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Quantum Computing + X HW5 高伯文 2024010734

[1]

We have derived that

$$E_+(R) = -\left(1+2\frac{D+X}{1+I}-\frac{2a}{R}\right)|E_0|$$

where $D=\frac{a}{R}-(1+\frac{a}{R})e^{-2R/a}$

$X=(1+\frac{R}{a})e^{-R/a}$

$I=\frac{1}{3}(R^2/a^2+3R/a+3)e^{-R/a}$

we will expand $E_+(R)$ as

$$E_+(R)=E_+(R^*)+\frac{1}{2}k(R-R^*)^2+O(R^2)$$

near the R^*. this is equivalent to calculating $\frac{d^2(E_+(R))}{dR^2}\Big|_{R=R^*}$

$$\frac{E_+(R)}{|E_0|}=-1+\frac{2a}{R}-2\frac{\frac{a}{R}-(1+\frac{a}{R})e^{-2R/a}+(1+\frac{R}{a})e^{-R/a}}{1+\frac{1}{3}(R^2/a^2+3R/a+3)e^{-R/a}}$$

$$=-1+\frac{2a}{R}-2\frac{\frac{a}{R}e^{R/a}+(1+\frac{R}{a})-(1+\frac{a}{R})e^{-R/a}}{e^{R/a}+\frac{1}{3}(R^2/a^2+3R/a+3)}$$

If we can get this k. we know that the potential of harmonic oscillator is $\frac{1}{2}\mu\omega^2X^2$. μ: reduced mass $=\frac{m_p}{2}$

$\Rightarrow \omega=\sqrt{\frac{2k}{m_p}}$, the calculation is left to the computer to do

The result is about

$\omega = 341863926673433$.

$E_{vibration} \approx 0.225\,eV$. Please refer to the code

[2]

(a) ① By applying the perturbation theory

$$H_0|0^{(0)}\rangle = E_0^{(0)}|0^{(0)}\rangle$$

$$H_0|0^{(1)}\rangle + \cancel{\lambda}X|0^{(0)}\rangle = E_0^{(0)}|0^{(1)}\rangle + E_0^{(1)}|0^{(0)}\rangle$$

$$H_0|0^{(2)}\rangle + X|0^{(1)}\rangle = E_0^{(0)}|0^{(2)}\rangle + E_0^{(1)}|0^{(1)}\rangle + E_0^{(2)}|0^{(0)}\rangle$$

$$E_0^{(1)} = \cancel{\langle 0\rangle}\langle 0^{(0)}|x|0^{(0)}\rangle$$

since $|0^{(0)}\rangle$ is an odd function

$E_0^{(1)}=0$

② $E_0^{(2)}=\langle 0^{(0)}|x|0^{(1)}\rangle$

we know that $|n^{(1)}\rangle=\sum_{m\neq n}\frac{\langle m^{(0)}|\cancel{V}x|n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}|m^{(0)}\rangle$

$\therefore \langle 0^{(0)}|x|0^{(1)}\rangle$

$=\langle 0^{(0)}|x\sum_{m\neq 0}\frac{\langle m^{(0)}|x|0^{(0)}\rangle}{E_0^{(0)}-E_m^{(0)}}|m^{(0)}\rangle$

$=\sum_{m\neq 0}\frac{|\langle m^{(0)}|x|0^{(0)}\rangle|^2}{E_0^{(0)}-E_m^{(0)}}$

$x=\sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)$

$\therefore$ only $\langle 1^{(0)}|x|0^{(0)}\rangle=\sqrt{\frac{\hbar}{2m\omega}}$

All in all $E_0^{(2)}=\frac{|\langle 1|x|0\rangle|^2}{E_0-E_1}=-\frac{1}{2m\omega^2}$

if we add λ^2 back

the second order energy shift is $-\frac{\lambda^2}{2m\omega^2}$,

③ Suppose we shift the origin of the harmonic oscillator

$$\cancel{\frac{\hbar^2}{2m}}\left(\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+\lambda X\right)\Psi=E\Psi$$

we can get

$$H' = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x+\frac{\lambda}{m\omega^2}\right)^2 - \frac{\lambda^2}{2m\omega^2}$$

which means E_0 is shifted by $-\frac{\lambda^2}{2m\omega^2}$, the result is the same as we got.

(b) Similarly

① $E^{(1)}_{0,0} = 0$ due to symmetry of ground state wave function

② $E^{(0)}_{0,0} = \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\omega = \hbar\omega$

$E^{(0)}_{1,0} = E^{(0)}_{0,1} = 2\hbar\omega$

~~③ Take $E_{1,0}$ as an examply~~ example

By using the same perturbation theory

~~$H_0|0^{(2)}\rangle$~~

$$H_0|0^{(1)}\rangle + m\omega^2 xy|0^{(0)}\rangle = E_0^{(0)}|0^{(1)}\rangle + E_0^{(1)}|0^{(0)}\rangle \quad \text{"1"}$$

$$H_0|0^{(2)}\rangle + m\omega^2 xy|0^{(1)}\rangle = E_0^{(0)}|0^{(2)}\rangle + E_0^{(1)}|0^{(1)}\rangle + E_0^{(2)}|0^{(0)}\rangle \quad \text{"2"}$$

$$E_0^{(2)} = \langle 0^{(0)}| m\omega^2 xy|0^{(1)}\rangle$$

From equation "1"

$$|0^{(1)}\rangle = \sum_{m\neq 0} \frac{\langle m^{(0)}|m\omega^2 xy|0^{(0)}\rangle}{E_0^{(0)}-E_m^{(0)}}|m^{(0)}\rangle$$

$$E_0^{(2)} = \sum_{m\neq 0}\frac{|\langle m^{(0)}|m\omega^2 xy|0^{(0)}\rangle|^2}{E_0^{(0)}-E_m^{(0)}}$$

$x = \sqrt{\frac{\hbar}{2m\omega}}(a_x+a_x^{\dagger})$ $y = \sqrt{\frac{\hbar}{2m\omega}}(a_y+a_y^{\dagger})$

∴ $\langle m^{(0)}|$ can only be $\langle 1,0|$ or $\langle 0,1|$ or $\langle 1,1|$ if we want it to be nonzero

$$E_0^{(2)} = m^2\omega^4\left[\frac{\left(\frac{\hbar}{2m\omega}\right)^2}{E_0^{(0)}-E_2^{(0)}} + \frac{\left(\sqrt{\frac{\hbar}{2m\omega}}\right)^2}{E_0^{(0)}-E_1^{(1)}}\right]$$

$$= m^2\omega^4\left[\frac{\frac{\hbar^2}{4m^2\omega^2}}{-2\hbar\omega} - \frac{\frac{\hbar}{2m\omega}}{\hbar\omega}\right]$$

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

The lowest three eigenstates of ~~$H = H_0 + V$~~ H_0 are

$|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$

which represents the tensor product of $|0\rangle$ and $|1\rangle$ states for 1D-harmonic oscillator

and the corresponding zeroth-order energies are

$E^{(0)}_{0,0} = \hbar\omega$ $E^{(0)}_{1,0} = E^{(0)}_{0,1} = 2\hbar\omega$

$E^{(1)}_{0,0} = \langle 0^{(0)}| m\omega^2 xy|0^{(0)}\rangle = 0$

due to symmetry

$$H_0|1^{(1)}\rangle + m\omega^2 xy|1^{(0)}\rangle = E_1^{(0)}|1^{(1)}\rangle + E_0^{(1)}|1^{(0)}\rangle$$

where $|1^{(0)}\rangle = |1,0\rangle + |0,1\rangle$

$\langle 1,0|m\omega^2 xy|1,0\rangle = \langle 0,1|m\omega^2 xy|0,1\rangle = 0$

$\langle 1,0|m\omega^2 xy|0,1\rangle = m\omega^2\langle 1|x|0\rangle\langle 0|y|1\rangle$

$= m\omega^2\cdot\frac{\hbar}{2m\omega} = \frac{1}{2}\hbar\omega$

∴ $E_0^{(1)} = \frac{1}{2}\hbar\omega$.

and the first order energy shift is

$\alpha E_0^{(1)} = \frac{1}{2}\hbar\omega\alpha$

③ The exact solution

$$\frac{1}{2}m\omega^2 x^2 + \frac{1}{2}m\omega^2 y^2 + \alpha m\omega^2 xy = \frac{1}{2}m\omega^2 (x, y)\begin{pmatrix}1 & \alpha\\ \alpha & 1\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}$$

$$\begin{vmatrix}1-\lambda & \alpha\\ \alpha & (1-\lambda)\end{vmatrix} = 0 \Rightarrow (1-\lambda)^2 = \alpha^2$$

$1-\lambda = \pm\alpha$ $\lambda = 1\pm\alpha$

∴ the first order shift of energy for $|1,0\rangle$, and $|0,1\rangle$ are both $\frac{1}{2}\hbar\omega\alpha$, which achieves the same result.

【3】

(a) For a single particle

$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$

① If the spins of two particles are symmetric the spatial wave function must be anti-symmetric

$$\Psi_{spatial} = \frac{1}{\sqrt{2}}\left[\phi_i(x_1)\phi_j(x_2) - \phi_j(x_1)\phi_i(x_2)\right]$$

⇒ minimum ⇒ $i=1, j=2$

lowest energy $E_{min} = (1^2+2^2)\frac{\pi^2\hbar^2}{2mL^2}$

$= \frac{5\pi^2\hbar^2}{2mL^2}$

② If the spins of two particles are anti-symmetric, the spatial wave function must be symmetric

$$\Psi_{spatial} = \frac{1}{\sqrt{2}}\left[\phi_i(x_1)\phi_j(x_2)+\phi_j(x_1)\phi_j(x_2)\right]$$

we can let $i=j=1$

$$\Rightarrow E_{min} = \frac{\pi^2\hbar^2}{mL^2}$$

(b) ① Let $\Psi_1 = \frac{1}{\sqrt{2}}(|1,2\rangle - |2,1\rangle)$

$$E_0^{(1)} = \langle \Psi_1 | V | \Psi_1 \rangle$$

$$= \langle \Psi_1 | -\lambda\delta(x_1-x_2) | \Psi_1 \rangle$$

$$= -\lambda\int |\Psi(x,x)|^2 dx$$

$$\Psi_1(x,x) = \frac{1}{\sqrt{2}}\left[\phi_1(x)\phi_2(x) - \phi_2(x)\phi_1(x)\right]$$

$$= 0$$

$\Rightarrow E_0^{(1)} = 0$ $\because$ spin symmetry

② Let $\Psi_1^{(x_1,x_2)} = \frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_1(x_2)+\phi_1(x_2)\phi_1(x_1)\right]$

$$\therefore E_0^{(1)} = -\lambda\int_{-\infty}^{+\infty}(\phi_1(x))^4 dx$$

we know that $\phi_1(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$

$$\therefore E_0^{(1)} = -\frac{4\lambda}{L^2}\int_0^L \sin^4\left(\frac{\pi x}{L}\right)dx$$

$$= -\frac{4\lambda}{\pi L}\int_0^{\pi}\sin^4\theta\, d\theta$$

$$= -\frac{4\lambda}{\pi L}\cdot\frac{1}{4}\left(1+\frac{1}{2}\right)\pi$$

$$= -\frac{3\lambda}{2L}$$

$$\therefore E \approx E_{min}^{(0)} + E_0^{(1)}$$

$$= \frac{\pi^2\hbar^2}{mL^2} - \frac{3\lambda}{2L}$$

【4】 Please refer to the code

【5】

(a) $a_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} c_j e^{2\pi i jk/N}$

~~we need to prove~~

$$\{a_j, a_k^+\} = 0$$

$$a_j a_k^+ = \frac{1}{N}\left(\sum_{m=1}^{N} c_m e^{2\pi i mj/N}\right)\left(\sum_{n=1}^{N} c_n^+ e^{-2\pi i nk/N}\right)$$

$$= \frac{1}{N}\sum_{m,n} c_m c_n^+ e^{2\pi i(mj-nk)/N}$$

similarly

$$a_k a_j^+ = \frac{1}{N}\sum_{n,m} c_n c_m^+ e^{2\pi i(nk-mj)/N}$$

① $$a_j \cdot a_k = \frac{1}{N}\left(\sum_{m=1}^{N} c_m e^{2\pi i mj/N}\right)\left(\sum_{n=1}^{N} c_n e^{2\pi i nk/N}\right)$$

$$= \frac{1}{N}\sum_{m,n} c_m \cdot c_n e^{2\pi i(mj+nk)/N}$$

since $\{c_m, c_n\} = 0$

$\Rightarrow a_j \cdot a_k + a_k a_j = 0$

$\Rightarrow \{a_j, a_k\} = 0$

② similarly, we will have $\{a_j^+, a_k^+\} = 0$ since ~~$\{c_j, c_k^+\}$~~ $\{c_m^+, c_n^+\} = 0$

③ For $\{a_j, a_k^+\}$

~~$\{c_j, c_k^+\} = \delta_{jk}$~~ $\{c_m, c_n^+\} = \delta_{mn} I$.

$\therefore$ There are some terms left

$$a_j a_k^+ + a_k^+ a_j = \frac{1}{N}\sum_{m=n=t}\left(c_t c_t^+ e^{2\pi i t(k-j)/N} + c_t^+ c_t e^{2\pi i t(k-j)/N}\right)$$

$$= \frac{1}{N}\sum_{t=1}^{N} e^{2\pi i t(k-j)/N}\cdot I$$

$$= \begin{cases} I, & k=j \\ 0, & k\neq j \end{cases}$$

$$= \delta_{k,j} I$$

∴ a_k operators satisfy the fermionic anti-commutation relations.

(b) $c_j c_{j+1}$

$$= \frac{1}{N}\left(\sum_{m=0}^{N-1} a_m e^{-2\pi i jm/N}\right)\left(\sum_{n=0}^{N-1} a_n e^{-2\pi i (j+1)n/N}\right)$$

$$= \frac{1}{N}\sum_{m,n} a_m a_n e^{-2\pi i [j(m+n)+n]/N}$$

Sum over j

$$\Rightarrow \sum_{j=1}^{N} c_j c_{j+1}$$

$$= \frac{1}{N}\sum_{m,n}\left(a_m a_n e^{-2\pi i n/N} \cdot \sum_{j=1}^{N} e^{-2\pi i (m+n) j/N}\right)$$

$$= \cancel{\tfrac{N}{N}}\sum_{m+n=N} a_m a_n e^{-2\pi i n/N}$$

Similarly

$$\sum c_{j+1}^\dagger c_j^\dagger = \sum_{m+n=N} a_m^\dagger a_n^\dagger e^{2\pi i n/N}$$

$$\sum c_j^\dagger c_{j+1} = \sum_{m=n} a_m^\dagger a_n e^{-2\pi i n/N}$$

$$\sum c_{j+1}^\dagger c_j = \sum_{m=n} a_m^\dagger a_n e^{2\pi i m/N}$$

$$\therefore \sum c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j = \sum_{k=0}^{N-1} a_k^\dagger a_k \, 2\cos\left(\frac{2\pi k}{N}\right)$$

$\sum c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger$ * notice $e^{2\pi i m/N} = e^{-2\pi i n/N}$ if $m+n=N$

$$= \sum_{m+n}\left(a_m a_n + a_m^\dagger a_n^\dagger\right) e^{-2\pi i n/N}$$

$$c_j^\dagger c_j = \frac{1}{N}\left(\sum_m a_m^\dagger e^{+2\pi i jm/N}\right)\left(\sum_n a_n e^{-2\pi i jn/N}\right)$$

$$\sum_{j=1}^{N} c_j^\dagger c_j = \cancel{\tfrac{N}{N}}\sum_{m=n} a_m^\dagger a_n = \sum_k a_k^\dagger a_k$$

⇒ The Hamiltonian can be written as

$$H = \sum_k a_k^\dagger a_k \left(2B - 2J\cos\frac{2\pi k}{N}\right)$$

$$\pm J\sum_k \left(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger\right) e^{\pm 2\pi i k/N}$$

$e^{-2\pi i k/N}$ $e^{2\pi i k/N}$

anti

the cos part will be 0

due to symmetry

~~(b)~~

$$H = \sum_{k>0} \left(a_k^\dagger \ a_{-k}\right)\begin{pmatrix} B - J\cos\frac{2\pi k}{N} & \cancel{J e^{2\pi i k/N}} \ iJ\sin\frac{2\pi k}{N} \\ -iJ\cancel{e^{2\pi i k/N}}\sin\frac{2\pi k}{N} & -B + J\cos\frac{2\pi k}{N}\end{pmatrix}\begin{pmatrix} a_k \\ a_{-k}^\dagger\end{pmatrix}$$

(c) Suppose we only consider one of the k (fix k), $\sin\frac{2\pi k}{N}$

$$\left(a_k^\dagger \ a_{-k}\right)\begin{pmatrix} B - J\cos\frac{2\pi k}{N} & iJ\cancel{e^{2\pi i k/N}} \\ -iJ\cancel{e^{2\pi i k/N}}\sin\frac{2\pi k}{N} & -B + J\cos\frac{2\pi k}{N}\end{pmatrix}\begin{pmatrix} a_k \\ a_{-k}^\dagger\end{pmatrix}$$

a_k & a_{-k} are coupled.

suppose the 2×2 matrix is

$$\begin{pmatrix} A & iB \\ -iB & -A\end{pmatrix} \qquad A = B - J\cos\frac{2\pi k}{N} \qquad B = J\sin\frac{2\pi k}{N}$$

then the eigenvalues are

$$(A-\lambda)(-A-\lambda) = B^2$$

$$\lambda_{1,2} = \pm\sqrt{A^2+B^2}$$

for $\lambda_1 = \sqrt{A^2+B^2}$

$$\begin{pmatrix} A - \sqrt{A^2+B^2} & iB \\ -iB & -A-\sqrt{A^2+B^2}\end{pmatrix}\vec{v}_1 = 0$$

$$\vec{v}_1 = \begin{pmatrix} iB \\ \sqrt{A^2+B^2} - A\end{pmatrix}\frac{1}{\sqrt{2(B^2+A^2) - 2A\sqrt{A^2+B^2}}}$$

similarly for $\lambda_2 = -\sqrt{A^2+B^2}$

$$\vec{v}_2 = \begin{pmatrix} iB \\ -A-\sqrt{A^2+B^2}\end{pmatrix}\frac{1}{\sqrt{2(A^2+B^2) + 2A\sqrt{A^2+B^2}}}$$

$$\vec{v}_1 = \begin{pmatrix} iB \\ \lambda - A\end{pmatrix}\cdot\frac{1}{\sqrt{(\lambda-A)^2 - B^2}} \quad \text{or} \quad \begin{pmatrix} \frac{B}{\sqrt{(\lambda-A)^2-B^2}} \\ -i\frac{\lambda-A}{\sqrt{(\lambda-A)^2-B^2}}\end{pmatrix}$$

so we can just let

$$u = \frac{B}{\sqrt{(\lambda-A)^2-B^2}} \qquad v = \frac{\lambda-A}{\sqrt{(\lambda-A)^2-B^2}}$$

(d) The energy of a single particle is $E = \sqrt{A^2+B^2} = \sqrt{B^2+J^2-2BJ\cos\frac{2\pi k}{N}}$

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The minimum is gained when $\cos\frac{2\pi k}{N} \to 0$, which is $k \to 0$

when $N \to \infty$ we can take the two eigenstates, and let $k \to 0$

$\Rightarrow E_{gap} = 2E_{k\to 0} = 2|J-B|$

Ⅱ6Ⅱ The 2 electrons are described by

(a) $|1,\uparrow\rangle$, $|1,\downarrow\rangle$, $|2,\uparrow\rangle$, $|2,\downarrow\rangle$

① Total spin $=0$:

$|1100\rangle$ $|1001\rangle$ $|0110\rangle$ $|0011\rangle$

Total spin $=1$:

$|1010\rangle$, $|0101\rangle$

② For Spatial reflection, if two electrons occupy the same spatial state, it is even. otherwise, it is odd:

even:

$|1100\rangle$, $|0011\rangle$

odd:

others

(b) For these state, only two states that have same spin & spatial parity can evolute to each other by H, so, we can setup a form

total spin \ spatial	even	odd
~~even~~ 0	$\lvert 1100\rangle$ $\lvert 0011\rangle$	$\lvert 1001\rangle$ $\lvert 0110\rangle$
~~odd~~ 1	0	$\lvert 1010\rangle$ $\lvert 0101\rangle$

$\therefore$ only the entries corresponding to two state in the same cell can be non-zero.