变分原理

这一章的作业思路相对简单，只是拿试探波函数代入计算能量。

第一题

1.

$$\langle V\rangle = 2\alpha A^2\int_0^\infty x e^{-2bx^2}dx$$

$$= 2\alpha A^2\left(-\frac{1}{4b}e^{-2bx^2}\right)\Big|_0^\infty$$

$$= \frac{a}{\sqrt{2b\pi}}$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{a}{\sqrt{2\pi b}}$$

$$\frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha}{\sqrt{2\pi}}b^{-3/2} \doteq 0.$$

$$\Downarrow$$

$$b^{\frac{3}{2}} = \frac{\alpha}{\sqrt{2\pi}}\frac{m}{\hbar^2};$$

$$b = \left(\frac{m\alpha}{\sqrt{2\pi}\hbar^2}\right)^{\frac{2}{3}}$$

代入Mathematica中计算得，

$$\langle H_{min}\rangle = \frac{3}{2}\left(\frac{\alpha^2\hbar^2}{2\pi m}\right)^{\frac{1}{3}}$$

$$\langle H\rangle = \langle T\rangle + \langle V\rangle = 6\frac{\hbar^2}{ma^2} - 3\frac{\alpha}{a}.$$

$$\frac{\partial\langle H\rangle}{\partial a} = -12\frac{\hbar^2}{ma^3} + 3\frac{\alpha}{a^2} = 0 \Rightarrow a = \frac{4\hbar^2}{m\alpha}.$$

$$\langle H\rangle_{min} = -\frac{3m\alpha^2}{8\hbar^2} > -\frac{m\alpha^2}{2\hbar^2}$$

4. 展开，得

$$\sum_{n=1}^{\infty} c_n\langle\psi_1, \psi\rangle = c_1 = 0.$$

(a)

$$\langle H\rangle = \sum_{n=2}^{\infty} E_n |c_n|^2 \geq E_{fe}\sum_{n=2}^{\infty}|c_n|^2 = E_{fe}.$$

(b)

$$1 = |A|^2\int_{-\infty}^{\infty} x^2 e^{-2bx^2}\,dx = |A|^2 \frac{1}{8b}\sqrt{\frac{\pi}{2b}} \Rightarrow A = \ldots$$

$$\langle T\rangle = -\frac{\hbar^2}{2m}|A|^2\int_{-\infty}^{\infty} x e^{-bx^2}\frac{d^2}{dx^2}(x e^{-bx^2})\,dx$$

$$\Rightarrow -2bxe^{-bx^2} - 4bxe^{-bx^2} + 4b^2x^3e^{-bx^2}$$

$$\langle V\rangle = \frac{1}{2}m\omega^2|A^2|\int_{-\infty}^{\infty} x^2 e^{-2bx^2}x^2\,dx = \frac{3m\omega^2}{8b}$$

$$\langle H\rangle = 0 \Rightarrow b = \frac{m\omega}{2\hbar}.$$

$$\langle H\rangle_{min} = \frac{3\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{3m\omega^2}{8}\frac{2\hbar}{m\omega} = \frac{3}{2}\hbar\omega.$$

第二题

5.

ψ^0_{gs} .

$\langle \psi^0_{gs} | H | \psi^0_{gs} \rangle \geq E^0_{gs}$

但 $H = H^0 + H'$

故 $\langle \psi^0_{gs} | H | \psi^0_{gs} \rangle = \langle \psi^0_{gs} | H^0 | \psi^0_{gs} \rangle + \langle \psi^0_{gs} | H' | \psi$

但 $\langle \psi^0_{gs} | H' | \psi^0_{gs} \rangle$ 是一阶修正.

故 $E^0_{gs} + E^1_{gs} \geq E_{gs}$.

6. $E^2_{gs} = \sum_{m \neq gs} \frac{|\langle \psi^0_m | H' | \psi_{gs} \rangle|^2}{E^0_{gs} - E^0_m}$

分母为负 $\Rightarrow E^2_{gs} < 0$.

~~6.~~

第三、四题（连着上面）

(x^2+b^2)

代入MMA中，得：$\frac{1}{2}m\omega^2 b^2$

$$\langle H\rangle = \frac{\hbar^2}{4mb^2} + \frac{1}{2}m\omega^2 b^2$$

$$\frac{\partial\langle H\rangle}{\partial b} = -\frac{\hbar^2}{2mb^3} + m\omega^2 b = 0 \Rightarrow b^2 = \frac{1}{\sqrt{2}}\frac{\hbar}{m\omega}$$

$$\langle H\rangle_{min} = \frac{\hbar^2}{4m}\frac{\sqrt{2}m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{1}{\sqrt{2}}\frac{\hbar}{m\omega} = \frac{\sqrt{2}}{2}\hbar\omega > \frac{1}{2}\hbar\omega$$

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3. $$\psi(x) = \begin{cases} A(x+a/2) & (-a/2 < x < 0 \\ A(a/2-x) & (0 < x < \frac{a}{2}) \\ 0 & (其它 \end{cases}$$

$$1 = |A^2|\, 2\int_0^{\frac{a}{2}}\left(\frac{a}{2}-x\right)^2 dx = \frac{a^3}{12}A^2$$

$$\Downarrow$$

$$A = \sqrt{\frac{12}{a^3}}$$

$$\langle T\rangle = \frac{-\hbar^2}{2m}\int\psi\left[A\delta\left(x+\frac{a}{2}\right) - 2A\delta(x) + A\delta\left(x-\frac{a}{2}\right)\right]d$$

$$= \frac{\hbar^2}{m}A^2\frac{a}{2} = 6\frac{\hbar^2}{ma^2}$$

$$\langle V\rangle = -\alpha\int|\psi|^2\delta(x)\,dx = -\alpha|\psi(0)|^2 = -\frac{3\alpha}{a}$$

第五题

(5) $\langle V\rangle = 2\alpha A^2 \int_0^\infty x^4 e^{-2bx^2} dx$

$= 2\alpha A^2 \frac{3}{8(2b)^2}\sqrt{\frac{\pi}{2b}}$

$= \frac{3\alpha}{16b^2}$

$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}$

$\frac{\partial\langle H\rangle}{\partial b} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8b^3} = 0$

$\Downarrow$

$b^3 = \frac{3\alpha m}{4\hbar^2} \qquad b = \left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}}$

$\langle H\rangle_{min}$ = 代入 $= \frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{\frac{1}{3}}$