Part 2: Electrons in Solids

Comparison: Electrons and phonons

Movement of nuclei in a lattice

- Movement is confined around fixed positions
- Quasi-Momentum is in the 1BZ
- Ions are distinguishable, cannot be exchanged
- Solutions are Bosonic Quasiparticle in 1BZ only

Electrons in a periodic potential

- Wavefunction $\psi(x) = \langle x | \psi \rangle$ may extend over entire lattice
- Momentum can take any value
- Indistinguishable, can be exchanged
- Solutions are Fermionic Quasiparticle in "Bands"

“Second quantization”: description by creation and annhihilation operators

Recapitulation of Phonons: Bosonic description

Oscillator modes:

$$\hat{n} = \hat{a}\hat{a}^{\dagger} \qquad [\hat{a}^{\dagger}, \hat{a}] = 1$$

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^{+})^{n}|0\rangle$$

For general set of quantum numbers:

$$[\hat{a}^{\alpha}_{\vec{k}_1}, \hat{a}^{\beta\,\dagger}_{\vec{k}_2}] = \delta_{\alpha\beta}\delta_{\vec{k}_1\vec{k}_2}$$

$$\left\langle \hat{a}^{\alpha\,\dagger}_{\vec{k}_1}(0)\hat{a}^{\beta}_{\vec{k}_2}(t) \right\rangle = \delta_{\alpha,\beta}\delta_{\vec{k}_1,\vec{k}_2}\frac{e^{-it\omega^{\alpha}_{\vec{k}_1}}}{e^{\beta\hbar\omega^{\alpha}_{\vec{k}_1}}-1}$$

"Second quantization" for Fermions: annihilation and creation of particles with $\hat{c}_\alpha, \hat{c}_\alpha^\dagger$

Pauli Principle: $\hat{n}_\alpha = \hat{c}_\alpha^\dagger \hat{c}_\alpha$ can only be 0 or 1

Anticommutation: $\left\{\hat{c}_\alpha, \hat{c}_\beta^\dagger\right\} = \hat{c}_\alpha \hat{c}_\beta^\dagger + \hat{c}_\beta^\dagger \hat{c}_\alpha = \delta_{\alpha\beta}$

Basis states: $\left|\alpha\right\rangle = \hat{c}_\alpha^\dagger \left|0\right\rangle$

General single particles states: $\left|\psi\right\rangle = \sum_{\left|\alpha\right\rangle} \left|\alpha\right\rangle\left\langle\alpha\middle|\psi\right\rangle = \sum_{\left|\alpha\right\rangle} \psi_\alpha \left|\alpha\right\rangle$

Many-body wavefunctions are automatically anti-symmetric

For bosons and fermions: any single-particle operator can be expressed in terms of $\hat{b}_\alpha, \hat{b}_\alpha^\dagger$

We know: Operators are defined by their action on a basis $|\beta\rangle$

$$\hat{\Omega}|\psi\rangle = \sum_\beta \hat{\Omega}|\beta\rangle\langle\beta|\psi\rangle$$

$$\hat{\Omega} = \sum_{\alpha\beta} \Omega_{\alpha\beta}|\alpha\rangle\langle\beta| \quad \text{where} \quad \Omega_{\alpha\beta} = \langle\alpha|\hat{\Omega}|\beta\rangle$$

Now define:

$$\hat{\Omega} = \sum_{\alpha\beta} \Omega_{\alpha\beta}\hat{b}_\alpha^\dagger \hat{b}_\beta$$

Action of a single particle operator $\hat{\Omega} = \sum_{\alpha\beta} \Omega_{\alpha\beta} \hat{b}_\alpha^\dagger \hat{b}_\beta$

On a two (or more) particle state $|\alpha\beta\rangle = \hat{b}_\alpha^\dagger \hat{b}_\beta^\dagger |0\rangle$

Interactions: additional energy if two quantum numbers are occupied

$$\hat{H}_{\text{int}} = \sum_{\alpha\beta} H_{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta$$

General two-body operators:

Continuous quantum numbers $\left|\varphi\right\rangle = \int d^3\vec{r}\,\left|\vec{r}\right\rangle\left\langle\vec{r}\,\middle|\,\varphi\right\rangle = \int d^3\vec{r}\;\varphi(\vec{r})\left|\vec{r}\right\rangle$

Define fermionic field operators $\hat{\Psi}^\dagger(\vec{r})$ to create particle at position $\vec{r}$

$$\left|\vec{r}\right\rangle = \hat{\Psi}^\dagger(\vec{r})\left|0\right\rangle$$

Anti-commutation relations: $\left\{\hat{\Psi}(\vec{r}_1), \hat{\Psi}^\dagger(\vec{r}_2)\right\} = \delta(\vec{r}_1 - \vec{r}_2)$

Operators in continuous real space

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$

Expressed in terms of field operators:

$$\hat{H} = \int d^3\vec{r}\,\hat{\Psi}^\dagger(\vec{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\hat{\Psi}(\vec{r})$$

Momentum space and periodic potential $U(\vec{r}) = U(\vec{r} + \vec{R})$

Momentum states are plane waves: $$\left|\vec{p}\right\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\vec{r}\; e^{i\vec{p}\cdot\vec{r}/\hbar} \left|\vec{r}\right\rangle$$

Define momentum creation operators:

$$\hat{c}^\dagger(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{r}\; e^{i\vec{k}\cdot\vec{r}}\, \hat{\Psi}^\dagger(\vec{r})$$