Second quantization: Application

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Here we discuss how to apply the second quantization method on several many body systems.

1. The Hamiltonian in terms of field operator

The true power of field operators is that they can provide a complete and closed description of a dynamical system of identical particles without invoking any wave functions or the Schrödinger equation. Since the dynamics of a quantum system is determined by its Hamiltonian, our next step is to get the Hamiltonian in terms of field operators. Let us start with a system of non-interacting particles. The many-particle Hamiltonian is just the sum over all one-particle Hamiltonians. In the Schrödinger wave field, we have

$$\begin{aligned}
\langle\psi|[\frac{1}{2m}\hat{\boldsymbol{p}}^2+\hat{V}(\hat{\boldsymbol{r}})]|\psi\rangle &= \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \langle\psi|\boldsymbol{r}_1\rangle\langle\boldsymbol{r}_1|\frac{1}{2m}\hat{\boldsymbol{p}}^2+\hat{V}^{(1)}(\hat{\boldsymbol{r}})]|\boldsymbol{r}_2\rangle\langle\boldsymbol{r}_2|\psi\rangle \\
&= \iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \langle\psi|\boldsymbol{r}_1\rangle[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}_2}{}^2+V^{(1)}(\boldsymbol{r}_2)]\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\langle\boldsymbol{r}_2|\psi\rangle \\
&= \int d\boldsymbol{r}_1 \langle\psi|\boldsymbol{r}_1\rangle[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}_1}{}^2+V^{(1)}(\boldsymbol{r}_1)]\langle\boldsymbol{r}_1|\psi\rangle \\
&= \int d\boldsymbol{r}\,\psi^*(\boldsymbol{r})[-\frac{\hbar^2}{2m}\nabla^2+V^{(1)}(\boldsymbol{r})]\psi(\boldsymbol{r})
\end{aligned}$$

Using the quantum field operator, the Hamiltonian is given by

$$\hat{H}^{(1)} = \int d\boldsymbol{r}\,\hat{\psi}^+(\boldsymbol{r})[-\frac{\hbar^2}{2m}\nabla^2+V^{(1)}(\boldsymbol{r})]\hat{\psi}(\boldsymbol{r}).$$

This Hamiltonian can also be expressed in terms of the creation and annihilation operators

$$
\begin{aligned}
\hat{H}^{(1)} &= \sum_{\boldsymbol{k},\boldsymbol{k}'} \hat{b}_{\boldsymbol{k}}{}^{+} \hat{b}_{\boldsymbol{k}'} \int d\boldsymbol{r} \phi_{\boldsymbol{k}}{}^{*}(\boldsymbol{r})[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\boldsymbol{r})]\phi_{\boldsymbol{k}'}(\boldsymbol{r}) \\
&= \sum_{\boldsymbol{k},\boldsymbol{k}'} \hat{b}_{\boldsymbol{k}}{}^{+} \hat{b}_{\boldsymbol{k}'} \int d\boldsymbol{r} \phi_{\boldsymbol{k}}{}^{*}(\boldsymbol{r}) \varepsilon_{\boldsymbol{k}'} \phi_{\boldsymbol{k}'}(\boldsymbol{r}) \\
&= \sum_{\boldsymbol{k},\boldsymbol{k}'} \varepsilon_{\boldsymbol{k}'} \hat{b}_{\boldsymbol{k}}{}^{+} \hat{b}_{\boldsymbol{k}'} \delta_{\boldsymbol{k}',\boldsymbol{k}} \\
&= \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}}{}^{+} \hat{b}_{\boldsymbol{k}}
\end{aligned}
$$

where $\varepsilon_{\boldsymbol{k}}$ is the energy of the one-particle state $\phi_{\boldsymbol{k}}(\boldsymbol{r})$.

$$
\hat{\psi}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r}), \qquad \hat{\psi}^{+}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}}{}^{+} \phi_{\boldsymbol{k}}{}^{*}(\boldsymbol{r})
$$

and

$$
[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\boldsymbol{r})]\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_k \phi_{\boldsymbol{k}}(\boldsymbol{r})
$$

Next we consider the interaction between particles. Using the field operator,

$$
\begin{aligned}
\hat{H}^{(2)} &= \frac{1}{2}\iint d\boldsymbol{r}_1 d\boldsymbol{r}_2 \int d\boldsymbol{r}\, \hat{\psi}^{+}(\boldsymbol{r}_1)\hat{\psi}^{+}(\boldsymbol{r}_2) V^{(2)}(\boldsymbol{r}_1 - \boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_1) \\
&= \frac{1}{2V}\sum_{\boldsymbol{k},\boldsymbol{k}'\boldsymbol{q}} V^{(2)}(\boldsymbol{q}) \hat{b}_{\boldsymbol{k}+\boldsymbol{q}}{}^{+} \hat{b}_{\boldsymbol{k}'-\boldsymbol{q}}{}^{+} \hat{b}_{\boldsymbol{k}'} \hat{b}_{\boldsymbol{k}}
\end{aligned}
$$

where

$$
\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad \hat{\psi}^{+}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{k}} \hat{b}_{\boldsymbol{k}}{}^{+} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}
$$

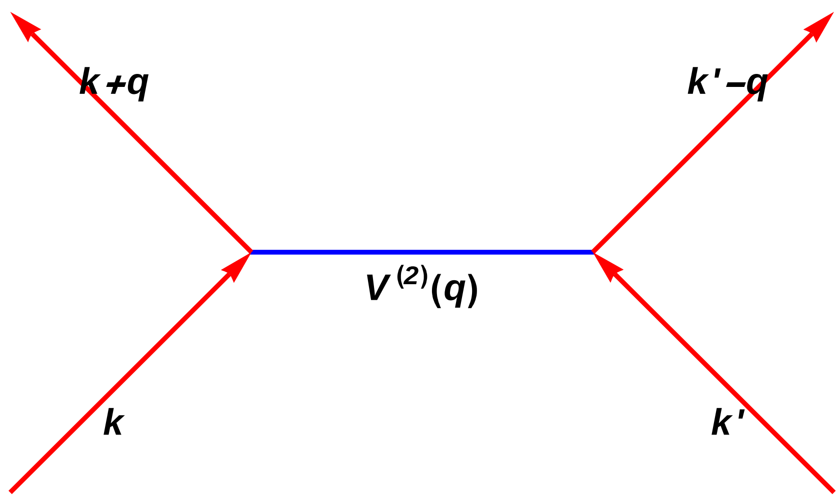


Fig. Two particles with wave vectors ***k*** and ***k***' can interact and thereby exchange momentum q. After this interaction the particles have wave vectors $\boldsymbol{k}+\boldsymbol{q}$ and $\boldsymbol{k}'-\boldsymbol{q}$. The amplitude of the process is proportional to the Fourier component $V^{(2)}(\boldsymbol{q})$ of the interaction potential.

2. Expression of operators in terms of quantum field operator

(a) Density operator

Schrödinger wave field:

$$\rho(x) = \psi^*(x)\psi(x)$$

The density operator (second quantization)

$$\hat{\rho}(x) = \hat{\psi}^+(x)\hat{\psi}(x)$$

where $\hat{\psi}(x)$ is a quantum field operator. The expectation value of density operator for the state given by

$$\left|\Phi\right\rangle = \hat{b}_k^{\ +}\left|\Phi_0\right\rangle, \qquad \left\langle\Phi\right| = \left\langle\Phi_0\right|\hat{b}_k$$

is obtained as

$$\begin{aligned}
\overline{\rho}(x) &= \langle \Phi | \hat{\psi}^+(x)\, \hat{\psi}(x) | \Phi \rangle \\
&= \langle \Phi_0 | \hat{b}_k \sum_{\mu,\nu} \hat{b}_\mu{}^+ \phi_\mu{}^*(x) \hat{b}_\nu \phi_\nu(x)\, \hat{b}_k{}^+ | \Phi_0 \rangle \\
&= \sum_{\mu,\nu} \phi_\mu{}^*(x)\phi_\nu(x) \langle \Phi_0 | \hat{b}_k \hat{b}_\mu{}^+ \hat{b}_\nu \hat{b}_k{}^+ | \Phi_0 \rangle \\
&= \sum_{\mu,\nu} \phi_\mu{}^*(x)\phi_\nu(x) \langle \Phi_0 | (\hat{b}_\mu{}^+ \hat{b}_k + \delta_{\mu,k})(\hat{b}_k{}^+ \hat{b}_\nu + \delta_{\nu,k} | \Phi_0 \rangle \\
&= \sum_{\mu,\nu} \phi_\mu{}^*(x)\phi_\nu(x) \delta_{\mu,k}\delta_{\nu,k} \langle \Phi_0 | \Phi_0 \rangle \\
&= \phi_k{}^*(x)\phi_k(x)
\end{aligned}$$

(b) Position operator

The position operator is defined by

$$\hat{x} = \int dx \psi^+(x) x \psi(x)$$

The expectation value $\langle \Phi | \hat{x} | \Phi \rangle$ is obtained as

$$\begin{aligned}
\langle \Phi | \hat{x} | \Phi \rangle &= \langle \Phi | \int dx \psi^+(x) x \psi(x) | \Phi \rangle \\
&= \sum_{\mu,\nu} \int dx \phi_\mu{}^*(x) x \phi_\nu(x) \langle \Phi_0 | \hat{b}_k \hat{b}_\mu{}^+ \hat{b}_\nu \hat{b}_k{}^+ | \Phi_0 \rangle \\
&= \sum_{\mu,\nu} \int dx \phi_\mu{}^*(x) x \phi_\nu(x) \delta_{\mu,k}\delta_{\nu,k} \\
&= \int dx \phi_k{}^*(x) x \phi_k(x)
\end{aligned}$$

(c) Potential energy

The average potential energy is given by

$$\int dx \psi^*(x) V(x) \psi(x)$$

The corresponding operator is

$$\hat{V}_{op} = \int dx \psi^+(x) V(x) \hat{\psi}(x)$$

The expectation value $\langle \Phi | \hat{V}_{op} | \Phi \rangle$ is

$$\langle\Phi|\hat{V}_{op}|\Phi\rangle = \sum_{\mu,\nu}\int dx\phi_\mu{}^*(x)V(x)\phi_\nu(x)\langle\Phi|\hat{b}_\mu{}^+\hat{b}_\nu|\Phi\rangle$$
$$= \sum_{\mu,\nu}\int dx\phi_\mu{}^*(x)V(x)\phi_\nu(x)\delta_{\mu,k}\delta_{\nu,k}$$
$$= \int dx\phi_k{}^*(x)V(x)\phi_k(x)$$

where

$$\langle\Phi|\hat{b}_\mu{}^+\hat{b}_\nu|\Phi\rangle = \langle\Phi_0|\hat{b}_k\hat{b}_\mu{}^+\hat{b}_\nu\hat{b}_k{}^+|\Phi\rangle$$
$$= \langle\Phi_0|\hat{b}_\mu{}^+\hat{b}_k + \delta_{\mu,k})(\hat{b}_k{}^+\hat{b}_\nu + \delta_{\nu,k}|\Phi_0\rangle$$
$$= \delta_{\mu,k}\delta_{\nu,k}$$

(d) Kinetic energy

Schrödinger wave field;

$$-\frac{\hbar^2}{2m}\int d\boldsymbol{r}\psi^*(\boldsymbol{r})\nabla^2\psi(\boldsymbol{x})$$

The corresponding operator;

$$-\frac{\hbar^2}{2m}\int d\boldsymbol{r}\hat{\psi}^+(\boldsymbol{r})\nabla^2\hat{\psi}(\boldsymbol{r}) = \sum_{\mu,\nu}\hat{b}_\mu{}^+\hat{b}_\nu(-\frac{\hbar^2}{2m})\int d\boldsymbol{r}\phi_\mu{}^*(\boldsymbol{r})\nabla^2\phi_\nu(\boldsymbol{r})$$
$$= \sum_{\mu,\nu}E_\nu\hat{b}_\mu{}^+\hat{b}_\nu\int d\boldsymbol{r}\phi_\mu{}^*(\boldsymbol{r})\phi_\nu(\boldsymbol{r})$$
$$= \sum_{\mu,\nu}E_\nu\hat{b}_\mu{}^+\hat{b}_\nu\delta_{\mu,\nu}$$
$$= \sum_{\mu}E_\mu\hat{b}_\mu{}^+\hat{b}_\mu$$

where

$$-\frac{\hbar^2}{2m}\nabla^2\phi_\nu(\boldsymbol{r}) = E_\nu\phi_\nu(\boldsymbol{r}) \qquad \text{(Schrödinger equation)}$$

(e) Coulomb interaction

The Schrödinger field operator is given by

$$\frac{1}{2}\iint dxdx'\hat{\psi}^{+}(x)\hat{\psi}^{+}(x')\frac{e^2}{|x-x'|}\hat{\psi}(x')\hat{\psi}(x)$$
$$=\sum_{\alpha,\beta,\gamma,\delta}\frac{1}{2}\iint dxdx'\phi_\alpha{}^*(x)\phi_\beta{}^*(x')\frac{e^2}{|x-x'|}\phi_\gamma(x')\phi_\delta(x)\hat{b}_\alpha{}^{+}\hat{b}_\beta{}^{+}\hat{b}_\gamma\hat{b}_\delta$$

The expectation

$$\langle\Phi|\frac{1}{2}\iint dxdx'\hat{\psi}^{+}(x)\hat{\psi}^{+}(x')\frac{e^2}{|x-x'|}\hat{\psi}(x')\hat{\psi}(x)|\Phi\rangle$$

$$\langle\Phi|\frac{1}{2}\iint dxdx'\hat{\psi}^{+}(x)\hat{\psi}^{+}(x')\frac{e^2}{|x-x'|}\hat{\psi}(x')\hat{\psi}(x)|\Phi\rangle$$
$$=\sum_{\alpha,\beta,\gamma,\delta}\frac{1}{2}\iint dxdx'\phi_\alpha{}^*(x)\phi_\beta{}^*(x)\frac{e^2}{|x-x'|}\phi_\gamma(x')\phi_\delta(x)\langle\Phi|\hat{b}_\alpha{}^{+}\hat{b}_\beta{}^{+}\hat{b}_\gamma\hat{b}_\delta|\Phi\rangle$$

$$|\Phi\rangle=\hat{b}_{\mu_1}{}^{+}\hat{b}_{\mu 2}{}^{+}|\Phi_0\rangle, \qquad \langle\Phi|=\langle\Phi_0|\hat{b}_{\mu_2}\hat{b}_{\mu_1}$$

$$\langle\Phi|\hat{b}_\alpha{}^{+}\hat{b}_\beta{}^{+}\hat{b}_\gamma\hat{b}_\delta|\Phi\rangle=\langle\Phi_0|\hat{b}_{\mu_2}\hat{b}_{\mu_1}\hat{b}_\alpha{}^{+}\hat{b}_\beta{}^{+}\hat{b}_\gamma\hat{b}_\delta\hat{b}_{\mu_1}{}^{+}\hat{b}_{\mu 2}{}^{+}|\Phi_0\rangle$$
$$=\delta_{\mu_1,\delta}\delta_{\gamma,\mu_2}|\Phi_0\rangle$$

since

$$\hat{b}_\gamma\hat{b}_\delta\hat{b}_{\mu_1}{}^{+}\hat{b}_{\mu 2}{}^{+}|\Phi_0\rangle=\hat{b}_\gamma(\hat{b}_{\mu_1}{}^{+}\hat{b}_\delta+\delta_{\mu_1,\delta})\hat{b}_{\mu 2}{}^{+}|\Phi_0\rangle$$
$$=\delta_{\mu_1,\delta}\hat{b}_\gamma\hat{b}_{\mu 2}{}^{+}|\Phi_0\rangle$$
$$=\delta_{\mu_1,\delta}(\hat{b}_{\mu 2}{}^{+}\hat{b}_\gamma+\delta_{\gamma,\mu_2})|\Phi_0\rangle$$
$$=\delta_{\mu_1,\delta}\delta_{\gamma,\mu_2}|\Phi_0\rangle$$

and

$$\hat{b}_{\mu_2}\hat{b}_{\mu_1}\hat{b}_\alpha{}^{+}\hat{b}_\beta{}^{+}|\Phi_0\rangle=\delta_{\alpha,\mu_1}\delta_{\mu_2,\beta}|\Phi_0\rangle.$$

Thus we get

$$\langle\Phi|\frac{1}{2}\iint dxdx'\hat{\psi}^{+}(x)\hat{\psi}^{+}(x')\frac{e^2}{|x-x'|}\hat{\psi}(x')\hat{\psi}(x)|\Phi\rangle$$

$$=\sum_{\alpha,\beta,\gamma,\delta}\frac{1}{2}\iint dxdx'\phi_\alpha^{*}(x)\phi_\beta^{*}(x)\frac{e^2}{|x-x'|}\phi_\gamma(x')\phi_\delta(x)\delta_{\mu_1,\delta}\delta_{\gamma,\mu_2}\delta_{\alpha,\mu_1}\delta_{\mu_2,\beta}$$

$$=\frac{1}{2}\iint dxdx'\phi_{\mu_1}^{*}(x)\phi_{\mu_2}^{*}(x)\frac{e^2}{|x-x'|}\phi_{\mu_2}(x')\phi_{\mu_1}(x)$$

(f) Calculation of the interaction *V* for charged bosons

$$\hat{H}_{\text{int}}=\frac{e^2}{2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\iint d\boldsymbol{r}'d\boldsymbol{r}''\phi_{\boldsymbol{k}_1}^{*}(\boldsymbol{r}')\phi_{\boldsymbol{k}_2}^{*}(\boldsymbol{r}'')\frac{e^{-\mu|\boldsymbol{r}'-\boldsymbol{r}''|}}{|\boldsymbol{r}'-\boldsymbol{r}''|}\phi_{\boldsymbol{k}_4}(\boldsymbol{r}'')\phi_{\boldsymbol{k}_3}(\boldsymbol{r}')\hat{b}_{\boldsymbol{k}_1}^{+}\hat{b}_{\boldsymbol{k}_2}^{+}\hat{b}_{\boldsymbol{k}_4}\hat{b}_{\boldsymbol{k}_3}$$

Here we use

$$\phi_{\boldsymbol{k}}=\frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$I=\frac{e^2}{2}\iint d\boldsymbol{r}'d\boldsymbol{r}''\phi_{\boldsymbol{k}_1}^{*}(\boldsymbol{r}')\phi_{\boldsymbol{k}_2}^{*}(\boldsymbol{r}'')\frac{e^{-\mu|\boldsymbol{r}'-\boldsymbol{r}''|}}{|\boldsymbol{r}'-\boldsymbol{r}''|}\phi_{\boldsymbol{k}_4}(\boldsymbol{r}'')\phi_{\boldsymbol{k}_3}(\boldsymbol{r}')$$

$$=\frac{e^2}{2V^2}\iint d\boldsymbol{r}'d\boldsymbol{r}''e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}'}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}''}\frac{e^{-\mu|\boldsymbol{r}'-\boldsymbol{r}''|}}{|\boldsymbol{r}'-\boldsymbol{r}''|}e^{i\boldsymbol{k}_4\cdot\boldsymbol{r}''}e^{i\boldsymbol{k}_3\cdot\boldsymbol{r}'}$$

$$=\frac{e^2}{2V^2}\iint d\boldsymbol{r}'d\boldsymbol{r}''e^{-i(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}''}\frac{e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_3)\cdot(\boldsymbol{r}'-\boldsymbol{r}'')}e^{-\mu|\boldsymbol{r}'-\boldsymbol{r}''|}}{|\boldsymbol{r}'-\boldsymbol{r}''|}$$

We use the new variables, $\boldsymbol{x}=\boldsymbol{r}''$, $\boldsymbol{y}=\boldsymbol{r}'-\boldsymbol{r}''$ and $\boldsymbol{q}=\boldsymbol{k}_1-\boldsymbol{k}_3$ Then we get

$$I=\frac{e^2}{2V^2}\iint d\boldsymbol{x}d\boldsymbol{y}e^{-i(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{x}}\frac{e^{-i\boldsymbol{q}\cdot\boldsymbol{y}}}{y}e^{-\mu y}$$

$$=\frac{e^2}{2V^2}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}\int d\boldsymbol{y}\frac{e^{-i\boldsymbol{q}\cdot\boldsymbol{y}}}{y}e^{-\mu y}$$

$$=\frac{e^2}{2V^2}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}\frac{4\pi}{q^2+\mu^2}$$

where

$$\int d\boldsymbol{y}\frac{e^{-i\boldsymbol{q}\cdot\boldsymbol{y}}}{y}e^{-\mu y} = 2\pi\int ye^{-\mu y}dy\int_0^\pi \sin\theta d\theta e^{-iqy\cos\theta}$$

$$= \frac{4\pi}{q}\int_0^\infty dye^{-\mu y}\sin(qy)$$

$$= \frac{4\pi}{q}\frac{q}{q^2+\mu^2}$$

$$= \frac{4\pi}{q^2+\mu^2}$$

The last integral corresponds to the Laplace transform of $\sin(qy)$. Finally we get

$$\hat{H}_{\text{int}} = \frac{e^2}{2V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}\frac{4\pi}{q^2+\mu^2}\hat{b}_{\boldsymbol{k}_1}{}^{+}\hat{b}_{\boldsymbol{k}_2}{}^{+}\hat{b}_{\boldsymbol{k}_4}\hat{b}_{\boldsymbol{k}_3}$$

3. The interaction between two fermions with spin 1/2
(Sakurai and Napolitano)

The interaction between two fermions with spin 1/2 can be expressed by

$$\hat{H}_{\text{int}} = \frac{e^2}{2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\iint d\boldsymbol{r}'d\boldsymbol{r}''\phi_{\boldsymbol{k}_1\lambda_1}{}^{*}(\boldsymbol{r}')\phi_{\boldsymbol{k}_2\lambda_2}{}^{*}(\boldsymbol{r}'')\frac{e^{-\mu|\boldsymbol{r}'-\boldsymbol{r}''|}}{|\boldsymbol{r}'-\boldsymbol{r}''|}\phi_{\boldsymbol{k}_4\lambda_2}(\boldsymbol{r}'')\phi_{\boldsymbol{k}_3\lambda_1}(\boldsymbol{r}')$$

Using the quantum field operator for fermion with spin 1/2

$$\hat{\psi}(\boldsymbol{r}) = \sum_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k}\lambda}\phi_{\boldsymbol{k}}(\boldsymbol{r})$$

with

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

the interaction can be rewritten as

$$\hat{H}_{\text{int}} = \frac{e^2}{2V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}\frac{4\pi}{q^2+\mu^2}\hat{a}_{\boldsymbol{k}_1\lambda_1}{}^{+}\hat{a}_{\boldsymbol{k}_2\lambda_2}{}^{+}\hat{a}_{\boldsymbol{k}_4\lambda_2}\hat{a}_{\boldsymbol{k}_3\lambda_1},$$

where λ indicates the electron spin. The diagrammatic representation of $\hat{H}_{\text{int}}$ is given by

The total Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{H}_{\rm int}(\boldsymbol{q} = 0) + \hat{H}_{\rm int}(\boldsymbol{q} \neq 0)$$

where

$$\hat{H}_0 = \sum_{\boldsymbol{k},\lambda} E_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k},\lambda}{}^{+} \hat{a}_{\boldsymbol{k},\lambda}$$

The diagrammatic representation in the momentum space is shown below.

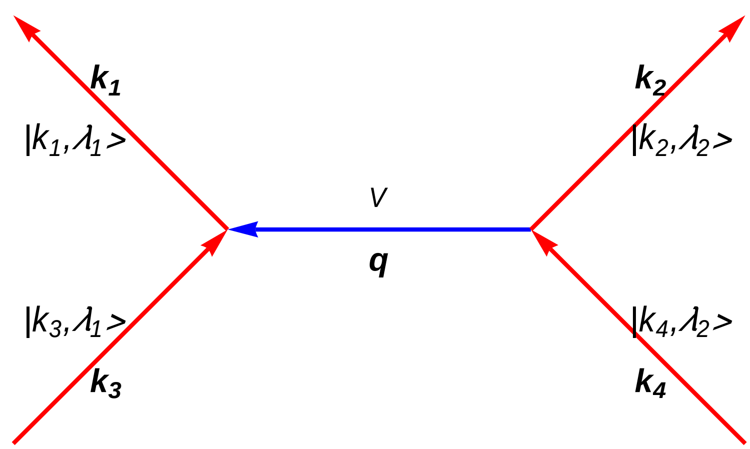
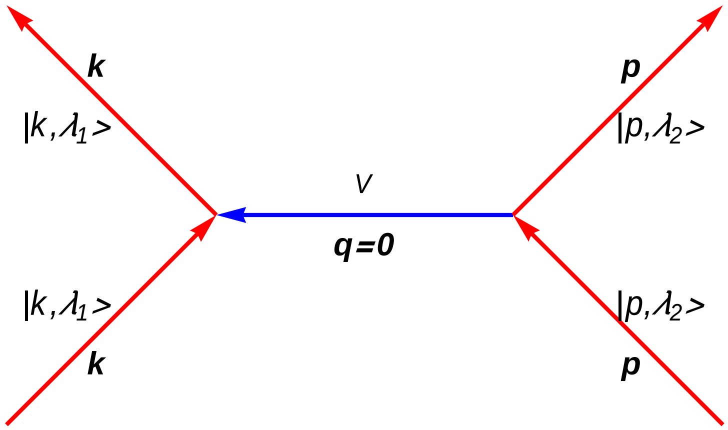


Fig. Diagrammatic representation of the momentum-space matrix element for $\hat{H}_{\rm int}(\boldsymbol{q} \neq 0)$. $\boldsymbol{k}_1 = \boldsymbol{k}_3 + \boldsymbol{q}$. $\boldsymbol{k}_4 = \boldsymbol{k}_2 + \boldsymbol{q}$. $\boldsymbol{q} = \boldsymbol{k}_1 - \boldsymbol{k}_3 = \boldsymbol{k}_4 - \boldsymbol{k}_2$

4. Evaluation of $\hat{H}_{\rm int}(\boldsymbol{q} = 0)$



In the above expression, we redefine $\boldsymbol{k}_3 = \boldsymbol{k}$, and $\boldsymbol{k}_4 = \boldsymbol{p}$. Then the term of $\hat{H}_{\text{int}}$ for which $\boldsymbol{q} = 0$ become

$$\begin{aligned}
\hat{H}_{\text{int}}(\boldsymbol{q}=0) &= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\boldsymbol{k}\lambda_1,\boldsymbol{p}\lambda_2} \hat{a}_{\boldsymbol{k}\lambda_1}{}^{+}\hat{a}_{\boldsymbol{p}\lambda_2}{}^{+}\hat{a}_{\boldsymbol{p}\lambda_2}\hat{a}_{\boldsymbol{k}\lambda_1} \\
&= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\boldsymbol{k}\lambda_1,\boldsymbol{p}\lambda_2} \hat{a}_{\boldsymbol{k}\lambda_1}{}^{+}\hat{a}_{\boldsymbol{p}\lambda_2}{}^{+}\hat{a}_{\boldsymbol{k}\lambda_1}\hat{a}_{\boldsymbol{p}\lambda_2} \\
&= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\boldsymbol{k}\lambda_1,\boldsymbol{p}\lambda_2} \hat{a}_{\boldsymbol{k}\lambda_1}{}^{+}(\hat{a}_{\boldsymbol{k}\lambda_1}\hat{a}_{\boldsymbol{p}\lambda_2}{}^{+} - \delta_{\boldsymbol{k},\boldsymbol{p}}\delta_{\lambda_1\lambda_2})\hat{a}_{\boldsymbol{p}\lambda_2} \\
&= \frac{e^2}{2V}\frac{4\pi}{\mu^2}\sum_{\boldsymbol{k}\lambda_1,\boldsymbol{p}\lambda_2} [\hat{a}_{\boldsymbol{k}\lambda_1}{}^{+}\hat{a}_{\boldsymbol{k}\lambda_1}\hat{a}_{\boldsymbol{p}\lambda_2}{}^{+}\hat{a}_{\boldsymbol{p}\lambda_2} - \delta_{\boldsymbol{k},\boldsymbol{p}}\delta_{\lambda_1\lambda_2}\hat{a}_{\boldsymbol{k}\lambda_1}{}^{+}\hat{a}_{\boldsymbol{p}\lambda_2}] \\
&= \frac{e^2}{2V}\frac{4\pi}{\mu^2}(\hat{N}^2 - \hat{N})
\end{aligned}$$

5. Reformulation of $\hat{H}_{\text{int}}(\boldsymbol{q} \neq 0)$

The $\hat{H}_{\text{int}}(\boldsymbol{q}=0)$ term vanishes in the limit of $V \to \infty$. The $\hat{H}_{\text{int}}(\boldsymbol{q} \neq 0)$ term can be redefined as

$$\boldsymbol{k}_3 = \boldsymbol{k}, \qquad \boldsymbol{k}_4 = \boldsymbol{p}$$

$$\boldsymbol{k}_1 = \boldsymbol{k}_3 + \boldsymbol{q} = \boldsymbol{k} + \boldsymbol{q}, \qquad \boldsymbol{k}_4 = \boldsymbol{k}_2 + \boldsymbol{q} = \boldsymbol{p}$$

or

$$\boldsymbol{k}_2 = \boldsymbol{p} - \boldsymbol{q}$$

Then the total Hamiltonian is expressed by

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}(\boldsymbol{q} \neq 0)$$

with

$$\hat{H}_0 = \sum_{\boldsymbol{k},\lambda} E_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k},\lambda}{}^{+} \hat{a}_{\boldsymbol{k},\lambda}$$

and

$$\hat{H}_{\text{int}}(\boldsymbol{q} \neq 0) = \frac{e^2}{2V} \sum_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}{}' \sum_{\lambda_1,\lambda_2} \frac{4\pi}{q^2} \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\lambda_1}{}^{+} \hat{a}_{\boldsymbol{p}-\boldsymbol{q},\lambda_2}{}^{+} \hat{a}_{\boldsymbol{p},\lambda_2} \hat{a}_{\boldsymbol{k},\lambda_1}$$

where the notation $\sum'$ indicates that the terms with $\boldsymbol{q} = 0$ are to be omitted. Here we assume that the screening parameter $\mu = 0$.

6. Quantum box (fermions)

We consider a quantum box with the volume $V = L^3$ (cube with side L). The quantum state is defined by $|\boldsymbol{k}\rangle$ with $k_x = \frac{2\pi}{L} n_x$, $k_y = \frac{2\pi}{L} n_y$, and $k_z = \frac{2\pi}{L} n_z$ (n_x, n_y, n_z are integers). The wave function is given by

$$\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}},$$

The quantum field operator is defined by

$$\hat{\psi}(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{a}_{\boldsymbol{k}}(t).$$

Note that the annihilation and creation operators are defined by

$$\frac{1}{\sqrt{V}}\int d\boldsymbol{r}\hat{\psi}(\mathbf{r},t)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{1}{\sqrt{V}}\int d\boldsymbol{r}\sum_{\boldsymbol{k}'}\frac{1}{\sqrt{V}}e^{i(\boldsymbol{k}'-\boldsymbol{k})'\cdot\boldsymbol{r}}\hat{a}_{\boldsymbol{k}'}(t)$$
$$= \frac{1}{V}\sum_{\boldsymbol{k}'}\int d\boldsymbol{r}e^{i(\boldsymbol{k}'-\boldsymbol{k})'\cdot\boldsymbol{r}}\hat{a}_{\boldsymbol{k}'}(t)$$
$$= \sum_{\boldsymbol{k}'}\hat{a}_{\boldsymbol{k}'}(t)\delta_{\boldsymbol{k}',\boldsymbol{k}}$$
$$= \hat{a}_{\boldsymbol{k}}(t)$$

or

$$\hat{a}_{\boldsymbol{k}}(t) = \frac{1}{\sqrt{V}}\int d\boldsymbol{r}\hat{\psi}(\mathbf{r},t)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad \hat{a}_{\boldsymbol{k}}^{+}(t) = \frac{1}{\sqrt{V}}\int d\boldsymbol{r}\hat{\psi}^{+}(\mathbf{r},t)e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

where

$$\frac{1}{V}\int d\boldsymbol{r}e^{i(\boldsymbol{k}'-\boldsymbol{k})'\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k}',\boldsymbol{k}}.$$

The commutation relation:

$$[\hat{a}_k(t),\hat{a}_{k'}{}^{+}(t)]_{+} = [\frac{1}{\sqrt{V}}\int d\mathbf{r}\hat{\psi}(\mathbf{r},t)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}},\frac{1}{\sqrt{V}}\int d\mathbf{r}'\hat{\psi}^{+}(\mathbf{r}',t)e^{i\boldsymbol{k}'\cdot\boldsymbol{r}'}]_{+}$$
$$= \frac{1}{V}\int d\boldsymbol{r}\int d\boldsymbol{r}'e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}'\cdot\boldsymbol{r}'}[\hat{\psi}(\mathbf{r},t),\hat{\psi}^{+}(\mathbf{r}',t)]_{+}$$
$$= \frac{1}{V}\int d\boldsymbol{r}\int d\boldsymbol{r}'e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}'\cdot\boldsymbol{r}'}\delta(\mathbf{r}-\mathbf{r}')$$
$$= \frac{1}{V}\int d\boldsymbol{r}e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}$$
$$= \delta_{\boldsymbol{k},\boldsymbol{k}'}$$

Similarly, we have

$$[\hat{a}_k(t),\hat{a}_{k'}(t)]_{+} = [\frac{1}{\sqrt{V}}\int d\mathbf{r}\hat{\psi}(\mathbf{r},t)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}},\frac{1}{\sqrt{V}}\int d\mathbf{r}'\hat{\psi}(\mathbf{r}',t)e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}]_{+}$$
$$= \frac{1}{V}\int d\boldsymbol{r}\int d\boldsymbol{r}'e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}[\hat{\psi}(\mathbf{r},t),\hat{\psi}(\mathbf{r}',t)]$$
$$= 0$$

At t =0, we have

$$\hat{a}_{\boldsymbol{k}}(t=0) = \hat{a}_{\boldsymbol{k}} = \frac{1}{\sqrt{V}} \int d\boldsymbol{r} \hat{\psi}(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$\hat{H}_0 = \int dr \{ \frac{\hbar^2}{2m} \nabla \psi^+(\boldsymbol{r}) \cdot \nabla \psi(\boldsymbol{r}) + V(\boldsymbol{r}) \psi^+(\boldsymbol{r}) \psi(\boldsymbol{r}) \}$$
$$= \sum_{\boldsymbol{k}} \frac{\hbar^2 \boldsymbol{k}^2}{2m} \hat{a}_{\boldsymbol{k}}{}^+ \hat{a}_{\boldsymbol{k}} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k}'-\boldsymbol{k}} \hat{a}_{\boldsymbol{k}'}{}^+ \hat{a}_{\boldsymbol{k}}$$

with

$$V_{\boldsymbol{k}} = \frac{1}{V} \int d\boldsymbol{r} V(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$

((The interaction Hamiltonian))

$$H_1 = \frac{1}{2} \int d\boldsymbol{r} \int d\boldsymbol{r}' \hat{\psi}^+(\boldsymbol{r}) \hat{\psi}^+(\boldsymbol{r}') U(|\boldsymbol{r}-\boldsymbol{r}'|) \hat{\psi}(\boldsymbol{r}') \hat{\psi}(\boldsymbol{r})$$
$$= \frac{1}{2} \sum_{\boldsymbol{k},\boldsymbol{p}} \sum_{\boldsymbol{k}',\boldsymbol{p}'} \delta_{\boldsymbol{k}+\boldsymbol{p},\boldsymbol{k}'+\boldsymbol{p}'} U(|\boldsymbol{p}-\boldsymbol{k}'|) \hat{a}_{\boldsymbol{p}'}{}^+ \hat{a}_{\boldsymbol{k}'}{}^+ \hat{a}_{\boldsymbol{k}} \hat{a}_{\boldsymbol{p}}$$

where

$$U(|\boldsymbol{k}|) = \frac{1}{V} \int dx e^{-i\boldsymbol{k}.\boldsymbol{r}} U(|\boldsymbol{r}|)$$

((Momentum operator))

$$\hat{\boldsymbol{P}} = \frac{1}{2} \int d\boldsymbol{r} \frac{\hbar}{i} \{ \hat{\psi}^+(\boldsymbol{r},t) \nabla \hat{\psi}(\boldsymbol{r},t) - \nabla \hat{\psi}^+(\boldsymbol{r},t) \hat{\psi}(\boldsymbol{r},t)$$

$$\hat{\boldsymbol{P}} = \sum_{\hbar} \hbar \boldsymbol{k} \hat{a}_k{}^+(t) \hat{a}_k{}^+(t)$$

7. Free electron Fermi gas model in metal

We consider the properties of a Fermi gas of non-interacting spin 1/2 fermions in their ground state. The ground state $|\Phi_0\rangle$ is characterized by all the momentum states being filled up to the Fermi momentum p_F. Then we have

$$n_{\boldsymbol{p}\uparrow} = \langle \Phi_0 | \hat{a}_{\boldsymbol{p}\uparrow}{}^{+} \hat{a}_{\boldsymbol{p}\uparrow} | \Phi_0 \rangle = \theta(p_F - |\boldsymbol{p}|) = \begin{cases} 1 & |\boldsymbol{p}| \le p_F \\ 0 & |\boldsymbol{p}| > p_F \end{cases}$$

and

$$n_{\boldsymbol{p}\uparrow} = n_{\boldsymbol{p}\downarrow} .$$

(a) The Fermi momentum: p_F

The Fermi momentum is determined by the condition that the total number of particles is given by

$$N = \sum_{\boldsymbol{p}} (n_{\boldsymbol{p}\uparrow} + n_{\boldsymbol{p}\downarrow}) = \frac{2}{(2\pi\hbar)^3} \frac{4\pi}{3} p_F{}^3 = \frac{V p_F{}^3}{3\pi^2 \hbar^3} = \frac{V k_F{}^3}{3\pi^2}$$

or

$$\frac{V p_F{}^3}{3\pi^2 \hbar^3} = N , \qquad\qquad p_F{}^3 = 3\pi^2 \hbar^3 n$$

or

$$k_F{}^3 = 3\pi^2 \frac{N}{V} = 3\pi^2 n$$

where n is the number density and k_F is the wave number ($p_F = \hbar k_F$).

(b) Average density

$$\langle \rho(\boldsymbol{r}) \rangle = \sum_{\sigma} \langle \Phi_0 | \hat{\psi}_\sigma{}^{+}(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}) | \Phi_0 \rangle$$
$$= \frac{1}{V} \sum_{\sigma, \boldsymbol{p}, \boldsymbol{p}'} \langle \Phi_0 | \hat{a}_{\boldsymbol{p}\sigma}{}^{+} \hat{a}_{\boldsymbol{p}'\sigma} | \Phi_0 \rangle \exp[\frac{-i(\boldsymbol{p} - \boldsymbol{p}') \cdot \boldsymbol{r}}{\hbar}]$$

where σ is the spin variable, and

$$\langle \Phi_0 | \hat{a}_{\boldsymbol{p}\sigma}{}^{+} \hat{a}_{\boldsymbol{p}'\sigma} | \Phi_0 \rangle = \delta_{\boldsymbol{p},\boldsymbol{p}'} n_{p,\sigma}$$

Then we have

$$\langle \rho(\boldsymbol{r}) \rangle = \frac{1}{V} \sum_{\sigma, \boldsymbol{p}} n_{\boldsymbol{p}\sigma} = n$$

Thus the density in the gas is uniform.

(c) One-particle density matrix

$$G_\sigma(\boldsymbol{r} - \boldsymbol{r}') = \langle \Phi_0 | \hat{\psi}_\sigma{}^+(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}') | \Phi_0 \rangle$$
$$= \frac{1}{V} \sum_{\boldsymbol{p}} n_{\boldsymbol{p},\sigma} \exp[-\frac{i}{\hbar} \boldsymbol{p} \cdot (\boldsymbol{r} - \boldsymbol{r}')]$$

Converting the sum to an integral. we get

$$G_\sigma(\boldsymbol{r} - \boldsymbol{r}') = \frac{1}{V} \frac{V}{(2\pi\hbar)^3} \int_0^{p_F} d\boldsymbol{p} \exp[-\frac{i}{\hbar} \boldsymbol{p} \cdot (\boldsymbol{r} - \boldsymbol{r}')]$$
$$= \frac{1}{4\pi^2\hbar^3} \int_0^{p_F} p^2 dp \int_0^{\pi} \sin\theta d\theta \exp[-\frac{i}{\hbar} p \cos\theta |\boldsymbol{r} - \boldsymbol{r}'|]$$
$$= \frac{1}{4\pi^2\hbar^3} \int_0^{p_F} p^2 dp \int_{-1}^{1} d\mu \exp[-\frac{i}{\hbar} p |\boldsymbol{r} - \boldsymbol{r}'| \mu]$$
$$= \frac{1}{2\pi^2\hbar^2 |\boldsymbol{r} - \boldsymbol{r}'|} \int_0^{p_F} p \sin(\frac{p}{\hbar} |\boldsymbol{r} - \boldsymbol{r}'|) dp$$
$$= \frac{p_F{}^3}{2\pi^2\hbar^3} \frac{(-x\cos x + \sin x)}{x^3}$$

or

$$G_\sigma(\boldsymbol{r} - \boldsymbol{r}') = \frac{3n}{2} \frac{\sin x - x\cos x}{x^3}$$

where

$$p_F{}^3 = 3\pi^2\hbar^3 n$$

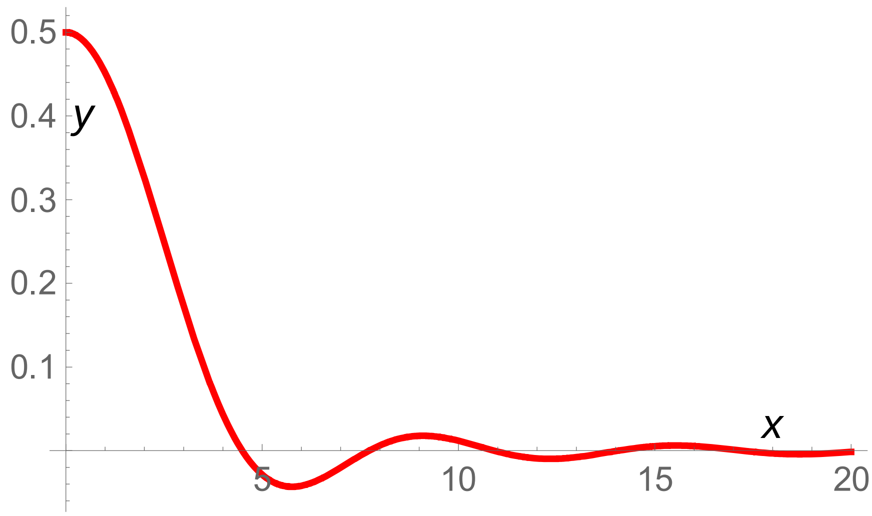


Fig. Plot of $y = \dfrac{G_\sigma}{n}$ as a function of $x = \dfrac{p_F}{\hbar}|\boldsymbol{r}-\boldsymbol{r}'|$.

(d) Pair correlation function

The **Pauli exclusion principle** is the quantum mechanical **principle** that states that two or more identical fermions (particles with half-integer spin) cannot occupy the same quantum state within a quantum system simultaneously.

Suppose that there is one fermion at the point $\boldsymbol{r}$. We calculate the relative probability of finding another particle at $\boldsymbol{r}'$. One way to formulate these problem is to remove (mathematically) a particle (with spin σ) at the point r from the system, leaving behind (N-1) particles in the state

$$|\Phi'(\boldsymbol{r},\sigma)\rangle = \hat{\psi}_\sigma(\boldsymbol{r})|\Phi_0\rangle$$

and ask for the density distribution of particles (with spin σ') in this new state. This density is

$$\begin{aligned}\langle\Phi'(\boldsymbol{r},\sigma)|\hat{\psi}_{\sigma'}^{+}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')|\Phi'(\boldsymbol{r},\sigma)\rangle &= \langle\Phi_0|\hat{\psi}_{\sigma}^{+}(\boldsymbol{r})\hat{\psi}_{\sigma'}^{+}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')\hat{\psi}_{\sigma}(\boldsymbol{r})|\Phi_0\rangle \\ &= \left(\frac{n}{2}\right)^2 g_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') \\ &= \left(\frac{n}{2}\right)^2 - [G_s((\boldsymbol{r}-\boldsymbol{r}')]^2\end{aligned}$$

9. Expectation value of $\hat{H}_0$

$$
\begin{aligned}
E^{(0)} &= \langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle \\
&= \frac{\hbar^2}{2m} \sum_{\boldsymbol{k},\sigma} k^2 \langle \Phi_0 | n_{\boldsymbol{k}\sigma} | \Phi_0 \rangle \\
&= \frac{\hbar^2}{2m} \sum_{\boldsymbol{k},\sigma} k^2 \theta(k_F - k) \\
&= \frac{\hbar^2}{2m} 2 \frac{V}{(2\pi)^3} \int_0^{k_F} 4\pi k^4 dk \\
&= \frac{\hbar^2}{2m} \frac{V}{\pi^2} \frac{1}{5} k_F{}^5
\end{aligned}
$$

$$
\begin{aligned}
N^{(0)} &= \langle \Phi_0 | \hat{N} | \Phi_0 \rangle \\
&= \sum_{\boldsymbol{k},\sigma} \langle \Phi_0 | n_{\boldsymbol{k}\sigma} | \Phi_0 \rangle \\
&= \sum_{\boldsymbol{k},\sigma} \theta(k_F - k) \\
&= 2 \frac{V}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk \\
&= \frac{V k_F{}^3}{3\pi^2}
\end{aligned}
$$

$$
E^{(0)} = \frac{3}{5} \varepsilon_F N
$$

or

$$
E^{(0)} = \frac{3}{5} \varepsilon_F N = \frac{3}{5} \frac{\hbar^2}{2m} k_F{}^2 N = \frac{3}{5} \frac{\hbar^2 N}{2m r_0{}^2} (\frac{9\pi}{4})^{2/3} = \frac{3}{5} \frac{\hbar^2 N}{2m a_B{}^2} \frac{1}{r_s{}^2} (\frac{9\pi}{4})^{2/3}
$$

or

$$
E^{(0)} = \frac{3}{5} \frac{e^2}{2a_B} \frac{N}{r_s{}^2} (\frac{9\pi}{4})^{2/3} = \frac{e^2}{2a_B} \frac{N}{r_s{}^2} 2.2099
$$

where

$$
\varepsilon_F = \frac{\hbar^2}{2m} k_F{}^2, \qquad r_0 = (\frac{9\pi}{4})^{1/3} \frac{1}{k_F}, \qquad r_s = \frac{r_0}{a_B}
$$

$$a_B = \frac{\hbar^2}{me^2} = 0.529177 \text{Å}.$$

The first-order energy shift

$$E^{(1)} = \langle \Phi_0 | \hat{H}_1 | \Phi_0 \rangle$$
$$= \frac{e^2}{2V} \sum_{\boldsymbol{kpq}}{}' \sum_{\sigma\sigma'} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1}{}^{+} \hat{a}_{\boldsymbol{p}-\boldsymbol{q},\sigma_2}{}^{+} \hat{a}_{\boldsymbol{p},\sigma_2} \hat{a}_{\boldsymbol{k},\sigma_1} | \Phi_0 \rangle$$

The states $\boldsymbol{p},\sigma_2$ and $\boldsymbol{k},\sigma_1$ must be inside the Fermi sea. Similarly, $\boldsymbol{k}+\boldsymbol{q},\sigma_1$ and $\boldsymbol{p}-\boldsymbol{q},\sigma_2$ must also be inside the Fermi sea. There are two possibilities.

$\boldsymbol{k}+\boldsymbol{q},\sigma_1 = \boldsymbol{k},\sigma_1,\quad \boldsymbol{p}-\boldsymbol{q},\sigma_2 = \boldsymbol{p},\sigma_2$ (the first pairing)

or

$\boldsymbol{p}-\boldsymbol{q},\sigma_2 = \boldsymbol{k},\sigma_1 \quad \boldsymbol{k}+\boldsymbol{q},\sigma_1 = \boldsymbol{p},\sigma_2$ (the second pairing)

The first pairing is forbidden because the term $\boldsymbol{q}=0$ is excluded from the sum. Then the matrix becomes

$$E^{(1)} = \frac{e^2}{2V} \sum_{\boldsymbol{kq}}{}' \sum_{\sigma\sigma'} \delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{p}} \delta_{\sigma_1,\sigma_2} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1}{}^{+} \hat{a}_{\boldsymbol{k},\sigma_1}{}^{+} \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1} \hat{a}_{\boldsymbol{k},\sigma_1} | \Phi_0 \rangle$$
$$= -\frac{e^2}{2V} \sum_{\boldsymbol{kq}}{}' \sum_{\sigma\sigma'} \delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{p}} \delta_{\sigma_1,\sigma_2} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1}{}^{+} \hat{a}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1} \hat{a}_{\boldsymbol{k},\sigma_1} \hat{a}_{\boldsymbol{k},\sigma_1} | \Phi_0 \rangle$$
$$= -\frac{e^2}{2V} \sum_{\boldsymbol{kq}}{}' \sum_{\sigma\sigma'} \delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{p}} \delta_{\sigma_1,\sigma_2} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{n}_{\boldsymbol{k}+\boldsymbol{q},\sigma_1} \hat{n}_{\boldsymbol{k},\sigma_1} | \Phi_0 \rangle$$
$$= -\frac{e^2}{2V} \sum_{\boldsymbol{kq}}{}' \sum_{\sigma\sigma'} \delta_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{p}} \delta_{\sigma_1,\sigma_2} \frac{4\pi}{q^2} \theta(k_F - |\boldsymbol{k}+\boldsymbol{q}|)\theta(k_F - k)$$

or

$$E^{(1)} = -\frac{e^2}{2V} \frac{4\pi V^2}{(2\pi)^6} 2 \int d\boldsymbol{k} \int d\boldsymbol{q} \frac{\theta(k_F - |\boldsymbol{k}+\boldsymbol{q}|)\theta(k_F - k)}{q^2}$$

It is convenient to change variables from $\boldsymbol{k}$ to $\boldsymbol{P} = \boldsymbol{k} + \frac{1}{2}\boldsymbol{q}$ in order to get the symmetric form;

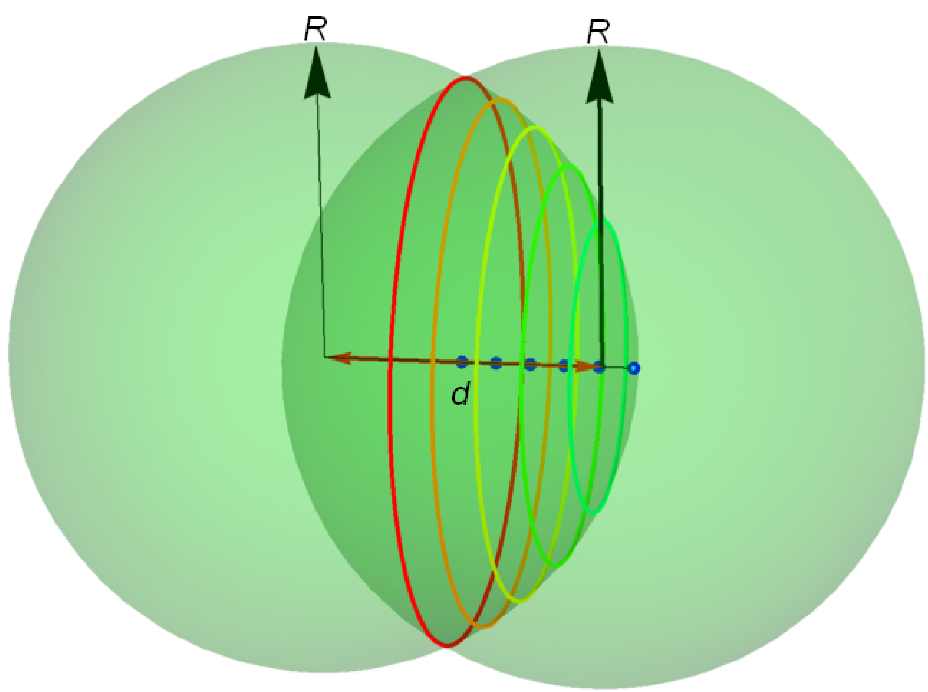
$$E^{(1)} = -\frac{4\pi e^2 V}{(2\pi)^6}\int \frac{1}{q^2} d\boldsymbol{q} \int d\boldsymbol{P}\theta(k_F - \left|\boldsymbol{P} + \frac{\boldsymbol{q}}{2}\right|)\theta(k_F - \left|\boldsymbol{P} - \frac{\boldsymbol{q}}{2}\right|)$$

We note that

$$\int d\boldsymbol{P}\theta(k_F - \left|\boldsymbol{P} + \frac{\boldsymbol{q}}{2}\right|)\theta(k_F - \left|\boldsymbol{P} - \frac{\boldsymbol{q}}{2}\right|) = \frac{4\pi}{3} k_F{}^3 (1 - \frac{3}{2}x + \frac{1}{2}x^3)\theta(1-x)$$

with $x = \frac{q}{2k_F}$. Thus we get

((**Note**)) **Mathematics: volume of the overlap of two spheres**



Let two spheres with the same radius R be located along the x-axis centered at (0,0,0) and (d,0,0), respectively. The equations of the two spheres are

$$x^2 + y^2 + z^2 = R^2, \qquad (1)$$

$$(x-d)^2 + y^2 + z^2 = R^2 \qquad (2)$$

Combining Eqs.(1) and (2) gives

$$(x-d)^2 - x^2 = 0$$

or

$$x = \frac{d}{2}$$

The intersection of the spheres is therefore a curve lying in a plane parallel to the yz-plane at $x = \frac{d}{2}$. Plugging this back into Eq.(1) gives

$$y^2 + z^2 = R^2 - \frac{d^2}{4}$$

which is a circle with radius $\sqrt{R^2 - \frac{d^2}{4}}$. The volume of the 3D lens common to the two spheres can be found by adding the two spherical caps. The volume is

$$\begin{aligned} V &= 2\int_{d/2}^{R} \pi(\sqrt{R^2 - x^2})^2 dx \\ &= 2\pi \int_{d/2}^{R} (R^2 - x^2) dx \\ &= 2\pi [R^2 x - \frac{1}{3}x^3]_{d/2}^{R} \\ &= \frac{4\pi}{3} R^3 (1 - \frac{3}{2}\alpha + \frac{1}{2}\alpha^3) \end{aligned}$$

with $\alpha = \frac{d}{2R}$

$$E^{(1)} = -\frac{4\pi e^2 V}{(2\pi)^6}\int \frac{1}{q^2} 4\pi q^2 dq \frac{4\pi}{3} k_F{}^3 (1 - \frac{3}{2}x + \frac{1}{2}x^3)\theta(1-x)$$

$$= -\frac{4\pi e^2 V}{(2\pi)^6} 4\pi \frac{4\pi}{3} k_F{}^3 (2k_F)\int_0^1 dx(1 - \frac{3}{2}x + \frac{1}{2}x^3)$$

$$= -\frac{(4\pi)^3 e^2 V}{(2\pi)^6}\frac{16}{9} k_F{}^4$$

$$= -\frac{e^2 N}{2r_0}\frac{3}{2\pi}(\frac{9\pi}{4})^{1/3}$$

$$= -\frac{e^2}{2a_B} N \frac{0.916331}{r_s}$$

or

$$E^{(1)} = -\frac{e^2}{2a_B} N \frac{0.916331}{r_s}$$

where

$$V = \frac{4\pi}{3} r_0{}^3 N, \qquad N = \frac{V k_F{}^3}{3\pi^2}, \qquad a_B = \frac{\hbar^2}{me^2} \text{ (Bohr radius)}$$

$$r_s = \frac{r_0}{a_B}, \qquad k_F = (\frac{9\pi}{4})^{1/3}\frac{1}{r_0}.$$

So the total energy is

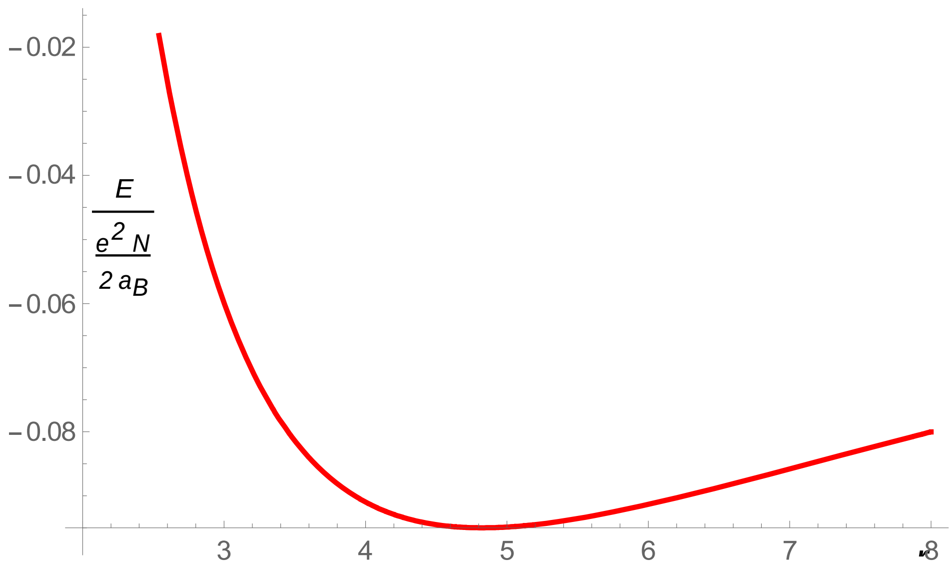
$$E = E^{(0)} + E^{(1)} = \frac{e^2 N}{2a_B}(\frac{1}{r_s{}^2} 2.099 - \frac{0.916331}{r_s})$$

with $\frac{e^2}{2a_B} = 13.6057$ eV. We make a plot of

$$\frac{E}{\frac{e^2 N}{2a_B}} = \frac{1}{r_s{}^2} 2.2099 - \frac{0.916331}{r_s}$$

as function of r_s . This function has a minimum (=-0.0949887) at r_s =4.82337.

Li:	$r_s = 3.22$
Na:	$r_s = 3.86$
K	$r_s = 4.87$
Rb	$r_s = 5.18$
Cs	$r_s = 5.57$



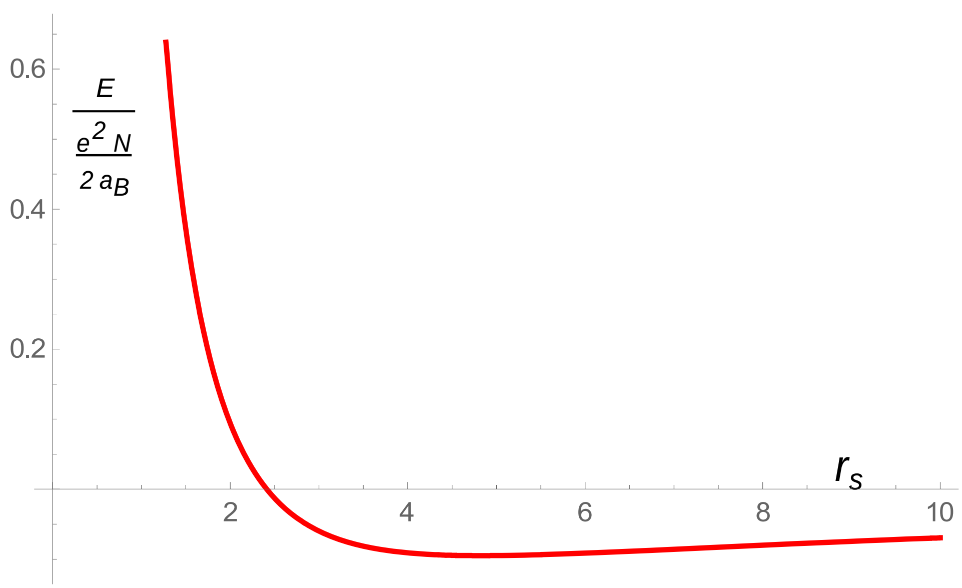


Fig. Plot of $\dfrac{E}{\dfrac{e^2 N}{2a_B}}$ as a function of $r_s = \dfrac{r_0}{a_B}$. Minimum value (=-0.0949887) at r_s =4.82337.

REFERENCES

H. Haken, Quantum Field Theory, Introduction (North-Holland, 1976).

D.J. Thouless, The Quantum mechanics of Many Body Systems (Academic Press, 1961).

A.L. Fetter and J.D. Walecka, Quantum Theory of Many-particle Systems (McGraw-Hill, 1971).

J.J. Sakurai and J. Naporitano, Modern Quantum Mechanics, second edition (Addison-Wesley, 2011).

A.M. Zagoskin, Quantum Theory of Many-Body Systems, Techniques and Applications, second edition (Springer, 2014).