# EXERCISES

## Second Quantization

# Second Quantization Recap

$$\hat{n}_s |n_1 \ldots n_s \ldots\rangle = n_s \, |n_1 \ldots n_s \ldots\rangle$$

$$\hat{I} = \sum_{n_1 \ldots n_s \ldots} C_{n_1 \ldots n_s \ldots} \, |n_1 \ldots n_s \ldots\rangle\langle n_1 \ldots n_s \ldots|$$

$$\langle n_1 \ldots n_s \ldots | n_1' \ldots n_s' \ldots\rangle = \delta_{n_1 n_1'} \ldots \delta_{n_s n_s'} \ldots$$

Bosons : $n_s = 0, 1, 2, \ldots$

Fermions: $n_s = 0, 1$

## Bosons:

$$a_s^{+} |n_1 \ldots n_s \ldots\rangle = \sqrt{n_s + 1} \, |n_1 \ldots n_s + 1 \ldots\rangle$$

$$a_s |n_1 \ldots n_s \ldots\rangle = \sqrt{n_s} \, |n_1 \ldots n_s - 1 \ldots\rangle$$

$$[a_s, a_{s'}] = [a_s^{+}, a_{s'}^{+}] = 0 \quad , \quad [a_s, a_{s'}^{+}] = \delta_{ss'}$$

## Fermions

$$a_s^+ |n_1 \cdots n_s \cdots\rangle = (-1)^{n_1+n_2+\cdots+n_{s-1}} |n_1 \cdots \overset{n_s}{\overset{\downarrow}{1}} \cdots\rangle \quad (n_s = 0)$$

$$= 0 \quad (n_s = 1)$$

$$a_s |n_1 \cdots n_s \cdots\rangle = (-1)^{n_1+n_2+\cdots+n_{s-1}} |n_1 \cdots 0 \cdots\rangle \quad (n_s = 1)$$

$$= 0 \quad (n_s = 0)$$

$$[a_s, a_{s'}]_+ = [a_s^+, a_{s'}^+]_+ = 0 \,, \qquad [a_s, a_{s'}^+]_+ = \delta_{ss'}$$

$$a_s^n = (a_s^+)^n = 0 \qquad n > 1$$

<u>All particles</u> (Fermions <u>and</u> Bosons)

$$\hat{n}_s |0\rangle = 0 \qquad a_s |0\rangle = \langle 0| a_s^+ = 0$$

$$\hat{n}_s = a_s^+ a_s \qquad \hat{N} = \sum_s \hat{n}_s = \sum_s a_s^+ a_s$$

## Momentum Eigenstates

$$\psi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \vec{k} \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \qquad \vec{p}|\vec{k}\rangle = \hbar\vec{k}|\vec{k}\rangle$$

Box normalization

$$\langle \vec{r} | \vec{r}' \rangle = \delta(\vec{r}-\vec{r}') = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}$$

$$\langle \vec{k} | \vec{k}' \rangle = \delta_{\vec{k}\vec{k}'} = \frac{1}{V}\int d^3r\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}$$

$$\int d^3r\, f(\vec{r})\,\delta(\vec{r}-\vec{r}') = f(\vec{r}') \implies \int d^3r\, \delta(\vec{r}-\vec{r}') = 1$$

$$\sum_{\vec{k}} f(\vec{k})\,\delta_{\vec{k}\vec{k}'} = f(\vec{k}') \Rightarrow \sum_{\vec{k}} \delta_{\vec{k}\vec{k}'} = 1$$

$$\boxed{\hat{I} = \sum_{\vec{k}} |\vec{k}\rangle\langle\vec{k}| = \int d^3r\, |\vec{r}\rangle\langle\vec{r}|}$$

← resolution of the identity

# Field Operators

particle located at $\vec{r}$ (4)

$$a_s^\dagger |0\rangle = |s\rangle \qquad \langle \vec{r} | s \rangle = \psi_s(\vec{r})$$

$$|\vec{r}\rangle = \sum_s |s\rangle\langle s|\vec{r}\rangle = \underbrace{\sum_s \psi_s^*(\vec{r})\, a_s^\dagger}_{\Psi^\dagger(\vec{r})} |0\rangle = \overbrace{\Psi^\dagger(\vec{r})\,|0\rangle}^{\text{particle located at } \vec{r}}$$

$$\therefore \quad \boxed{\begin{aligned} \Psi^\dagger(\vec{r}) &= \sum_s \psi_s^*(\vec{r})\, a_s^\dagger \\ \Psi(\vec{r}) &= \sum_s \psi_s(\vec{r})\, a_s \end{aligned}} \qquad \boxed{\begin{aligned} a_s &= \int d^3r\, \psi_s^*(\vec{r})\, \Psi(\vec{r}) \\ a_s^\dagger &= \int d^3r\, \psi_s(\vec{r})\, \Psi^\dagger(\vec{r}) \end{aligned}}$$

## Canonical Field commutation relations:

$$[\Psi(\vec{r}), \Psi(\vec{r}')]_\pm = [\Psi^\dagger(\vec{r}), \Psi^\dagger(\vec{r}')]_\pm = 0, \qquad [\Psi(\vec{r}), \Psi^\dagger(\vec{r}')]_\pm = \delta(\vec{r}-\vec{r}')$$

$\pm$
- $-$ bosons (commutation relations)
- $+$ Fermions (anticommutation relations)

Note !!

$$\Psi(\vec{r})|0\rangle = \langle 0|\Psi^\dagger(\vec{r}) = 0$$

Special case : single particle states are momentum states

$$s \longrightarrow \vec{k} \;, \quad \varphi_s(\vec{r}) \Rightarrow \varphi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$$\therefore \quad \Psi^{\dagger}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \, a^{\dagger}_{\vec{k}}$$

$$\Psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \, a_{\vec{k}}$$

$$a_{\vec{k}} = \frac{1}{\sqrt{V}} \int d^3r \; e^{-i\vec{k}\cdot\vec{r}} \, \Psi(\vec{r})$$

$$a^{\dagger}_{\vec{k}} = \frac{1}{\sqrt{V}} \int d^3r \; e^{i\vec{k}\cdot\vec{r}} \, \Psi^{\dagger}(\vec{r})$$

$$[a_{\vec{k}}, a_{\vec{k}'}]_{\pm} = [a^{\dagger}_{\vec{k}}, a^{\dagger}_{\vec{k}'}]_{\pm} = 0 \,, \qquad [a_{\vec{k}}, a^{\dagger}_{\vec{k}'}]_{\pm} = \delta_{\vec{k}\vec{k}'}$$

Exercise 1

Write relations for field operators of spin - 1/2 fermions (use $\vec{k}$ states)

Soln

Spin $\sigma = \uparrow \downarrow$ $\quad \uparrow: S_z = \frac{\hbar}{2} \quad \downarrow: S_z = -\frac{\hbar}{2}$

single particle state $\quad s: \vec{k}, \sigma \equiv |\vec{k}, \uparrow\rangle$ or $|\vec{k}, \downarrow\rangle$

$$a_s^{\dagger} \longrightarrow a_{\vec{k}\sigma}^{\dagger} : a_{\vec{k}\uparrow}^{\dagger}, \; a_{\vec{k}\downarrow}^{\dagger}$$

anticommutation relations:

$$[a_{\vec{k}\sigma}, a_{\vec{k}'\sigma'}]_+ = [a_{\vec{k}\sigma}^{\dagger}, a_{\vec{k}'\sigma'}^{\dagger}]_+ = 0, \qquad [a_{\vec{k}\sigma}, a_{\vec{k}'\sigma'}^{\dagger}] = \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'}$$

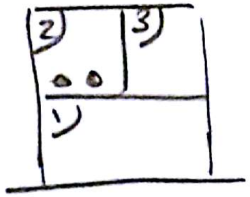
$$\Psi_{\sigma}^{\dagger}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k},\sigma} \varphi^{*}(\vec{r})\, a_{\vec{k}\sigma}^{\dagger}, \qquad \Psi_{\sigma}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k},\sigma} \varphi(\vec{r})\, a_{\vec{k}\sigma}$$

$$a_{\vec{k}\sigma}^{\dagger} = \frac{1}{\sqrt{V}} \int d^3r\, e^{i\vec{k}\cdot\vec{r}}\, \Psi_{\sigma}^{\dagger}(\vec{r}), \qquad a_{\vec{k}\sigma} = \frac{1}{\sqrt{V}} \int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, \Psi_{\sigma}(\vec{r})$$

$$[\Psi_{\sigma}(\vec{r}), \Psi_{\sigma'}(\vec{r}')]_+ = [\Psi_{\sigma}^{\dagger}(\vec{r}), \Psi_{\sigma'}^{\dagger}(\vec{r}')]_+ = 0, \qquad [\Psi_{\sigma}(\vec{r}), \Psi_{\sigma'}^{\dagger}(\vec{r}')] = \delta_{\sigma\sigma'}\, \delta(\vec{r}-\vec{r}')$$

## Exercise 2

Two identical bosons can occupy 3 single-particle states 1, 2, 3.




$|020\rangle$

(a) What is the dimensionality of the multiparticle Hilbert space?

Use notation $|n_1 n_2 n_3\rangle$. The states are

$|200\rangle, |020\rangle, |002\rangle, |110\rangle, |101\rangle, |011\rangle$

There are 6 basis states: dim. of Hilbert space $= 6$

(b) Express the following states in terms of creation operators acting on the vacuum state $|0\rangle$: $|200\rangle, |101\rangle, |002\rangle$

$$a_1^+|0\rangle = a_1^+|000\rangle = \sqrt{1}\,|100\rangle = |100\rangle$$

$$a_1^+ a_1^+|0\rangle = a_1^+|100\rangle = \sqrt{1+1}\,|200\rangle = \sqrt{2}\,|200\rangle$$

$$\therefore \quad |200\rangle = \frac{1}{\sqrt{2}}(a_1^+)^2|0\rangle$$

$$|101\rangle = a_1^+ a_3^+|0\rangle = a_3^+ a_1^+|0\rangle$$

$$|002\rangle = \frac{1}{\sqrt{2}}(a_3^+)^2|0\rangle$$

c) Consider now 5 bosons instead of 2. Write the state:

$|0\,5\,0\rangle$ using $a, a^{+}$ operators.

$$a_2^{+}|0\,0\,0\rangle = \sqrt{1}\,|0\,1\,0\rangle \quad , \quad (a_2^{+})^2|0\,0\,0\rangle = \sqrt{1}\,a_2^{+}|0\,1\,0\rangle = \sqrt{1}\sqrt{2}\,|0\,2\,0\rangle$$

$$(a_2^{+})^3|0\,0\,0\rangle = \sqrt{1}\sqrt{2}\sqrt{3}\,|0\,3\,0\rangle \quad \ldots \text{ etc.}$$

$$\therefore\ (a_2^{+})^5 = \sqrt{1}\cdots\sqrt{5}\,|0\,5\,0\rangle = \sqrt{5!}\,|0\,5\,0\rangle$$

$$\therefore\ |0\,5\,0\rangle = \frac{1}{\sqrt{5!}}(a_2^{+})^5|0\rangle$$

d) Write the state $|2\,0\,3\rangle$ as above

$$|2\,0\,3\rangle = \frac{1}{\sqrt{2!}}(a_1^{+})^2\,\frac{1}{\sqrt{3!}}(a_3^{+})^3|0\rangle$$

e) Write the general bosonic state $|n_1 \ldots n_s \ldots\rangle$ as above

$$|n_1 \ldots n_s \ldots\rangle = \frac{1}{\sqrt{n_1!}}(a_1^{+})^{n_1} \cdots \frac{1}{\sqrt{n_s!}}(a_s^{+})^{n_s} \cdots |0\rangle$$

Exercise 3

Consider two identical fermions occupying 5 orthonormal single-particle states $s = 1, 2, \dots, 5$.

a) What is the dimensionality of the multiparticle space?

$$\# \text{ of states} = C^5_2 = \frac{5 \times 4}{2 \times 1} = 10 \text{ states}$$

b) List all the states with sharp occupation numbers.

We use notation $|n_1 n_2 \dots n_5\rangle$. The states are,

$|11000\rangle$, $|10100\rangle$, $|10010\rangle$, $|10001\rangle$, $|01100\rangle$, $|01010\rangle$,
$|01001\rangle$, $|00110\rangle$, $|00101\rangle$, $|00011\rangle$

c) Write the state $|00110\rangle$, $|10001\rangle$ using creation and annihilation operators for fermions.

$$|00110\rangle = a_3^\dagger a_4^\dagger |0\rangle \quad , \quad |10001\rangle = a_1^\dagger a_5^\dagger |0\rangle$$

## Exercise 4

In a "normal ordered" product of operators, all creation operators stand to the left and all annihilation operators stand to the right. Put the following operators in normal ordered form (for bosons and fermions).

(a) $a_1 a_2^+$

Bosons: $a_1 a_2^+ = a_2^+ a_1$

Fermions: $a_1 a_2^+ = -a_2^+ a_1$

(b) $a_1 a_2 a_2^+ a_1^+$

Bosons: $[a_2, a_2^+] = 1 \rightarrow a_2 a_2^+ - a_2^+ a_2 = 1 \longrightarrow a_2 a_2^+ = 1 + a_2^+ a_2$

$\therefore a_1 a_2 a_2^+ a_1^+ = a_1 (1 + a_2^+ a_2) a_1^+ = a_1 a_1^+ + a_1 a_2^+ a_2 a_1^+$

Furthermore: $a_1$ commutes with $a_2^+, a_2$ : $[a_1, a_2^+] = [a, a_2] = 0$

$\therefore a_1 a_2^+ = a_2^+ a_1 \quad , \quad a_1 a_2 = a_2 a_1 \quad , \quad a_1 a_1^+ = 1 + a_1^+ a_1$

$\therefore a_1 a_2 a_2^+ a_1^+ = 1 + a_1^+ a_1 + a_2^+ a_2 a_1 a_1^+ = 1 + a_1^+ a_1 + a_2^+ a_2 (1 + a_1^+ a_1)$

$= 1 + a_1^+ a_1 + a_2^+ a_2 + a_2^+ a_2 a_1^+ a_1 = 1 + a_1^+ a_1 + a_2^+ a_2 + a_2^+ a_1^+ a_2 a_1$ #

**Fermions**: $[a_2, a_2^+]_+ = 1 \Rightarrow a_2 a_2^+ + a_2^+ a_2 = 1$

$\therefore\ a_2 a_2^+ = 1 - a_2^+ a_2$

$\therefore\ a_1 a_2 a_2^+ a_1^+ = a_1 (1 - a_2^+ a_2) a_1^+ = a_1 a_1^+ - a_1 a_2^+ a_2 a_1^+$

$[a_1, a_2^+]_+ = [a_1, a_2]_+ = 0 \quad \therefore\ a_1 a_2^+ = -a_2^+ a_1\ ,\quad a_1 a_2 = -a_2 a_1$

Furthermore, $a_1 a_1^+ = 1 - a_1^+ a_1$, Hence:

$$a_1 a_2 a_2^+ a_1^+ = 1 - a_1^+ a_1 + a_2^+ a_1 a_2 a_1^+ = 1 - a_1^+ a_1 - a_2^+ a_2 a_1 a_1^+$$

$$= 1 - a_1^+ a_1 - a_2^+ a_2 (1 - a_1^+ a_1) = 1 - a_1^+ a_1 - a_2^+ a_2 + a_2^+ a_2 a_1^+ a_1$$

$$= 1 - a_1^+ a_1 - a_2^+ a_2 - a_2^+ a_1^+ a_2 a_1$$

$\longleftarrow$ all operators normal ordered

(last term may be re-arranged)

Combining both results:

$$a_1 a_2 a_2^+ a_1^+ = 1 \pm a_1^+ a_1 \pm a_2^+ a_2 \pm a_2^+ a_1^+ a_2 a_1$$

upper sign Bosons

lower sign Fermions

**Note:** $\langle 0 | a_1 a_2 a_2^+ a_1^+ | 0 \rangle = 1$ For bosons and Fermions

Recall $\langle 0 | a^+ = a | 0 \rangle = 0$

## Exercise (5)

Show that the expectation value of a normal-ordered product of operators vanishes in the vacuum state $|0\rangle$.

**Soln**

A normal-ordered product has the form $a_s^+ a_{s'}^+ \cdots a_{s''} a_{s'''}$

The vacuum expectation value is $\langle 0| a_s^+ \cdots a_{s''} |0\rangle$

However: $\langle 0| a_s^+ = a_s|0\rangle$

$\therefore$ The (VEV) (Vacuum Expectation Value) vanishes.

**Exercise 6**

Evaluate the following expectation values for both fermions and bosons:

(a) $\langle 0| a_1 a_1^\dagger |0\rangle$ (b) $\langle 0| a_1 a_2 a_1^\dagger a_2^\dagger |0\rangle$

(c) $\langle 0| a_1 a_3^\dagger a_1^\dagger |0\rangle$ (d) $\langle 0| a_1 a_2 a_1 a_2 a_1^\dagger a_1^\dagger a_2^\dagger a_2^\dagger |0\rangle$

$\pm$
$+$ bosons
$-$ fermions

**Solution:**

(a) $\langle 0| a_1 a_1^\dagger |0\rangle = \langle 0| (1 \pm a_1^\dagger a_1) |0\rangle = \langle 0|0\rangle \pm \langle 0| \underbrace{a_1^\dagger a_1}_{n_1} |0\rangle$

$= 1 \pm 0 = 1$

(b) $\langle 0| a_1 a_2 a_1^\dagger a_2^\dagger |0\rangle = \langle 0| a_1 (\pm a_1^\dagger a_2) a_2^\dagger |0\rangle = \pm \langle 0| a_1 a_1^\dagger a_2 a_2^\dagger |0\rangle$

$= \pm \langle 0| a_1 a_1^\dagger (1 \pm a_2^\dagger a_2) |0\rangle = \pm \langle 0| a_1 a_1^\dagger |0\rangle \mp \langle 0| a_1 a_1^\dagger a_2^\dagger a_2 |0\rangle$ zero

$= \pm \langle 0| (1 - a_1^\dagger a_1) |0\rangle = \pm 1$

(c) $\langle 0| a_1 a_3^\dagger a_1^\dagger |0\rangle = \pm \langle 0| a_3^\dagger a_1 a_1^\dagger |0\rangle = 0$

(d) 0 (Fermions), $a_1^\dagger a_1^\dagger a_2^\dagger a_2^\dagger |0\rangle = \sqrt{2}\sqrt{2}\,|22\rangle = 2|22\rangle$

$\therefore$ VEV $= \langle 22| 2 * 2 |22\rangle = 4\langle 22|22\rangle = 4$ (bosons)

Exercise 7

What is the physical meaning of the following operators?

(a) $\sum_{s} a^{\dagger}_{s} a_{s}$  (b) $\sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}}$  (c) $\sum_{\vec{k},\sigma} a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma}$

(d) $\sum_{\vec{k}} (\hbar\vec{k})\, a^{\dagger}_{\vec{k}} a_{\vec{k}}$  (e) $\sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m}\right) a^{\dagger}_{\vec{k}} a_{\vec{k}}$

Note: $\sigma = \uparrow\downarrow$ (spin 1/2)

Soln

(a) $a^{\dagger}_{s} a_{s} = n_s \quad \therefore \quad \sum_{s} a^{\dagger}_{s} a_{s} = \sum_{s} \hat{n}_s = \hat{N}$ (total no. of particles)

(b) $\sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}} = \sum_{\vec{k}} \hat{n}_{\vec{k}} = \hat{N}$

(c) $\sum_{\vec{k},\sigma} a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma} = \sum_{\vec{k},\sigma} \hat{n}_{\vec{k}\sigma} = \sum_{\vec{k}} \left(\hat{n}_{\vec{k}\uparrow} + \hat{n}_{\vec{k}\downarrow}\right) = \hat{N}_{\uparrow} + \hat{N}_{\downarrow} = \hat{N}$

(d) $\sum_{\vec{k}} (\hbar\vec{k})\, a^{\dagger}_{\vec{k}} a_{\vec{k}} = \sum_{\vec{k}} (\hbar\vec{k})\, n_{\vec{k}} = \vec{P}$ ← total momentum of particles

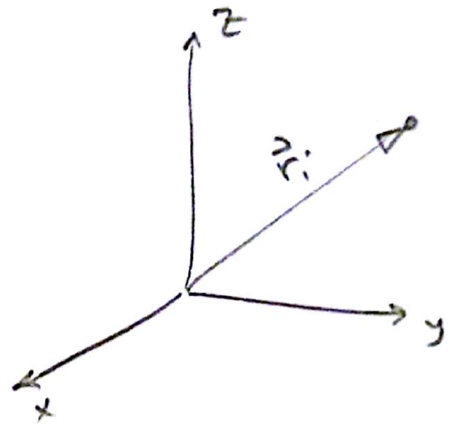
(e) $\sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) a^{\dagger}_{\vec{k}} a_{\vec{k}} = \sum_{\vec{k}} \left(\frac{\hbar^2 k^2}{2m}\right) \hat{n}_{\vec{k}} = \hat{K}$ ← total kinetic energy of particles of mass m each.

Exercise 7

The potential energy of a multi-particle system moving in an external potential is given by:

$$U_{ext} = \sum_{i=1}^{N} V_{ext}(\vec{r}_i)$$

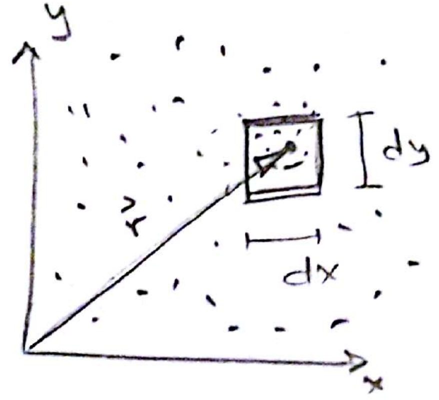
where $V_{ext}(\vec{r}_i)$ is the potential energy of particle number $i$, located at position $\vec{r}_i$.




Write $U_{ext}$ in terms of second quantized operators.

Soln

- Density of particles at point $\vec{r}$ is $\psi^{+}(\vec{r})\,\psi(\vec{r})$
- Divide space into small cubes of volume $dx\,dy\,dz$
- Number of particles in small cube with center at $\vec{r}$ is $dx\,dy\,dz\;\psi^{+}(\vec{r})\,\psi(\vec{r})$

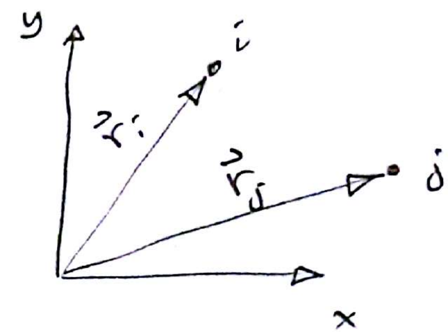



- ∴ $\hat{U}_{ext} = \int d\vec{r}\; V_{ext}(\vec{r})\,\psi^{+}(\vec{r})\,\psi(\vec{r})$

$d\vec{r} \equiv d^3r \equiv dx\,dy\,dz$

Exercise 8

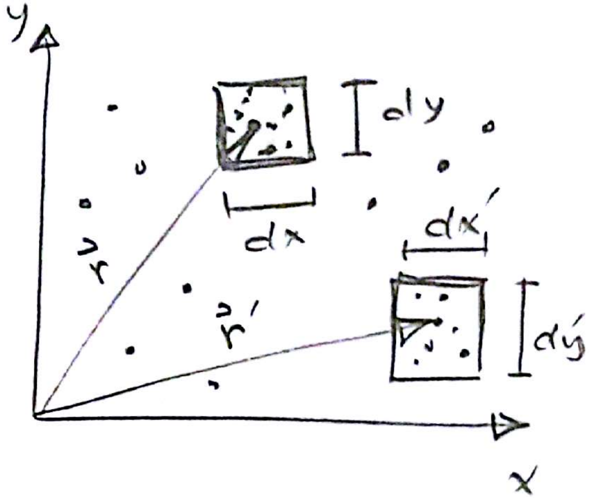
The interaction potential energy between a pair of particles is given by the potential energy $U_{ij} = V(\vec{r}_i - \vec{r}_j)$




The total inter-particle interaction energy is

$$U = \frac{1}{2} \sum_{i \neq j} V(\vec{r}_i - \vec{r}_j)$$

Write $\hat{U}$ using field operators.




Soln.

Interaction energy between particles in cubes at $\vec{r}, \vec{r}'$ is

$$\Delta \hat{U} = V(\vec{r} - \vec{r}') \underbrace{\left[\psi^{+}(\vec{r})\psi(\vec{r})\, d\vec{r}\right]}_{\#\text{ at } \vec{r}} \underbrace{\left[\psi^{+}(\vec{r}')\psi(\vec{r}')\, d\vec{r}'\right]}_{\#\text{ at } \vec{r}'}$$

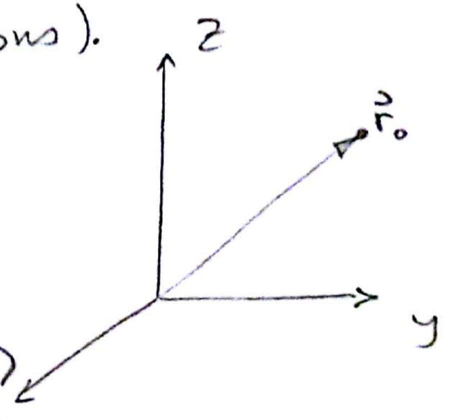
Integrating over $\vec{r}, \vec{r}'$:

$$\hat{U} = \frac{1}{2} \int d\vec{r} \int d\vec{r}' \; V(\vec{r} - \vec{r}') \; \psi^{+}(\vec{r})\psi(\vec{r})\psi^{+}(\vec{r}')\psi(\vec{r}')$$ Wrong order !!!

However, this is not the correct order of operators

Exercise 9

Find the inter-particle interaction energy $U$ for the single-particle state $\psi^\dagger(r_0)|0\rangle$ using the last operator. (Consider bosons).




**Soln** $U$ should come out as zero (particle does not interact with itself. However

$$\hat{U}\,\psi^\dagger(r_0)|0\rangle = \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\left[\psi^\dagger(\vec{r})\,\psi(\vec{r})\,\psi^\dagger(\vec{r}\,')\,\psi(\vec{r}\,')\right]\psi^\dagger(r_0)|0\rangle \quad \times$$

However, $[\psi(\vec{r}\,'), \psi^\dagger(\vec{r}_0)] = \delta(\vec{r}\,'-\vec{r}_0) \Rightarrow \psi(\vec{r}\,')\psi^\dagger(\vec{r}_0) = \delta(\vec{r}\,'-\vec{r}_0) + \psi^\dagger(\vec{r}_0)\psi(\vec{r}\,')$

$$\therefore\ \hat{U}\psi^\dagger(r_0)|0\rangle = \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\,\psi^\dagger(\vec{r})\,\psi(\vec{r})\,\psi^\dagger(\vec{r}\,')\left[\delta(\vec{r}\,'-\vec{r}_0) + \underbrace{\psi^\dagger(r_0)\,\psi(\vec{r}\,')}_{=0}\right]|0\rangle$$

$$= \frac{1}{2}\int d\vec{r}\ V(\vec{r}-\vec{r}_0)\,\psi^\dagger(\vec{r})\,\psi(\vec{r})\,\psi^\dagger(\vec{r}_0)|0\rangle$$

Again, $[\psi(\vec{r}), \psi^\dagger(\vec{r}_0)] = \delta(\vec{r}-\vec{r}_0) \Rightarrow \psi(\vec{r})\psi^\dagger(\vec{r}_0) = \delta(\vec{r}-\vec{r}_0) + \psi^\dagger(r_0)\psi(\vec{r})$

$$\therefore\ U\psi^\dagger(\vec{r}_0)|0\rangle = \frac{1}{2}\int d\vec{r}\ V(\vec{r}-\vec{r}_0)\,\psi^\dagger(\vec{r})\left[\delta(\vec{r}-\vec{r}_0) + \cancelto{0}{\psi^\dagger(\vec{r}_0)\,\psi(\vec{r})}\right]|0\rangle$$

$$= \frac{1}{2}V(\vec{r}_0-\vec{r}_0)\,\psi^\dagger(\vec{r}_0)|0\rangle = \frac{1}{2}V(0)\,\psi^\dagger(\vec{r}_0)|0\rangle \quad \text{which is not zero!}$$

Something is wrong!!

Exercise 10

Show that the operator $\hat{U} = \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\, \psi^{\dagger}(\vec{r})\psi^{\dagger}(\vec{r}\,')\psi(\vec{r}\,')\psi(\vec{r})$ gives zero when acting on the single-particle state $\psi^{\dagger}(r_0)|0\rangle$

Soln.

$$\hat{U}\psi^{\dagger}(\vec{r}_0)|0\rangle = \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\left[\psi^{\dagger}(\vec{r})\psi^{\dagger}(\vec{r}\,')\psi(\vec{r}\,')\psi(\vec{r})\right]\psi^{\dagger}(\vec{r}_0)|0\rangle$$

$$= \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\, \psi^{\dagger}(\vec{r})\psi^{\dagger}(\vec{r}\,')\psi(\vec{r}\,')\left(\cancel{\delta(\vec{r}-\vec{r}_0)}^{\,0} + \cancel{\psi^{\dagger}(r_0)\psi(\vec{r})}^{\,0}\right)|0\rangle$$

$$= 0$$

$\therefore$ The correct expression for $\hat{U}$ is:

$$\hat{U} = \frac{1}{2}\int d\vec{r}\int d\vec{r}\,'\, V(\vec{r}-\vec{r}\,')\, \psi^{\dagger}(\vec{r})\psi^{\dagger}(\vec{r}\,')\psi(\vec{r}\,')\psi(\vec{r})$$

*Note: It is important to keep this particular order for fermions!!

## Exercise 11

Show that the total kinetic energy operator $\hat{K} = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} a^{+}_{\vec{k}} a_{\vec{k}}$

can be written as $\hat{K} = \int d^3r \; \psi^{+}(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi(\vec{r})$

**Soln**

We use the identities from page 5: $\psi^{+}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} a^{+}_{\vec{k}}$

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} a_{\vec{k}}$$

$$\therefore \int d^3r \; \psi^{+}(\vec{r}) \left[-\frac{\hbar^2}{2m}\nabla^2\right] \psi(\vec{r}) = \int d^3r \underbrace{\left[\frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} a^{+}_{\vec{k}}\right]}_{\psi^{+}(\vec{r})} \left(-\frac{\hbar^2 \nabla^2}{2m}\right) \underbrace{\left[\frac{1}{\sqrt{V}} \sum_{\vec{k}'} e^{i\vec{k}'\cdot\vec{r}} a_{\vec{k}'}\right]}_{\psi(\vec{r})}$$

However, $\vec{\nabla} e^{i\vec{k}'\cdot\vec{r}} = i\vec{k}' e^{i\vec{k}'\cdot\vec{r}}$ and $\nabla^2 e^{i\vec{k}'\cdot\vec{r}} = -\vec{k}'^2 e^{i\vec{k}'\cdot\vec{r}}$ (Verify !!)

$$\therefore \text{R.H.S.} = \frac{1}{V} \sum_{\vec{k},\vec{k}'} \frac{+\hbar^2 k'^2}{2m} a^{+}_{\vec{k}} a_{\vec{k}'} \underbrace{\int d^3r \; e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}}_{V\delta_{\vec{k},\vec{k}'}}$$

$$= \frac{1}{V} \sum_{\vec{k}\vec{k}'} \frac{\hbar^2 k'^2}{2m} a^{+}_{\vec{k}} a_{\vec{k}'} \left(V \delta_{\vec{k},\vec{k}'}\right) = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} a^{+}_{\vec{k}} a_{\vec{k}}$$

QED

## Exercise 12

Write the operators $\hat{K}$, $\hat{U}_{ext}$, $\hat{U}$ using second quantization

**Soln**

For spin $\frac{1}{2}$ fermions, the creation operators are $\underbrace{a^{+}_{\vec{k}\uparrow},\ a^{+}_{\vec{k}\downarrow}}_{a^{+}_{\vec{k}\sigma}}$, $\underbrace{\psi^{+}_{\uparrow}(\vec{r}),\ \psi^{+}_{\downarrow}(\vec{r})}_{\psi^{+}_{\sigma}(\vec{r})}$

$$\therefore \quad \hat{K} = \sum_{\vec{k},\sigma} \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) a^{+}_{\vec{k}\sigma} a_{\vec{k}\sigma}$$

$$= \sum_{\sigma=\uparrow\downarrow} \int d^3r \; \psi^{+}_{\sigma}(\vec{r}) \left(\frac{-\hbar^2}{2m}\nabla^2\right) \psi_{\sigma}(\vec{r})$$

$$\hat{U}_{ext} = \sum_{\sigma} \int d^3r \; U_{ext}(\vec{r}) \, \psi^{+}_{\sigma}(\vec{r}) \psi_{\sigma}(\vec{r})$$

Note: Which are numbers and which are operators?

$$\hat{U} = \frac{1}{2} \int d^3r \int d^3r' \; V(\vec{r}-\vec{r}') \sum_{\sigma,\sigma'} \psi^{+}_{\sigma}(\vec{r}) \psi^{+}_{\sigma'}(\vec{r}') \psi_{\sigma'}(\vec{r}') \psi_{\sigma}(\vec{r})$$