PHY5410 FA22 HW06

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Problem 1 (11.3)**.** Define

$$a_x = \frac{1}{\sqrt{2}}(x - ip_x)$$
$$a_y = \frac{1}{\sqrt{2}}(y - ip_y)$$

Then

$$H = a_x^\dagger a_x + a_y^\dagger a_y + 1$$

Compare two the 1-D harmonic oscillators, using the technique of separation of variables, we have the wave functions for the three lowest lying energy levels:

$$\phi_{0,0}(x, y) = \frac{1}{\sqrt{\pi}} e^{-x^2/2} e^{-y^2/2}$$
$$\phi_{1,0}(x, y) = \sqrt{\frac{2}{\pi}} x e^{-x^2/2} e^{-y^2/2}$$
$$\phi_{0,1}(x, y) = \sqrt{\frac{2}{\pi}} y e^{-x^2/2} e^{-y^2/2}$$

where $\phi_{0,1}$ and $\phi_{1,0}$ are two degenerate states.

The perturbed hamiltonian is

$$H = H_0 + \frac{1}{2}\delta H_1$$
$$H_0 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2)$$
$$H_1 = xy(x^2 + y^2)$$

To avoid singularity of degenerated states, consider diagonalize the matrix $\langle \psi_{i,j} | H_1 | \psi_{k,l} \rangle$, $(i, j), (k, l) = (1, 0), (0, 1)$. Consider the following integrals

$$\int_{\mathbb{R}^2} \mathrm{d}x\, \mathrm{d}y\; x^2 y^2 (x^2 + y^2) e^{-x^2 - y^2} = \int_{\mathbb{R}^2} r\, \mathrm{d}r\, \mathrm{d}\theta \sin^2\theta \cos^2\theta r^6 e^{-r^2} = \frac{3}{4}\pi$$

We can verify that

$$\langle \psi_{0,0} | H_1 | \psi_{0,0} \rangle = 0$$
$$\langle \psi_{1,0} | H_1 | \psi_{1,0} \rangle = 0$$
$$\langle \psi_{0,1} | H_1 | \psi_{0,1} \rangle = 0$$
$$\langle \psi_{1,0} | H_1 | \psi_{0,1} \rangle = \langle \psi_{1,0} | H_1 | \psi_{0,1} \rangle = \frac{3}{2}$$

Note that

$$\begin{bmatrix} 0 & 3/2 \\ 3/2 & 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 3/2 & \\ & -3/2 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Define two new states to avoid singularity

$$\psi_1' = \frac{1}{\sqrt{2}}(\psi_{1,0} + \psi_{0,1})$$
$$\psi_2' = \frac{1}{\sqrt{2}}(\psi_{1,0} - \psi_{0,1})$$

which diagonalize H_1. Hence

$$E^1_{0,0} = 0$$
$$E^1_{1,1'} = \frac{3}{2}$$
$$E^1_{1,2'} = -\frac{3}{2}$$

Thus shifts are 0, $3\delta/4$ and $-3\delta/4$, correspondingly. Then we have first-order approximation equals to

$$E_{0,0} = 1$$
$$E_{1,1'} = 2 + \frac{3}{4}\delta$$
$$E_{1,2'} = 2 - \frac{3}{4}\delta$$

Problem 2 (11.5). Let

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x$$

Then

$$\psi^* H\psi = N^2\frac{\hbar^2}{m}\mu e^{-2\mu x^2} + N^2\left(\frac{1}{2}m\omega^2 - 2\frac{\hbar^2}{m}\mu^2\right)x^2 e^{-2\mu x^2}$$

Using the fact that

$$\int_{-\infty}^{\infty} e^{-\mu x^2}\,\mathrm{d}x = \sqrt{\pi}(2\mu)^{-1/2}$$
$$\int_{-\infty}^{\infty} x^2 e^{-\mu x^2}\,\mathrm{d}x = \frac{1}{2}\sqrt{\pi}(2\mu)^{-3/2}$$

Then the energy equals to

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\hbar^2}{2m}\mu + \frac{m\omega^2}{8}\frac{1}{\mu}$$

Easy to derive that E takes its minimum at $\mu = m\omega/2\hbar$. Then an approximation of the ground state energy is

$$E_0 = \frac{\hbar\omega}{2}$$

Problem 3 (11.7).

Remark. Since ψ_0, ψ_1 symmetric or antisymmetric on $\mathbb{R}$, the energy calculated on $(0, +\infty)$ is the same as $(-\infty, +\infty)$. Part (b) and (d) in this problem is solved by Mathematica.

(a) Note that

$$
\begin{aligned}
H\psi_0 &= \frac{\hbar^2}{m}\kappa_0 e^{-\kappa_0 x} - \frac{\hbar^2}{2m}\kappa_0^2 x e^{-\kappa_0 x} + V(x) x e^{-\kappa_0 x} \\
\psi_0^* H\psi_0 &= \frac{\hbar^2}{m}\kappa_0 x e^{-2\kappa_0 x} - \frac{\hbar^2}{2m}\kappa_0^2 x^2 e^{-2\kappa_0 x} + V(x) x^2 e^{-2\kappa_0 x}
\end{aligned}
$$

Since

$$
\begin{aligned}
\int_0^\infty \mathrm{d}x\, e^{-ax} &= \frac{1}{a} \\
\int_0^\infty \mathrm{d}x\, x e^{-ax} &= \frac{1}{a^2} \\
\int_0^\infty \mathrm{d}x\, x^2 e^{-ax} &= \frac{2}{a^3}
\end{aligned}
$$

we have

$$
\begin{aligned}
\langle\psi_0|H|\psi_0\rangle &= \frac{\hbar^2}{8\kappa_0 m} + V_0\int_0^a \mathrm{d}x x^2 e^{-2\kappa_0 x} = \frac{\hbar^2}{8\kappa_0 m} + V_0\left[\frac{1}{4\kappa_0^3} - e^{-2\kappa_0 a}\left(\frac{1}{4\kappa_0^3} + \frac{2a}{4\kappa_0^2} + \frac{a^2}{2\kappa_0}\right)\right] \\
\langle\psi_0|\psi_0\rangle &= \frac{1}{4\kappa_0^3} \\
\Rightarrow E &= V_0 + \frac{\hbar^2}{2m}\kappa_0^2 - V_0 e^{-2\kappa_0 a}(1 + 2a\kappa_0 + 2a^2\kappa_0^2)
\end{aligned}
$$

Minimize E w.r.t. κ_0, consider the derivative

$$
\frac{\partial E}{\partial \kappa_0} = \frac{\hbar^2}{m}\kappa_0 + 4V_0 a^3 \kappa_0^2 e^{-2\kappa_0 a} = 0
$$

Then κ_0 is the positive solution of

$$
\kappa_0 e^{-2\kappa_0 a} = -\frac{\hbar^2}{4V_0 a^3 m}
$$

(b) Using the orthogonality that $\langle\psi_0|\psi_1\rangle = 0$, we have

$$
\int_{-\infty}^{\infty} \mathrm{d}x\, x^2(x-n)e^{-(\kappa_0+\kappa_1)|x|} = \frac{4n}{(\kappa_0+\kappa_1)^2} = 0 \Rightarrow n = 0
$$

Then we have

$$
\begin{aligned}
E &= V_0 + \frac{\hbar^2}{6m}\kappa_1^2 - V_0\left[2a^2\kappa_1^2 + e^{-2\kappa_1 a}\left(1 + 2a\kappa_1 + 2a^2\kappa_1^2 + \frac{4}{3}a^3\kappa_1^3 + \frac{2}{3}a^4\kappa_1\right)\right] \\
\frac{\partial}{\partial\kappa_1}E &= \frac{\hbar^2}{3m}\kappa_1 + \frac{4}{3}a^5 V_0 \kappa_1^4 e^{-2a\kappa_1}
\end{aligned}
$$

Minimize E_0 w.r.t. $\kappa_1 > 0$, then κ_1 is the positive solution of

$$
\frac{\hbar^2}{3m} + \frac{4}{3}a^5 V_0 \kappa_1^3 e^{-2a\kappa_1} = 0
$$

(c) I give it up...

(d) Take $\psi_0 = xe^{-\kappa_0 x^2}$, we have

$$E = -\frac{2}{\sqrt{\pi}} a V_0 (2\kappa_0)^{1/2} + \frac{3\hbar^2}{2m}\kappa_0 + V_0 \operatorname{erf}[a(2\kappa_0)^{1/2}]$$
$$\frac{\partial}{\partial\kappa_0} E = \frac{3\hbar^2}{2m} + \frac{4}{\sqrt{\pi}} a^3 V_0 (2\kappa_0)^{1/2} e^{-2a^2\kappa_0}$$

Minimize E_0 w.r.t. $\kappa_0 > 0$, then κ_1 is the positive solution of

$$\frac{3\hbar^2}{2m} + \frac{4}{\sqrt{\pi}} a^3 V_0 (2\kappa_0)^{1/2} e^{-2a^2\kappa_0} = 0$$