固体理论, Homework 01

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1 简谐振子与二次量子化

对于一个简谐振子，

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{1.1}$$

构造产生及湮灭算符：

$$\hat{a} = \lambda\hat{x} + i\mu\hat{p}, \quad \hat{a}^\dagger = \lambda\hat{x} - i\mu\hat{p} \tag{1.2}$$

选择系数 λ 和 μ，使得它们满足玻色子产生湮灭算符的对易关系，并且 H 可以表示成

$$\hat{H} = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{1.3}$$

利用产生湮灭算符求解该简谐振子的能谱和能量本征态。

Solution:

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger] &= (\lambda\hat{x} + i\mu\hat{p})(\lambda\hat{x} - i\mu\hat{p}) - (\lambda\hat{x} - i\mu\hat{p})(\lambda\hat{x} + i\mu\hat{p}) \\
&= \lambda^2\hat{x}^2 + i\lambda\mu[\hat{p}, \hat{x}] + \mu^2\hat{p}^2 - (\lambda^2\hat{x}^2 - i\lambda\mu[\hat{p}, \hat{x}] + \mu^2\hat{p}^2) \\
&= 2i\lambda\mu[\hat{p}, \hat{x}] \\
&= 2i\lambda\mu \cdot (-i) \\
&= 2\lambda\mu
\end{aligned} \tag{1.4}$$

Since $[\hat{a}, \hat{a}^\dagger] = 1$, we have

$$\mu = \frac{1}{2\lambda} \tag{1.5}$$

thus

$$\begin{aligned}
\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) &= \omega\left(\lambda^2\hat{x}^2 + \lambda\mu + \mu^2\hat{p}^2 + \frac{1}{2}\right) \\
&= \omega\left(\lambda^2\hat{x}^2 - \frac{1}{2} + \frac{1}{4\lambda^2}\hat{p}^2 + \frac{1}{2}\right) \\
&= \omega\left(\lambda^2\hat{x}^2 + \frac{1}{4\lambda^2}\hat{p}^2\right)
\end{aligned} \tag{1.6}$$

Since $\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \hat{H}$, we get

$$\lambda^2 = \frac{1}{2}m\omega \tag{1.7}$$

$$\lambda = \sqrt{\frac{1}{2}m\omega}, \quad \mu = \frac{1}{\sqrt{2m\omega}} \tag{1.8}$$

i.e.

$$\boxed{\hat{a} = \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\hat{x} + i\frac{\hat{p}}{\sqrt{m\omega}}\right) \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\sqrt{m\omega}\hat{x} - i\frac{\hat{p}}{\sqrt{m\omega}}\right)} \tag{1.9}$$

Since

$$\hat{H} = \omega\left(\hat{n} + \frac{1}{2}\right) \tag{1.10}$$

$\hat{H}$ commutes with $\hat{n}$, thus shares the same eigenstates with $\hat{n}$.
Since

$$\hat{n}\,|n\rangle = n\,|n\rangle \tag{1.11}$$

we have

$$\hat{H}\,|n\rangle = \omega\left(\hat{n} + \frac{1}{2}\right)|n\rangle = \omega\left(n + \frac{1}{2}\right)|n\rangle \tag{1.12}$$

i.e.

$$\boxed{E_n = \omega\left(n + \frac{1}{2}\right)} \tag{1.13}$$

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle \tag{1.14}$$

The ground state could be obtained by

$$\langle x\,|\,a\,|\,0\rangle = 0 \tag{1.15}$$

thus

$$\frac{1}{\sqrt{2}}\,\langle x|\left(\sqrt{m\omega}x + \frac{\partial_x}{\sqrt{m\omega}}\right)|0\rangle = 0 \tag{1.16}$$

$$\frac{\sqrt{m\omega}}{\sqrt{2}}\left(x + \frac{\partial_x}{m\omega}\right)\langle x\,|\,0\rangle = 0 \tag{1.17}$$

$\therefore$

$$\langle x\,|\,0\rangle = \left(\frac{m\omega}{\pi}\right)^{1/4}\mathrm{e}^{-\frac{1}{2}m\omega x^2} \tag{1.18}$$

thus

$$\begin{aligned}\langle x\,|\,n\rangle &= \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle \\ &= \frac{1}{\sqrt{n!}}\left[\sqrt{\frac{m\omega}{2}}\left(x + \frac{\partial_x}{m\omega}\right)\right]^n\langle x\,|\,0\rangle\end{aligned} \tag{1.19}$$

$$\boxed{\langle x\,|\,n\rangle = \frac{1}{\sqrt{2^n n!}}H_n(\sqrt{m\omega}x)\,\langle x\,|\,0\rangle} \tag{1.20}$$

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考虑一个由三个电子组成的体系，三个电子分别占据 ϕ_1, ϕ_2 和 ϕ_3 三个轨道。

1. 写下一次量子化的费米子波函数 $\Psi(r_1, r_2, r_3)$ 并计算体系的能量（包括动能，势能及电子库伦相互作用能）。
2. 写下二次量子化的费米子波函数并计算体系的能量，并与上一问中结果进行比较。

Solution:

1.

$$\Psi(r_1, r_2, r_3) = \frac{1}{\sqrt{6}} \begin{vmatrix} \phi_1(r_1, \sigma_1) & \phi_1(r_2, \sigma_2) & \phi_1(r_3, \sigma_3) \\ \phi_2(r_1, \sigma_1) & \phi_2(r_2, \sigma_2) & \phi_2(r_3, \sigma_3) \\ \phi_3(r_1, \sigma_1) & \phi_3(r_2, \sigma_2) & \phi_3(r_3, \sigma_3) \end{vmatrix} \tag{2.1}$$

$$E = \left\langle \Psi \,\middle|\, \hat{H} \,\middle|\, \Psi \right\rangle = \sum_{i=1}^{3} \left\langle \phi_{i,\sigma_i} \,\middle|\, \hat{h}(i) \,\middle|\, \phi_{i,\sigma_i} \right\rangle + \langle 12 \,|\, 12 \rangle - \langle 12 \,|\, 21 \rangle + \langle 13 \,|\, 13 \rangle - \langle 13 \,|\, 31 \rangle + \langle 23 \,|\, 23 \rangle - \langle 23 \,|\, 32 \rangle \tag{2.2}$$

where

$$\hat{h}(i) = -\frac{1}{2}\nabla^2 + V(i) \tag{2.3}$$

$$\langle ij \,|\, kl \rangle = \left\langle \phi_i(r_1, \sigma_1)\phi_j(r_2, \sigma_2) \,\middle|\, \frac{1}{r_{12}} \,\middle|\, \phi_k(r_1, \sigma_1)\phi_l(r_2, \sigma_2) \right\rangle \tag{2.4}$$

2.

$$\Psi = \hat{a}^\dagger_{1,\sigma_1} \hat{a}^\dagger_{2,\sigma_2} \hat{a}^\dagger_{3,\sigma_3} \left| 0 \right\rangle \tag{2.5}$$

$$\hat{H} = \sum_{i,j=1}^{3} \hat{a}^\dagger_{i,\sigma_i} \left\langle \phi_{i,\sigma_i} \,\middle|\, \hat{h} \,\middle|\, \phi_{j,\sigma_j} \right\rangle \hat{a}_{j,\sigma_j} + \frac{1}{2} \sum_{i,j,k,l=1}^{3} \hat{a}^\dagger_{i,\sigma_i} \hat{a}^\dagger_{j,\sigma_j} \left\langle \phi_{i,\sigma_i}\phi_{j,\sigma_j} \,\middle|\, \hat{g} \,\middle|\, \phi_{k,\sigma_k}\phi_{l,\sigma_l} \right\rangle \hat{a}_{k,\sigma_k} \hat{a}_{l,\sigma_l} \tag{2.6}$$

Noticing that $i, j = k, l$

$$E = \left\langle \Psi \,\middle|\, \hat{H} \,\middle|\, \Psi \right\rangle = \sum_{i=1}^{3} \left\langle \phi_{i,\sigma_i} \,\middle|\, \hat{h}(i) \,\middle|\, \phi_{i,\sigma_i} \right\rangle + \langle 12 \,|\, 12 \rangle - \langle 12 \,|\, 21 \rangle + \langle 13 \,|\, 13 \rangle - \langle 13 \,|\, 31 \rangle + \langle 23 \,|\, 23 \rangle - \langle 23 \,|\, 32 \rangle \tag{2.7}$$