Second quantisation II

Reminder: 2nd quantisation

$C(n_1, n_2, \dots, t)$

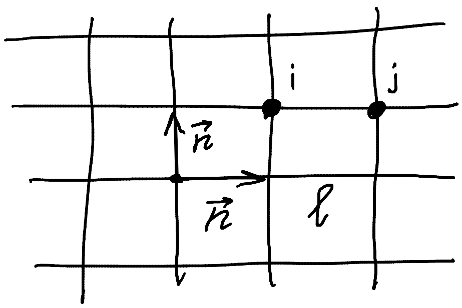
$|n_1 n_2 n_3 \dots\rangle$ – eigenstates

$\hat{a}_i^+$ and $\hat{a}_i$ – creation and annihilation operators

Bosons: $[\hat{b}_i, \hat{b}_k^+] = \delta_{ik}$; $[\hat{A}, \hat{B}] = 0$
for $\hat{A} = \hat{b}_i$, $\hat{B} = \hat{b}_k$
or $\hat{A} = \hat{b}_i^+$, $\hat{B} = \hat{b}_k^+$

Fermions: $\{\hat{a}_i, \hat{a}_k^+\} = \delta_{ik}$; $\{\hat{A}, \hat{B}\} = 0$
for $\hat{A} = \hat{a}_i$, $\hat{B} = \hat{c}_k$
$\hat{A} = \hat{a}_i^+$, $\hat{B} = \hat{a}_k^+$

Examples of Hamiltonians in the 2nd quantisation representation



(Ion crystal)

The Ham-n of conducting el-s

$$\hat{H} = -\sum_{\substack{\text{Neighb.}\\ \text{pairs } i \text{ and } j}} J\, \hat{a}_i^+ a_j$$

It is convenient to label sites by their coordinates $\vec{r}$

$$\hat{H} = -\sum_{\vec{r}, \vec{n}} J\, \hat{a}_{\vec{r}}^+ \hat{a}_{\vec{r}+\vec{n}}$$

Introduce $\hat{a}_k = \frac{1}{\sqrt{\ }} \sum \hat{a}_{\vec{r}}\, e^{i\vec{k}\vec{r}}$ (1)

Introduce $\hat{a}_{k} = \frac{1}{\sqrt{N}} \sum_{\vec r} \hat{a}_{\vec r}\, e^{i\vec k \vec r}$ (1)

(because we are looking at plane waves)

Let as express $\hat{a}_{r}$ through $\hat{a}_{k}$ (it somewhat resembles Fourier transform)

Multiply (1) by $e^{-i\vec k \vec R}$ and sum wrt $\vec k$

$$\sum_{\vec k} e^{i\vec k(\vec r - \vec R)} = N\,\delta_{\vec r \vec R}$$

$$\sum_{\vec k} \hat{a}_{\vec k}\, e^{-i\vec k \vec R} = \frac{1}{\sqrt{N}} \sum_{\vec r} N\,\delta_{\vec r \vec R}\, \hat{a}_{\vec r} \equiv \sqrt{N}\, \hat{a}_{\vec R}$$

$$\hat{a}_{\vec r} = \frac{1}{\sqrt{N}} \sum_{\vec k} e^{-i\vec k \vec r}\, \hat{a}_{k}$$

Respectively

$$\begin{cases} \hat{a}^{+}_{k} = \frac{1}{\sqrt{N}} \sum_{\vec r} \hat{a}^{+}_{\vec r}\, e^{-i\vec k \vec r} \\ \hat{a}^{+}_{\vec r} = \frac{1}{\sqrt{N}} \sum_{\vec k} \hat{a}^{+}_{\vec k}\, e^{i\vec k \vec r} \end{cases}$$

$$\hat{H} = -J \sum_{\vec r, \vec n} \vec a^{+}_{r}\, \vec a_{\vec r + \vec n} =$$

$$= -J \sum_{\vec k, \vec k'} \frac{1}{N} \hat{a}^{+}_{\vec k}\, \hat{a}_{\vec k'} \underbrace{\sum_{\vec r, \vec n} e^{i\vec k \vec r}\, e^{-i\vec k'(\vec r + \vec n)}}$$

$$\parallel \quad \cdots\, e^{-ik_x l} + e^{ik_x l} + e^{-ik_y l} + e^{ik_y l} + e^{-ik_z l} + e^{ik_z l}) =$$

$\vec{k},\vec{k}'$ $\qquad$ $\vec{r},\vec{n}$

$$N\sum_{\vec{n}} \delta_{\vec{k}\vec{k}'}\, e^{-i\vec{k}\vec{n}} \underset{3D}{=} N\,\delta_{\vec{k}\vec{k}'}\overbrace{\left(e^{-ik_x l}+e^{ik_x l}+e^{-ik_y l}+e^{ik_y l}+e^{-ik_z l}+e^{ik_z l}\right)}^{\vec{r},\vec{n}} =$$

$$= 2N\,\delta_{\vec{k}\vec{k}'}\left(\cos(k_x l)+\cos(k_y l)+\cos(k_z l)\right)$$

$$\hat{H} = -2J\sum_{\vec{k}}\left(\cos(k_x l)+\cos(k_y l)+\cos(k_z l)\right)\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$$

$$\equiv \sum_{\vec{k}} \hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}} E_{\vec{k}}\,,\quad E_{\vec{k}} = -2J\left(\cos(k_x l)+\cos(k_y l)+\cos(k_z l)\right)$$

Continuum limit ($l\to 0$, i.e. $kl \ll 1$)

$$\hat{H} = -2J\sum_{\vec{k}}\Big(\underset{\text{Drop this}}{3} - \frac{(k_x l)^2}{2} - \frac{(k_y l)^2}{2} - \frac{(k_z l)^2}{2}\Big)\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$$

$$\longrightarrow J l^2 \sum_{\vec{k}}\left(k_x^2+k_y^2+k_z^2\right)\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}$$

Note: We did not consider spin. In general, electrons with spin ↑ and spin ↓ behave as 2 independent subsystems

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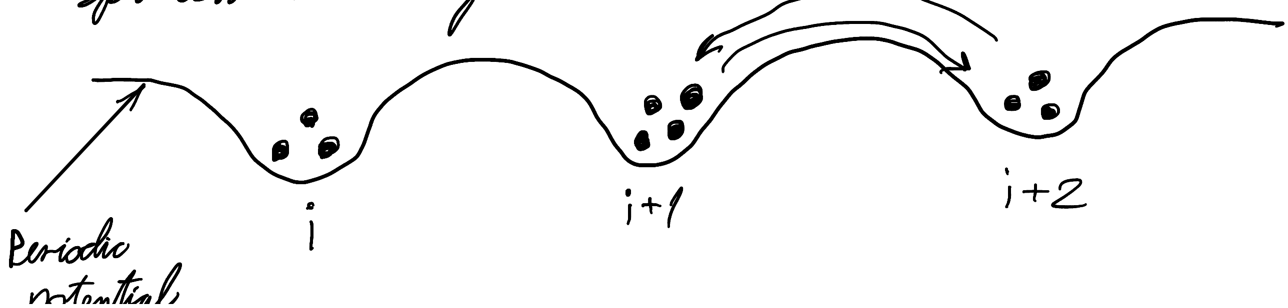
$\boxed{\text{Bose – Hubbard model}}$

Spinless interacting bosons on a lattice



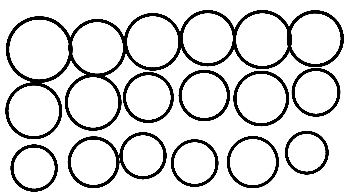
Periodic potential

The interaction energy on a site $\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i-1)-\mu\sum_i n_i$

$\hat{n}_i = b_i^+ b_i$ (an arbitrary quadratic function)

$$\hat{H}=\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i-1)-\mu\sum_i \hat{n}_i - t\sum_{\langle ij\rangle} b_i^+ b_j$$

Granulated superconductor



There are $\hat{N}_i$ Cooper pairs on each site (grain) i

The interaction energy $B(\hat{N}_i-N)^2$

Coulomb energy

(Cooper pair = a pair of electrons bound by interaction)

$$\hat{H}=B\sum_i(\hat{N}_i-N)^2 - t\sum_{\langle ij\rangle} b_i^+ b_j \quad ; \hat{N}_i = b_i^+ b_i$$

(Possibly explain superconductor - insulator transition)

Assume $t\to 0$, basically $t=0$

$|NN\ldots\rangle$ - ground state

$|NN\ldots N\ N{+}1\ N\ldots\rangle$ (or $N-1$) - energy B (degeneracy N)

$|\ldots N{+}1\ldots N{+}1\ldots\rangle$ - energy $2B$ (degeneracy $\frac{N!}{2!(N-2)!}=\frac{N(N-1)}{2}$)

$|NN\ldots N\ N{+}2\ N\ldots\rangle$ - energy $4B$ (degeneracy N)

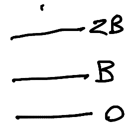
⋮

— 2B

— B

Sharp hugely degenerate levels

allow hopping



Sharp hugely degenerate levels

They get broadened if we allow hopping

Reduced space of excitations: 1 hopping boson

$$\mathcal{H}_{eff} = B - t\sum_{\langle i,j\rangle} b_i^+ b_j$$

(Fermionic) Hubbard model

$$\hat{H} = U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - t\sum_{\langle i,j\rangle,\sigma} \hat{a}^+_{i\sigma}\hat{a}_{j\sigma}$$

Consider a generic Hamiltonian with the kinetic energy and the potential energy and interactions between N particles. In the 1-st quantisation representation

$$\hat{H} = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\partial^2_{r_i} + V(\vec{r}_i)\right) + \frac{1}{2}\sum_{i\neq j} U(\vec{r}_i - \vec{r}_j)$$

acts on the many-body wavefunction $\Psi(\vec{r}_1, \dots, \vec{r}_N, t)$

In the second quantisation representation it has the form

$$\hat{H} = \sum_k \underbrace{\varepsilon_k}_{\frac{k^2}{2m}} \hat{a}^+_k a_k + \sum_{k,p} \hat{a}^+_k \hat{a}_p \int \psi_k^*(\vec{r}) V(\vec{r}) \psi_p(\vec{r})\, d\vec{r}$$

$$+ \frac{1}{2}\sum_{k_1,k_2,p_1,p_2} \hat{a}^+_{k_1}\hat{a}^+_{k_2}\hat{a}_{p_2}\hat{a}_{p_1} \int \psi^*_{k_1}(\vec{r})\psi^*_{k_2}(\vec{r}')U(\vec{r}-\vec{r}')\psi_{p_2}(\vec{r}')\psi_{p_1}(\vec{r})\, d\vec{r}\, d\vec{r}'$$

In a box of volume V with periodic boundary

$1 \quad ikr$

In a box of volume V with pe... conditions $\psi_k = \frac{1}{\sqrt{V}} e^{ikr}$

Fourier - transform the interaction term

$$\frac{1}{V^2}\int e^{-ir(k_1-p_1)} e^{ir'(p_2-k_2)} U(r-r')\, dr\, dr' =$$

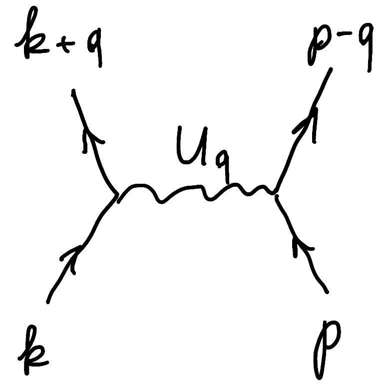
$$= \frac{1}{V^2}\int e^{-i(r-r')(k_1-p_1)} e^{ir'(p_1+p_2-k_1-k_2)} U(r-r')\, dr\, dr' =$$

$$= \frac{1}{V^2}\int e^{ir'(p_1+p_2-k_1-k_2)} dr' \int U(\xi) e^{-i\xi(k_1-p_1)} d\xi =$$

$$= \frac{1}{V}\, \delta_{p_1+p_2,\, k_1+k_2}\, U_{k_1-p_1}$$

$$\hat{H} = \sum_k \varepsilon_k \hat{a}_k^+ \hat{a}_k + \sum_{k,p} \hat{a}_k^+ \hat{a}_p \frac{1}{V} U_{k-p}$$

$$+ \frac{1}{2}\sum_{k,p,q} \hat{a}^+_{k+q} \hat{a}^+_{p-q} \hat{a}_p \hat{a}_k \frac{1}{V} U_q$$



<u>Ψ - operators</u>

It is often convenient to introduce Ψ-operators

$$\hat{\psi}(\vec{r}) = \sum_i \hat{a}_i \psi_i(\vec{r}) \quad \Big| = \frac{1}{\sqrt{V}}\sum_i \hat{a}_i e^{i\vec{k}\vec{r}}$$

$-i\vec{k}\vec{r}$

$$\hat{\psi}(\vec{r}) = \sum_i \hat{a}_i \, \psi_i(\vec{r}) \qquad = \frac{1}{\sqrt{V}} \sum_i \hat{a}_i \, e^{\dots}$$

$$\hat{\psi}^+(\vec{r}) = \sum_i \hat{a}_i^+ \, \psi_i^*(\vec{r}) \qquad = \frac{1}{\sqrt{V}} \sum_i \hat{a}_i^+ \, e^{-i\vec{k}\vec{r}}$$

Used often

The commutation relations:

*) Bosons

$$[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = \sum_{i,j} \psi_i(\vec{r}) \psi_j^*(\vec{r}\,') \underbrace{[\hat{a}_i, \hat{a}_j^+]}_{= \delta_{ij}} =$$

$$= \sum_i \psi_i(\vec{r}) \psi_i^*(\vec{r}\,') = \sum_i \langle \vec{r} | i \rangle \langle i | \vec{r}\,' \rangle \equiv \langle \vec{r} | \vec{r}\,' \rangle \to \delta(\vec{r} - \vec{r}\,')$$

$$\boxed{[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = \delta(\vec{r} - \vec{r}\,')}$$

*) Fermions

Similarly, $\boxed{\{\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')\} = \delta(\vec{r} - \vec{r}\,')}$

In terms of $\hat{\psi}$ and $\hat{\psi}^+$ the Hamiltonian is given by

$$\hat{H} = \int \left[- \hat{\psi}^+(\vec{r}) \frac{\partial_{\vec{r}}^2}{2m} \hat{\psi}(\vec{r}) + V(\vec{r}) \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}) \right] d\vec{r}$$

$$+ \frac{1}{2} \int \hat{\psi}^+(\vec{r}_1) \hat{\psi}^+(\vec{r}_2) \, U(\vec{r}_1 - \vec{r}_2) \, \hat{\psi}(\vec{r}_2) \hat{\psi}(\vec{r}_1) \, d\vec{r}_1 d\vec{r}_2$$

The naive expectation for the interaction term:

$$\frac{1}{2} \int \hat{\psi}^+(\vec{r}_1) \hat{\psi}(\vec{r}_1) \, U(\vec{r}_1 - \vec{r}_2) \, \hat{\psi}^+(\vec{r}_2) \hat{\psi}(\vec{r}_2) \, d\vec{r}_1 d\vec{r}_2$$

However, it allows for one particle to interact with

However, it allows for one particle to interact with itself. In order to disallow for that, we may rearrange the Ψ-operators in such a way that two Ψ^+s are followed by two Ψs.

The difference between the two operators will be just an effective shift of the chemical potential $\frac{1}{2}\int \hat{\Psi}^+(\vec{r})\, \hat{\Psi}(\vec{r})\, U(0)\, d\vec{r}$.