Operators in second quantization

1) One particle and an opeartor $\hat{A}$ acting on one particle

Let $|k\rangle$ – one-particle state (e.g. wavefunction with a momentum $\vec{k}$), forming a complete orthonormal basis

$|\xi\rangle$ – any arbitrary one-particle state.

$$\hat{A}|\xi\rangle = \sum_{k'} \hat{A}|k'\rangle\cdot\langle k'|\xi\rangle = \sum_{k'',k'} |k''\rangle\cdot\underbrace{\langle k''|\hat{A}|k'\rangle}_{A_{k''k'}}\cdot\langle k'|\xi\rangle = \sum_{k'',k'} |k''\rangle\cdot A_{k''k'}\cdot\langle k'|\xi\rangle$$

$$\hat{1} = \sum_k |k\rangle\langle k|$$

The result of $\hat{A}|\xi\rangle$ is expressed via matrix elements $A_{k''k'}$.

Using second quantization for the state $|\xi\rangle$:

$$|\xi\rangle = \sum_k |k\rangle\cdot\langle k|\xi\rangle = \sum_k \langle k|\xi\rangle\cdot|k\rangle = \sum_k \langle k|\xi\rangle\cdot\hat{a}^+_k|0\rangle$$

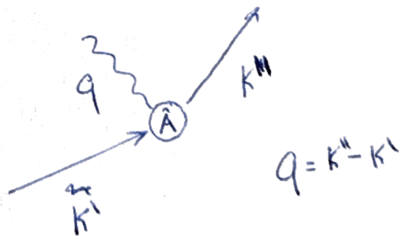
$$|k\rangle = \hat{a}^+_k|0\rangle$$

Then $$\hat{A}|\xi\rangle = \sum_{k'',k'} \underbrace{|k''\rangle}_{\hat{a}^+_{k''}|0\rangle}\cdot A_{k''k'}\langle k'|\xi\rangle = \sum_{k'',k'} A_{k''k'}\cdot\langle k'|\xi\rangle\cdot\hat{a}^+_{k''}|0\rangle$$

$$= \sum_{k',k'',k'''} A_{k''k'''}\cdot\langle k'|\xi\rangle\cdot\delta_{k''',k'}\cdot\hat{a}^+_{k''}|0\rangle$$

$$= \sum_{k',k'',k'''} A_{k''k'''}\langle k'|\xi\rangle\cdot\hat{a}^+_{k''}\cdot\underbrace{\delta_{k''',k'}|0\rangle}_{\hat{a}_{k'''}\hat{a}^+_{k'}|0\rangle} = \sum_{k'',k'''} A_{k''k'''}\cdot\hat{a}^+_{k''}\hat{a}_{k'''}\cdot\underbrace{\sum_{k'}\langle k'|\xi\rangle\cdot\hat{a}^+_{k'}|0\rangle}_{|\xi\rangle}$$

Thus, $$\boxed{\hat{A} = \sum_{k',k''} \langle k'|\hat{A}|k''\rangle\cdot\hat{a}^+_{k''}\cdot\hat{a}_{k'}}$$



$q = k'' - k'$

Feynman diagram

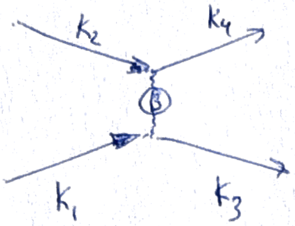
Examples: momentum: $\hat{p}_x = -i\hbar\frac{\partial}{\partial x} = \hbar\cdot\sum_{k_x} k_x\cdot\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$

energy: $\hat{K} = \frac{\hat{p}^2}{2m} = \frac{\hbar^2}{2m}\cdot\sum_{\vec{k}} k^2\cdot\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$

number of particles: $\hat{N} = \sum_{\vec{k}} \hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$; Coulomb pot. $\hat{V} = \frac{e^2}{r} = \sum_{\vec{k},\vec{q}} \frac{4\pi e^2}{q^2}\cdot\hat{a}^+_{\vec{k}}\,\hat{a}_{\vec{k}-\vec{q}}$

2) Operator $\hat{B}$ acts on two particles

Analogously,
$$\hat{B} = \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} \langle k_4\, k_3 | \hat{B} | k_2 k_1 \rangle \cdot \hat{a}^+_{k_4} \hat{a}^+_{k_3} \hat{a}_{k_2} \hat{a}_{k_1}$$



Example: Coulomb potential $\hat{V} = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} = \frac{1}{\Omega} \int \frac{4\pi e^2}{q^2} e^{i\vec{q}\vec{r}} d\vec{q}$

$$\langle k_4\, k_3 | \hat{V} | k_2 k_1 \rangle = \int \frac{e^{-i\vec{k}_4\vec{r}_1 - i\vec{k}_3\vec{r}_2}}{(\sqrt{\Omega})^2} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \frac{e^{i\vec{k}_2\vec{r}_2}}{\sqrt{\Omega}} \frac{e^{i\vec{k}_1\vec{r}_1}}{\sqrt{\Omega}} d\vec{r}_1 d\vec{r}_2$$

$$= \frac{4\pi e^2}{\Omega} \int \frac{1}{q^2} d\vec{q} \cdot \underbrace{\frac{1}{\Omega}\int e^{i(\vec{k}_1 - \vec{k}_4 + \vec{q})} d\vec{r}_1}_{\substack{\delta_{\vec{k}_1 - \vec{k}_4, -\vec{q}} \\ (\vec{k}_4 = \vec{k}_1 + \vec{q})}} \cdot \underbrace{\frac{1}{\Omega}\int e^{i(\vec{k}_2 - \vec{k}_3 - \vec{q})} d\vec{r}_2}_{\substack{\delta_{\vec{k}_2 - \vec{k}_3, \vec{q}} \\ (\vec{k}_3 = \vec{k}_2 - \vec{q})}}$$

$$= \sum_{\vec{q}} \frac{4\pi e^2}{\Omega q^2} \cdot \delta_{\vec{k}_1 - \vec{k}_4, -\vec{q}} \cdot \delta_{\vec{k}_2 - \vec{k}_3, \vec{q}}$$

$$\hat{B} = \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \frac{4\pi e^2}{\Omega q^2} \cdot \hat{a}^+_{\vec{k}_1 + \vec{q}}\, \hat{a}^+_{\vec{k}_2 - \vec{q}} \cdot \hat{a}_{\vec{k}_2} \hat{a}_{\vec{k}_1}$$

The Fröhlich Hamiltonian (interaction of electrons and phonons, : polarons)

$$\hat{H}_F = \cancel{\frac{p^2}{2m}} + \sum_{\vec{k}} \hbar\omega_{\vec{k}} \left(\hat{b}^+_k \hat{b}_k + \frac{1}{2} \right) + \sum_{\vec{k}, \vec{p}} V^{(F)}_{\vec{k}} \left(\hat{b}^+_k + \hat{b}_{-k} \right) \hat{c}^+_{\vec{p}-\vec{k}}\, \hat{c}_{\vec{p}} + \sum_{\vec{p}} \varepsilon_{\vec{p}} \cdot \hat{c}^+_{\vec{p}} \hat{c}_{\vec{p}}$$