$$\langle \hat{H} \rangle \Big|_{\lambda = \lambda_{min}} = \frac{1}{2} \hbar \omega$$

The variational ground state wavefunction is :

$$\phi_{\lambda = \lambda_{min}}(x) = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$$

They are equal to the exact results we learnt in QMI course because we have guessed the correct form of the wavefunction ($\sim e^{-\lambda x^2}$) in the beginning

1.5

The trial wavefunction is the same as problem 1.4.

$$\phi(x) = A e^{-\lambda x^2} \qquad A = \left(\frac{2\lambda}{\pi}\right)^{1/4} \qquad \text{Normalization constant}$$

The expectation value of Hamiltonian is :

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \phi^*(x)\, \hat{H}\, \phi(x)\, dx$$

$$= A^2 \int_{-\infty}^{\infty} e^{-\lambda x^2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + ax^4\right) e^{-\lambda x^2} dx$$

For kinetic energy part,

$$A^2 \int_{-\infty}^{\infty} e^{-\lambda x^2} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) e^{-\lambda x^2} dx = \frac{\hbar^2}{2m}\lambda \qquad \text{(already computed in 1.4)}$$

For potential energy part,

$$A^2 \int_{-\infty}^{\infty} e^{-\lambda x^2}\, ax^4\, e^{-\lambda x^2} dx$$

$$= aA^2 \int_{-\infty}^{\infty} x^4 e^{-2\lambda x^2} dx$$

$$= aA^2 \sqrt{\frac{\pi}{2\lambda}} \frac{3}{(4\lambda)^2} \qquad \left(\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \frac{(2n-1)(2n-3)\cdots 1}{(2\alpha)^n} \right)$$

$$= \frac{3a}{16\lambda^2}$$

$$\langle \hat{H} \rangle = \frac{\hbar^2}{2m}\lambda + \frac{3a}{16\lambda^2}$$

Let λ_{min} be the optimal value of λ. To find the minimum of $\langle \hat{H} \rangle$,

$$\frac{\partial}{\partial \lambda} \langle \hat{H} \rangle \Big|_{\lambda = \lambda_{min}} = 0$$

$$\frac{\hbar^2}{2m} - \frac{3a}{8\lambda_{min}^3} = 0$$

$$\lambda_{min} = \left(\frac{3ma}{4\hbar^2}\right)^{1/3}$$

1.5

The estimated G.S. energy

$$= \frac{\hbar^2}{2m}\left(\frac{3ma}{4\hbar^2}\right)^{1/3} + \frac{3a}{16}\left(\frac{4\hbar^2}{3ma}\right)^{2/3}$$

$$= \left[\frac{1}{2}\left(\frac{3}{4}\right)^{1/3} + \frac{3}{16}\left(\frac{4}{3}\right)^{2/3}\right]\left(\frac{\hbar^4 a}{m^2}\right)^{1/3}$$

$$\approx 0.6814\left(\frac{\hbar^4 a}{m^2}\right)^{1/3}$$