AGT; Sheet 11; Marc Hauer, Angelo Brade; 04.01.2025

<u>Exercise 3:</u>

Let $V_0 = L_x L_y L_z$ and $\phi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{V_0}} e^{i\vec{k}\cdot\vec{x}}$.

1.: Boundary conditions: $\phi_{\vec{k}}(x,y,z) = \phi_{\vec{k}}(x+L_x, y, z) = \phi_{\vec{k}}(x, y+L_y, z) = \phi_{\vec{k}}(x,y,z+L_z)$

Thus for x: $\phi_{\vec{k}}(x,y,z) = \phi_{\vec{k}}(x+L_x, y, z)$

$$\Rightarrow \quad e^{i(k_x\cdot x + k_y\cdot y + k_z\cdot z)} = e^{i(k_x\cdot(x+L_x) + k_y\cdot y + k_z\cdot z)}$$

$$\Rightarrow \quad \exp[ik_x x] = \exp[ik_x(x+L_x)] \quad | \text{ multiplying by } 1 = e^{i2\pi n_x}$$

$$\Rightarrow \quad 2\pi\cdot n_x + k_x\cdot x = k_x(x+L_x)$$

$$\Rightarrow \quad 2\pi\cdot n_x = k_x\cdot L_x$$

$$\Rightarrow \quad k_x = 2\pi\frac{n_x}{L_x}$$

Analogously this is done for y and z. Thus:

$$\vec{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right). \quad \square$$

2.:

$$\langle \phi_{\vec{k}} | \phi_{\vec{k}'} \rangle = \int_{\mathbb{R}} d\vec{x}^3\, \phi^*_{\vec{k}}(\vec{x})\, \phi_{\vec{k}'}(\vec{x}) \quad | \text{ boundary conditions: } \mathbb{R} = \Omega = V_0$$

$$= \int_{V_0} d\vec{x}^3 \frac{1}{\sqrt{V_0}} e^{-i\vec{k}\cdot\vec{x}} \cdot \frac{1}{\sqrt{V_0}} e^{i\vec{k}'\cdot\vec{x}}$$

I:
$$= \frac{1}{V_0}\int_{V_0} dx^3\, e^{i\vec{x}\cdot(\vec{k}'-\vec{k})}$$

$$= \frac{1}{V_0}\int_{V_0} dx^3 \exp\left(i\left[\frac{x}{L_x}(n_x'-n_x) + \frac{y}{L_y}(n_y'-n_y) + \frac{z}{L_z}(n_z'-n_z)\right]\right)$$

$$= \frac{1}{V_0}\int_{L_x} e^{i\frac{x}{L_x}(n_x'-n_x)}dx \int_{L_y} e^{i\frac{y}{L_y}(n_y'-n_y)}dy \int_{L_z} e^{i\frac{z}{L_z}(n_z'-n_z)}dz \quad | \; \delta(a\cdot x) = \frac{1}{a}\delta(x)$$

$$= \frac{1}{V_0} L_x\,\delta(n_x'-n_x)\, L_y\,\delta(n_y'-n_y)\, L_z\,\delta(n_z'-n_z) \quad | \; n_i \in \mathbb{N} \Rightarrow \delta(n_i'-n_i) = \delta_{n_i' n_i}$$

$$= \delta_{n_x' n_x}\,\delta_{n_y' n_y}\,\delta_{n_z' n_z} \quad \square$$

From (I) we could allready see, that $\langle \phi_{k'} | \phi_k \rangle = \delta_{k'k}$.

3.: Let $\hat{T}+\hat{U}=\hat{H}=-\frac{\hbar^2}{2m}\Delta+\hat{V}(x)$, thus $\hat{T}=-\frac{\hbar^2}{2m}\Delta$.

$$\Rightarrow \langle k'|\hat{T}|k\rangle = \langle k'|(-\tfrac{\hbar^2}{2m})\Delta|k\rangle \quad | \; \Delta|x\rangle = |x\rangle\Delta$$
$$= -\frac{\hbar^2}{2m}\langle k'|x\rangle\Delta\langle x|k\rangle \qquad | \; \langle x|k\rangle = \phi_{\vec{k}}(\vec{x})$$
$$= -\frac{\hbar^2}{2m}\langle k'|x\rangle\Delta\frac{1}{\sqrt{V_0}}e^{i\vec{k}\vec{x}}$$
$$= \frac{\hbar^2}{2m}\langle k'|x\rangle\vec{k}^2\frac{1}{\sqrt{V_0}}e^{i\vec{k}\vec{x}}$$
$$= \frac{\hbar^2}{2m}\vec{k}^2\langle k'|k\rangle$$
$$= \frac{\hbar^2}{2m}\vec{k}^2\delta_{k'k}$$

$\square$

4.:

$$\frac{1}{V_0}U_{\vec{k}-\vec{k}'} = \langle\vec{k}'|U|\vec{k}\rangle$$
$$= \int_{\mathbb{R}} dx^3\, \phi^*_{\vec{k}'}(\vec{x})U(x)\phi_{\vec{k}}(\vec{x}) \quad | \text{boundary conditions}$$
$$= \int_{V_0} dx^3\,\frac{1}{V_0}U(x)e^{i\vec{x}(\vec{k}-\vec{k}')}$$
$$= \int_{\mathbb{R}} d\vec{x}^3\,U(x)e^{i\vec{x}(\vec{k}-\vec{k}')}$$
$$= \mathcal{F}[U(x)](\vec{k}-\vec{k}')$$

$\square$

5.:

With $\langle x|\vec{p},k\rangle = \phi_{\vec{p},\vec{k}}(x) = \frac{1}{\sqrt{V_0}}e^{i\vec{x}\vec{p}}e^{i\vec{x}\vec{k}}$ and $U(\vec{x}-\vec{x}') = \frac{1}{V_0}\sum_{\vec{q}} e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}$ follows:

$$\langle\vec{p}',\vec{k}'|U(\vec{x}-\vec{x}')|\vec{p},\vec{k}\rangle = \int_{V_0} d^3x\,\frac{1}{V_0}e^{ix(\vec{p}'-\vec{p})}e^{ix(\vec{k}'-\vec{k})}\frac{1}{V_0}\sum_{\vec{q}} U_{\vec{q}}\,e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}$$
$$= \frac{1}{V_0}\sum_{\vec{q}} U_{\vec{q}}\int_{\mathbb{R}} dx^3\, e^{ix(\vec{p}'-\vec{p})}e^{ix(\vec{k}'-\vec{k})}e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}$$

i dont exactly know what is happening with this term

$$= \frac{1}{V_0}\sum_{\vec{q}} U_{\vec{q}}\,\delta_{\vec{q},\vec{p}-\vec{p}'}\,\delta_{\vec{q},\vec{k}-\vec{k}'}$$

$\square$

6.: Let $\hat{H} = \hat{T} + \hat{U} + \hat{V}$.

Find $\hat{T}$: $\langle \vec{k}' | \hat{T} | \vec{k} \rangle = \frac{\hbar^2}{2m} \vec{k}^2 \delta_{\vec{k}',\vec{k}}$

$$\Rightarrow \hat{T} = \sum_{\vec{k},\vec{k}'} \langle \vec{k}' | \hat{T} | \vec{k} \rangle |\vec{k}'\rangle\langle\vec{k}| \quad | \quad \sum_{\alpha} |i_\alpha\rangle\langle j_\alpha| = \hat{a}_i^+ \hat{a}_j$$

$$= \sum_{\vec{k},\vec{k}'} \frac{\hbar^2}{2m} \vec{k}^2 \delta_{\vec{k}',\vec{k}} \hat{a}_{k'}^+ \hat{a}_k$$

$$= \sum_{\vec{k}} \frac{(\hbar\vec{k})^2}{2m} \hat{a}_k^+ \hat{a}_k$$

Find $\hat{U}$: $\langle \vec{k}' | U | \vec{k} \rangle = \frac{1}{V_0} U_{\vec{k}'-\vec{k}}$

$$\Rightarrow \hat{U} = \sum_{\vec{k}',\vec{k}} \langle \vec{k}' | U | \vec{k} \rangle |\vec{k}'\rangle\langle\vec{k}|$$

$$= \sum_{\vec{k}',\vec{k}} \frac{1}{V_0} U_{\vec{k}'-\vec{k}} \hat{a}_{k'}^+ \hat{a}_k$$

$$= \frac{1}{V_0} \sum_{\vec{k}',\vec{k}} U_{\vec{k}'-\vec{k}} \hat{a}_{k'}^+ \hat{a}_k$$

Find $\hat{V}$: $\langle \vec{p}', \vec{k}' | V(\vec{x}-\vec{x}') | \vec{p}, \vec{k} \rangle = \frac{1}{V_0} \sum_{\vec{q}} V_{\vec{q}} \delta_{\vec{q},\vec{p}'-\vec{p}} \delta_{\vec{q},\vec{k}-\vec{k}'}$

From exercise 2 we know: $\hat{F} = \frac{1}{2} \sum_{\alpha\neq\beta} \sum_{i,j,k,l} \langle i,j | f | k,l \rangle |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta$

Thus: $\hat{V} = \frac{1}{2} \sum_{\alpha\neq\beta} \sum_{\vec{p}',\vec{p},\vec{k}',\vec{k}} \frac{1}{V_0} \sum_{\vec{q}} V_{\vec{q}} \delta_{\vec{q},\vec{p}'-\vec{p}} \delta_{\vec{q},\vec{k}-\vec{k}'} |p'\rangle_\alpha |k'\rangle_\beta \langle k|_\alpha \langle p|_\beta$

$$= \frac{1}{2} \sum_{\vec{p}',\vec{p},\vec{k}',\vec{k}} \frac{1}{V_0} \sum_{\vec{q}} V_{\vec{q}} \delta_{\vec{q},\vec{p}'-\vec{p}} \delta_{\vec{q},\vec{k}-\vec{k}'} \hat{a}_{\vec{p}'}^+ \hat{a}_{k'}^+ \hat{a}_{\vec{k}} \hat{a}_{\vec{p}}$$

$$= \frac{1}{2V_0} \sum_{\vec{k},\vec{p},\vec{q}} V_{\vec{q}} \hat{a}_{\vec{q}+\vec{p}}^+ \hat{a}_{\vec{k}-\vec{q}}^+ \hat{a}_{\vec{k}} \hat{a}_{\vec{p}}$$

Finally we construct $\hat{H}$:

$$\hat{H} = \sum_{\vec{k}} \frac{(\hbar\vec{k})^2}{2m} \hat{a}_k^+ \hat{a}_k + \frac{1}{V_0} \sum_{\vec{k}',\vec{k}} U_{\vec{k}'-\vec{k}} \hat{a}_{k'}^+ \hat{a}_k + \frac{1}{2V_0} \sum_{\vec{k},\vec{p},\vec{q}} V_{\vec{q}} \hat{a}_{\vec{q}+\vec{p}}^+ \hat{a}_{\vec{k}-\vec{q}}^+ \hat{a}_{\vec{k}} \hat{a}_{\vec{p}}$$

$\hat{T}$, the kinetic energy, is independent of other particles, thus only dependant on the own wave vector $\vec{k}$. $\hat{U}$, an arbitrary external potential, can be dependent of other particles, thus beeing also dependant on the other wave vectors $\vec{k}'$. In particular it is dependent of its own wave vector. This is not the case for $\hat{V}$, the two particle-potential. $\hat{V}$ describes the forces created by the other particle, thus there can't be any if the other particle would be identical in every way.