

# Introduction to Second Quantization

Based on Pathria's Book, Chapter 11

About the Green Function, I refer to Altland & Simons' Book, Chapter 7  
and Subir Sachdev's Book, Chapter 7

# Algebra of Second Quantization

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- The commutation relation of the Boson creation-annihilation relation is defined as following:

$$[a_i, a_j] = 0$$

$$[a_i^\dagger, a_j^\dagger] = 0$$

$$[a_i, a_j^\dagger] = \delta_{ij}$$

- For Fermions, the commutation relation is altered by anti-commutation relation.
- Number of the particle is the product of creation operator and annihilation operator:

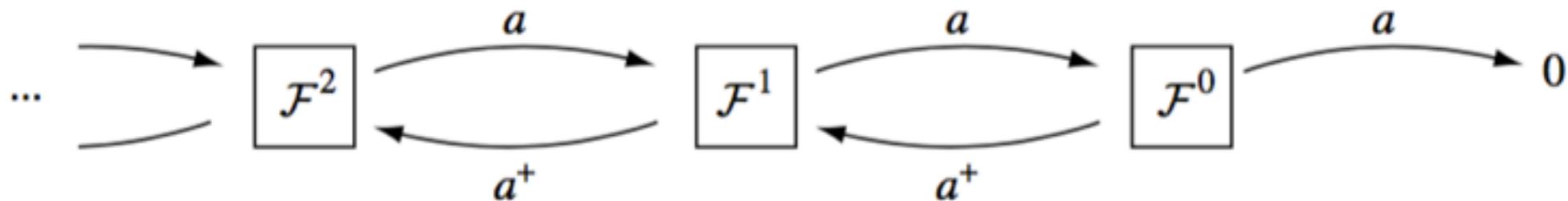
$$\hat{N} = \sum_i N_i = \sum_i a_i^\dagger a_i$$

# Algebra of Second Quantization

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- Vacuum state: State with no particles
- The creation-annihilation operators connects different subspace of the Fock space (the Hilbert space of many-body system)

$$a_i^\dagger |0\rangle = |i\rangle$$



- A many-body quantum state with determined particle number can be written as:

$$|\Psi\rangle = \prod_i \frac{1}{\sqrt{n_i!}} \left( a_i^\dagger \right)^{n_i} |0\rangle$$

# Algebra of Second Quantization

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- Representation transformation
- Suppose we have to orthonormal basis in the **single-particle Hilbert space**:

$$1 = \sum_i |i\rangle\langle i|$$

$$1 = \sum_\mu |\mu\rangle\langle \mu|$$

- One of the state can be expanded by another group of basis:

$$|\mu\rangle = \sum_i |i\rangle\langle i|\mu\rangle$$

$$a_\mu^\dagger |0\rangle = \sum_i \langle i|\mu\rangle a_i^\dagger |0\rangle \quad \Rightarrow \quad a_\mu^\dagger = \sum_i \langle i|\mu\rangle a_i^\dagger$$

- For example, the momentum representation and the real space representation

$$\psi^\dagger(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^\dagger \quad a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{V}} \int d^3x e^{i\mathbf{k}\cdot\mathbf{x}} \psi^\dagger(\mathbf{x})$$

# Algebra of Second Quantization

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- One-body operators
- Particle number operator

$$\hat{N} = \sum_i N_i = \sum_i a_i^\dagger a_i$$

- If we use the eigenstates of the operator  $\hat{O}$  , the second quantized form will be:

$$\hat{O} = \sum_i o_i a_i^\dagger a_i$$

- Do a representation transformation, then we get the result under arbitrary base state:

$$\hat{O} = \sum_{ij} \langle i | \hat{O}_1 | j \rangle a_i^\dagger a_j$$

# Examples of second quantization

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- Free electron system (plane wave, eigenstate of momentum)

$$H = \sum_{\mathbf{k}\sigma} \frac{\mathbf{k}^2}{2m} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$$

- Fermi Surface (Ground State of free electron gas)

$$|\text{FS}\rangle = \prod_{|\mathbf{k}| < k_F, \sigma} a_{\mathbf{k}\sigma}^\dagger |0\rangle$$

- Free electron gas in real space

$$H = \int d^3x \psi^\dagger(\mathbf{x}) \frac{-\nabla^2}{2m} \psi(\mathbf{x})$$

# Examples of second quantization

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- Tight Binding Approximation (Wannier function or Bloch momentum)

$$H = \sum_i \epsilon a_i^\dagger a_i + \sum_{\langle ij \rangle} (-t a_i^\dagger a_j + \text{h.c.})$$

$$a_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}}^\dagger \quad a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot\mathbf{R}_i} a_i^\dagger$$

- Energy band of 2D square lattice:

$$H = \sum_{\mathbf{k}} \{\epsilon - 2t [\cos(k_x a) + \cos(k_y a)]\} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

- What does the band of Graphene look like?

# Wave function and Schrödinger equation

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- Wave function is the inner product of a state with determined energy and particle number, and an eigenstate of many-body position

$$\psi_N(\mathbf{r}) = \frac{1}{\sqrt{N!}} \langle 0 | \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \cdots \psi(\mathbf{r}_N) | \psi_N \rangle$$

- why there is  $N!$  ?

$$\langle 0 | \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \cdots \psi(\mathbf{r}_N) \psi^\dagger(\mathbf{r}'_N) \cdots \psi^\dagger(\mathbf{r}'_2) \psi^\dagger(\mathbf{r}'_1) | 0 \rangle = \sum_{\mathcal{P}} \prod_i \delta^d(\mathbf{r}_i - \mathbf{r}'_{\mathcal{P}_i})$$

- Wave function is normalized:

$$\begin{aligned} & \int d^{3N}x \psi_N^*(\mathbf{x}_i) \psi_N(\mathbf{x}_i) \\ &= \frac{1}{N!} \int d^{3N}x \langle 0 | \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N) | \psi_N \rangle \langle \psi_N | \psi^\dagger(\mathbf{r}_N) \cdots \psi^\dagger(\mathbf{r}_1) | 0 \rangle \\ &= \frac{1}{N!} \int d^{3N}x \langle \psi_N | \psi^\dagger(\mathbf{r}_N) \cdots \psi^\dagger(\mathbf{r}_1) | 0 \rangle \langle 0 | \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N) | \psi_N \rangle \\ &= \frac{1}{N!} \int d^{3N}x \langle \psi_N | \psi^\dagger(\mathbf{r}_N) \cdots \psi^\dagger(\mathbf{r}_1) \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N) | \psi_N \rangle \\ &= \frac{1}{N!} \int d^{3N}x \langle \psi_N | \hat{N}(\hat{N}-1)(\hat{N}-2) \cdots | \psi_N \rangle \end{aligned}$$

# Wave function and Schrödinger equation

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- The wave function also satisfies the Schrödinger equation

$$\begin{aligned} E_N \psi_N(\mathbf{r}) &= \frac{1}{\sqrt{N!}} \langle 0 | \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N) \hat{H} | \psi_N \rangle \\ &= \frac{1}{\sqrt{N!}} \langle 0 | \sum_{i=1}^N \int d^3 \mathbf{r} \psi(\mathbf{r}_1) \cdots \\ &\quad \psi(\mathbf{r}_{i-1}) \delta(\mathbf{r} - \mathbf{r}_i) \psi(\mathbf{r}_{i+1}) \cdots \psi(\mathbf{r}_N) \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \psi(\mathbf{r}) | \psi_N \rangle \\ &= \frac{1}{\sqrt{N!}} \sum_{i=1}^N \left( -\frac{\hbar^2 \nabla_i^2}{2m} \right) \langle 0 | \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N) | \psi_N \rangle \\ &= \sum_{i=1}^N \left( -\frac{\hbar^2 \nabla_i^2}{2m} \right) \psi_N(\mathbf{r}) \end{aligned}$$

## \*Green function and spectrum function

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- Green Function is the grand canonical expectation value of creation-annihilation operators:

$$\langle T_\tau \psi(\mathbf{x}, \tau) \psi^\dagger(\mathbf{x}', \tau') \rangle \quad A(\mathbf{x}, \tau) = e^{\hat{H}\tau} A(\mathbf{x}) e^{-\hat{H}\tau}$$

- Fourier Transformation, we get Matsubara Frequencies.

$$C(i\omega_m) = \frac{1}{i\omega_m - \epsilon_{\mathbf{p}} + \mu}$$

- Lehmann Representation. By analytical continuum we can get the real time Retarded Green Function:

$$C^+(\mathbf{k}, \omega) = \frac{1}{\omega + i\delta - \epsilon_{\mathbf{k}} + \mu}$$

## \*Green function and spectrum function

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- Green function is an important tool to describe the many-body system.
- **Linear response** is a Retarded Green function, it is measurable quantity. And its analytical properties are also interesting.

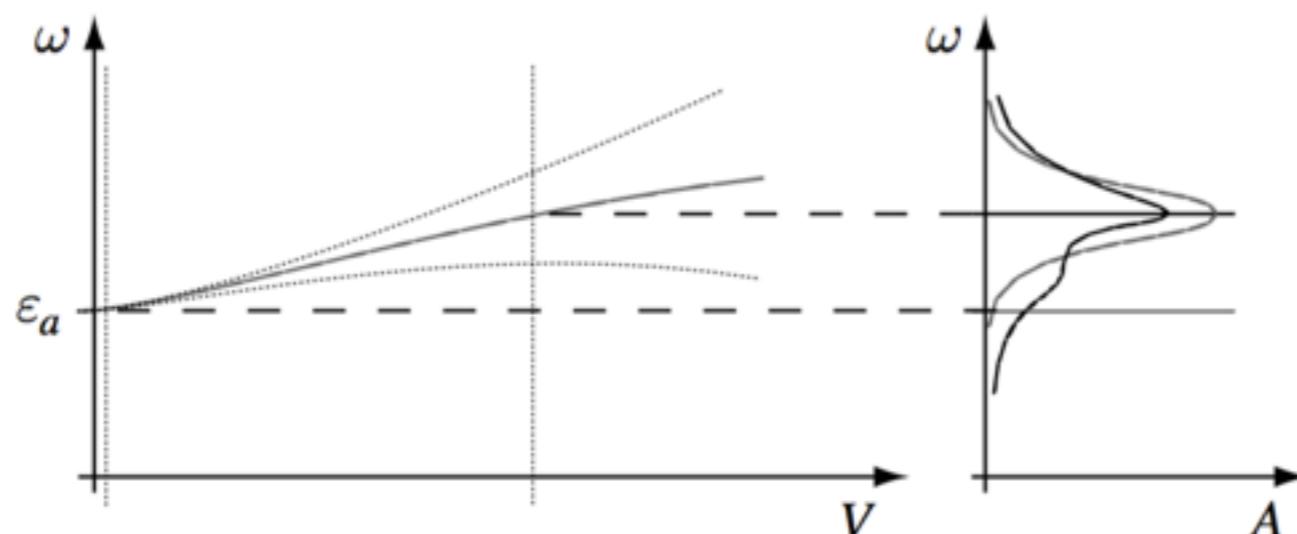
$$C^+(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = -i\Theta(t_1 - t_2)\langle [X_1(\mathbf{r}_1, t_1), X_2(\mathbf{r}_2, t_2)] \rangle$$

- Fourier Transformation of a free particle system

$$C^+(\mathbf{k}, \omega) = \frac{1}{\omega + i\delta - \epsilon_{\mathbf{k}} + \mu}$$

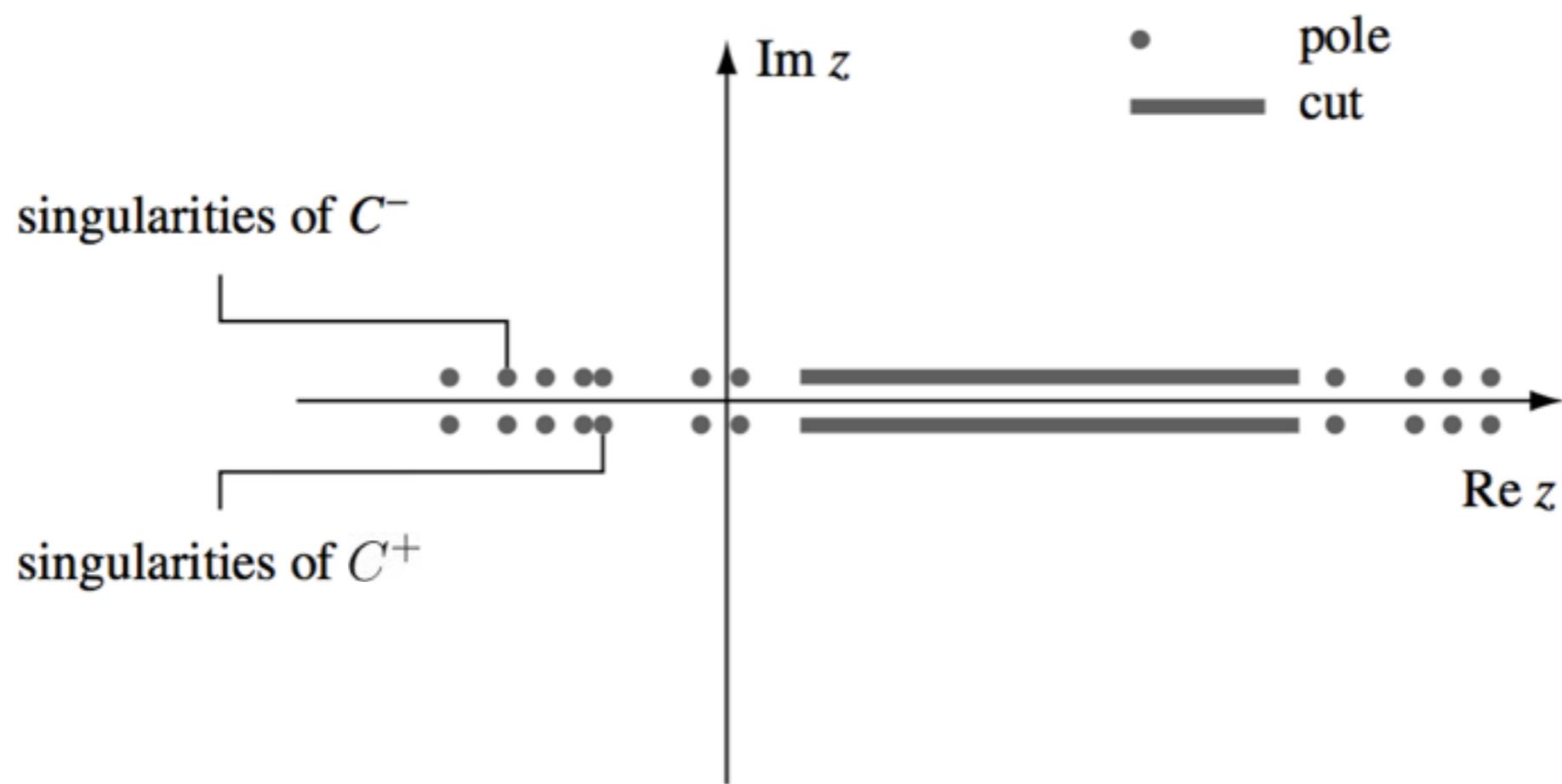
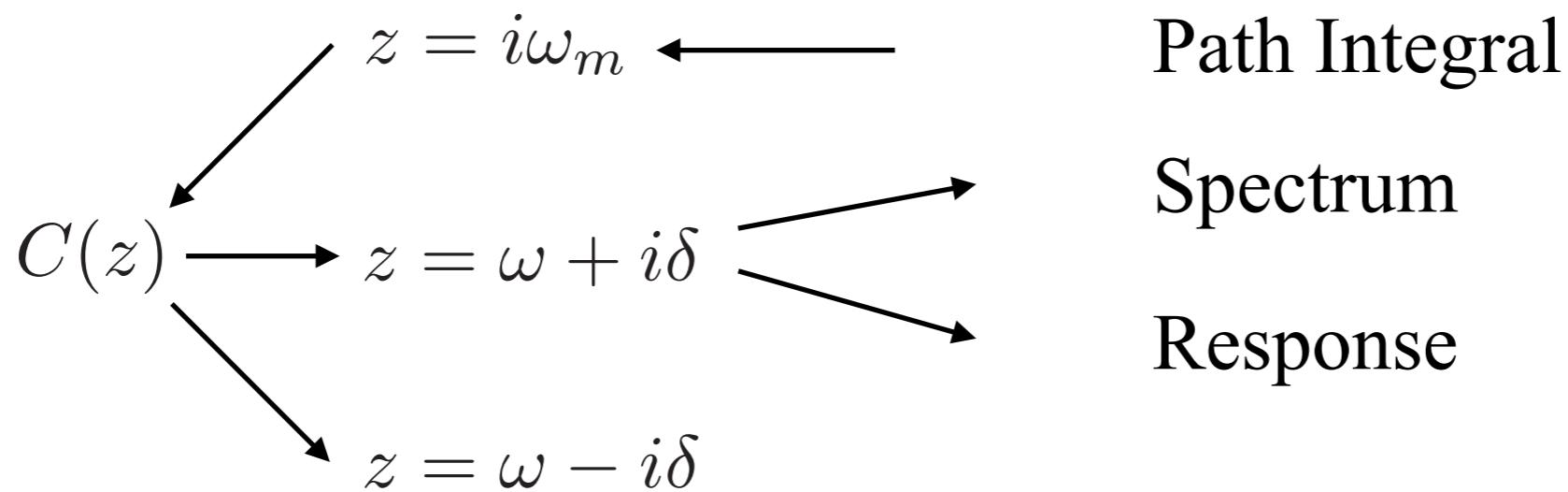
- Its imaginary part is the energy spectrum:

$$A(\mathbf{k}, \omega) = -2\Im C^+(\mathbf{k}, \omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}})$$



# \*Green function and spectrum function

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# Interacting System

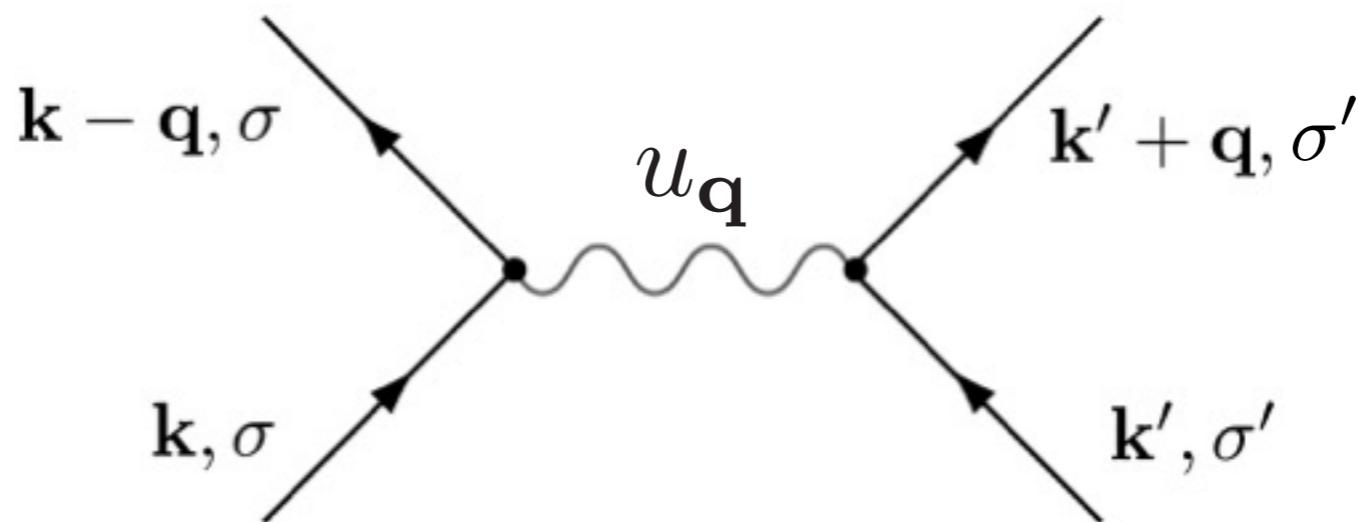
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- Potential energy operator

$$\hat{V} = \frac{1}{2} \int d^3x d^3y u(\mathbf{x} - \mathbf{y}) \rho(\mathbf{x}) \rho(\mathbf{y})$$

- Fourier transformation of the interacting potential

$$H = \sum_{\mathbf{k}\sigma} \frac{\mathbf{k}^2}{2m} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2L^3} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} u_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}\sigma}^\dagger a_{\mathbf{k}'-\mathbf{q}\sigma'}^\dagger a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma}$$



# Low temperature behaviour of imperfect Bose gas

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- Scattering length and  $\mathbf{q}=0$  approximation
- Scattering length is the Fourier transformation of the potential:

$$a(\mathbf{q}) = \frac{m}{4\pi\hbar^2} \int d^3x u(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}}$$

- If we neglect all the term with non-zero momentum transfer (**Maybe that's just the result of pseudo-potential approximation**)

$$H = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{2\pi a\hbar^2}{mV} \left[ \sum_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}^\dagger a_{\mathbf{p}} a_{\mathbf{p}} + \sum_{\mathbf{p}_1 \neq \mathbf{p}_2} (a_{\mathbf{p}_1}^\dagger a_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_2} a_{\mathbf{p}_1} + \textcircled{a_{\mathbf{p}_1}^\dagger a_{\mathbf{p}_2}^\dagger a_{\mathbf{p}_1} a_{\mathbf{p}_2}}) \right]$$

- The energy of the system is the function of  $\{n_{\mathbf{p}}\}$

$$E\{n_{\mathbf{p}}\} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} n_{\mathbf{p}} + \frac{2\pi a\hbar^2}{mV} \left[ 2N^2 - N - \sum_{\mathbf{p}} n_{\mathbf{p}}^2 \right]$$

# Low temperature behaviour of imperfect Bose gas

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- The energy of the system is the function of  $\{n_{\mathbf{p}}\}$ . Notice that  $N^2 \gg N$

$$E\{n_{\mathbf{p}}\} = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} n_{\mathbf{p}} + \frac{2\pi a \hbar^2}{mV} \left[ 2N^2 - \sum_{\mathbf{p}} n_{\mathbf{p}}^2 \right]$$

- Zero temperature
- So the ground state is given by:

$$n_{\mathbf{p}} = \begin{cases} 0 & \mathbf{p} \neq 0 \\ N & \mathbf{p} = 0 \end{cases}$$

$$E_0 = \frac{2\pi a \hbar^2 N^2}{mV} \quad P_0 = - \left( \frac{\partial E_0}{\partial V} \right)_N = \frac{2\pi a \hbar^2 N^2}{V^2}$$

$$c_0^2 = \frac{dP_0}{d\rho_m} = \frac{1}{m} \frac{dP_0}{dn} = \frac{4\pi a \hbar^2 n}{m^2} \quad \mu_0 = \left( \frac{\partial E_0}{\partial N} \right)_V = \frac{4\pi a \hbar^2 N}{mV}$$

# Low temperature behaviour of imperfect Bose gas

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- Finite temperature
- We can use the particle number of BEC to estimate the interacting energy.
- The partition function:

$$Q_N(V, T) = \sum_{\{n_{\mathbf{p}}\}} \exp \left[ -\beta \left( \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} n_{\mathbf{p}} + \frac{2\pi a \hbar^2}{mV} (2N^2 - n_0^2) \right) \right]$$

$$\frac{n_0}{N} = 1 - \left( \frac{T}{T_c} \right)^{3/2}$$

- Use these equations, we can get the Helmholtz Free energy:

$$A(N, V, T) = A_{id}(N, V, T) + \frac{2\pi a \hbar^2 N^2}{mV} \left[ 1 + 2 \left( \frac{T}{T_c} \right)^{3/2} - \left( \frac{T}{T_c} \right)^3 \right]$$

$$A(N, V, T) = A_{id}(N, V, T) + \frac{2\pi a \hbar^2 N}{m} \left( \frac{1}{v} + \frac{2}{v_c} - \frac{v}{v_c^2} \right)$$

# Low temperature behaviour of imperfect Bose gas

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$$A(N, V, T) = A_{id}(N, V, T) + \frac{2\pi a \hbar^2 N}{m} \left( \frac{1}{v} + \frac{2}{v_c} - \frac{v}{v_c^2} \right)$$

- Chemical potential and transition chemical potential

$$\mu = \mu_{id} + \frac{4\pi a \hbar^2}{m} \left( \frac{1}{v} + \frac{1}{v_c} \right)$$

$$\mu_c = \frac{8\pi a \hbar^2}{m \lambda_T^3} \zeta \left( \frac{3}{2} \right)$$

- When the temperature is zero, the result is the same as we obtained earlier.

## \*Interactions on ultracold atomic Bose–Einstein condensates

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- Quantum gas in a magnetic trap. Gross-Pitevskii energy functional

$$E\{\Psi(\mathbf{x})\} = \int d^3x \left[ \frac{\hbar^2}{2m} |\nabla\Psi(\mathbf{x})|^2 + V(\mathbf{x})|\Psi(\mathbf{x})|^2 + \frac{2\pi a\hbar^2}{m} |\Psi(\mathbf{x})|^4 \right]$$

- Gross-Pitevskii equation

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{x}) + V(\mathbf{x})\Psi(\mathbf{x}) + \frac{4\pi a\hbar^2}{m} |\Psi(\mathbf{x})|^2 \Psi(\mathbf{x}) = \mu \Psi(\mathbf{x})$$

- If we neglect the kinetic term, the configuration of field  $\Psi(\mathbf{x})$  will be:

$$\Psi(\mathbf{x}) = \sqrt{\frac{\mu - V(\mathbf{x})}{u_0}}$$

- particle number and energy will be:

$$N = \frac{8\pi}{15} \left( \frac{2\mu}{m\omega_0^2} \right)^{3/2} \frac{\mu}{u_0} \quad E = \frac{5}{7} \mu N$$

- Feshbach Resonance

# Low lying states of an imperfect Bose gas

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- Consider the terms with non-zero momentum transfer:

$$\sum_{\mathbf{p} \neq 0} u(\mathbf{p}) \left( a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_{\mathbf{p}} a_{-\mathbf{p}} \right)$$

- Since we are considering about the low lying properties, the operators  $a_0^\dagger$  and  $a_0$  can be treated as complex numbers:

$$a_0 = a_0^\dagger = \sqrt{N}$$

- The interacting potential  $u(\mathbf{p})$  can be considered as a constant  $u_0/V$
- Interaction term is a 4-operator product, and since the single particle ground state is macroscopically occupied, we can neglect all the terms with more than 2 operators with  $\mathbf{p} \neq 0$ .

# Low lying states of an imperfect Bose gas

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- So the effective Hamiltonian will be:

$$H = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{u_0}{2V} \left[ N^2 + N \sum_{\mathbf{p} \neq 0} (2a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}}) \right]$$

- Scattering length: second order perturbation, we get the relation between the scattering length and interaction term (**T-Matrix?**) :

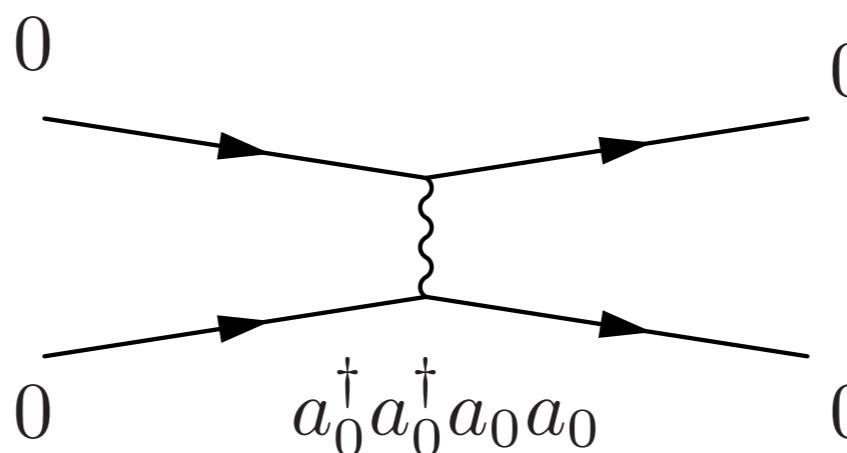
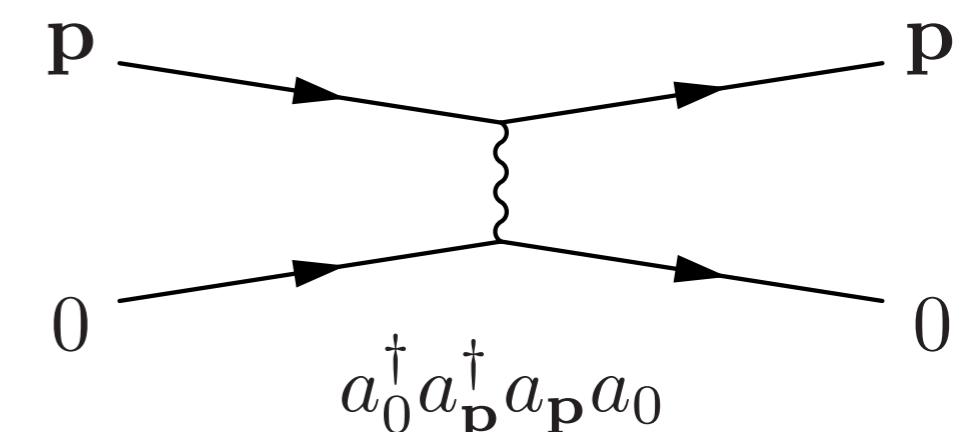
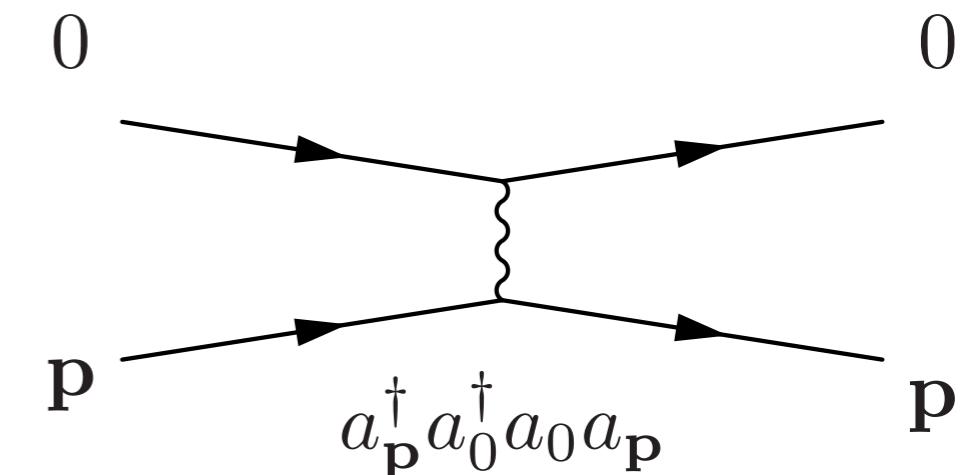
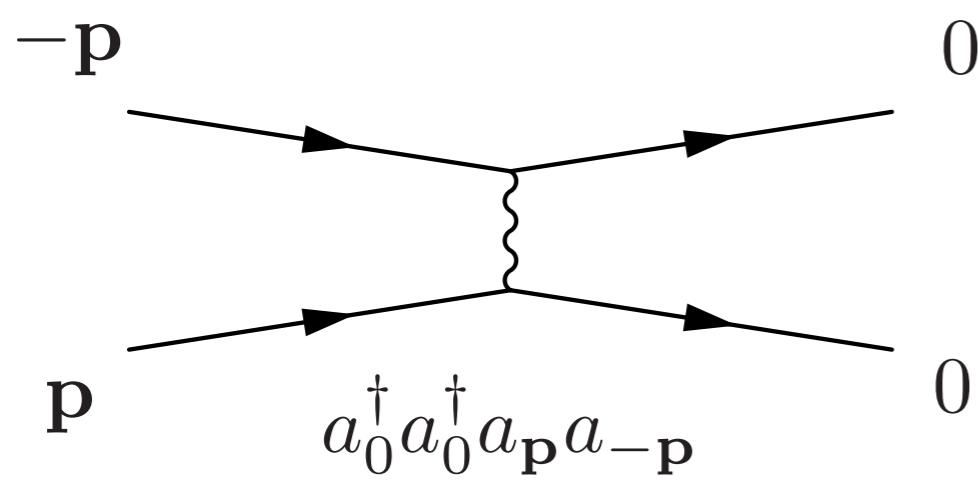
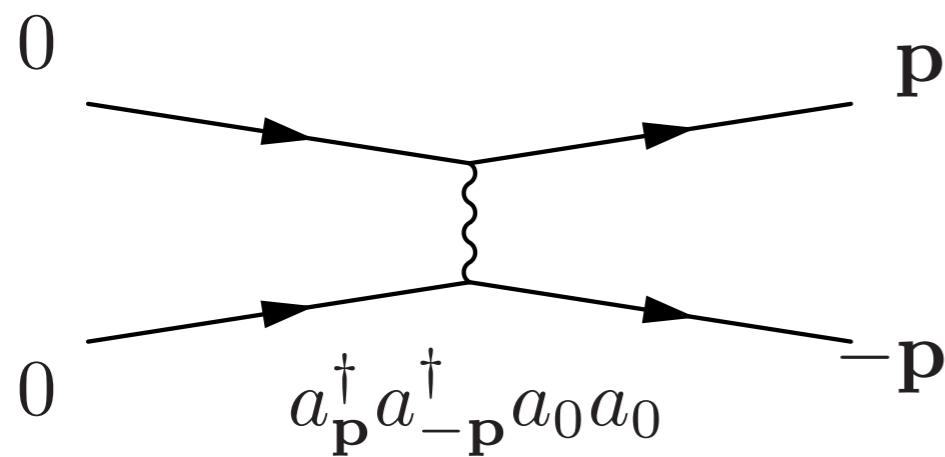
$$u_0 \simeq \frac{4\pi a \hbar^2}{m} \left( 1 + \frac{4\pi a \hbar^2}{V} \sum_{\mathbf{p} \neq 0} \frac{1}{p^2} \right)$$

- Use the scattering length to rewrite the Hamiltonian:

$$\begin{aligned} H &= \frac{2\pi a \hbar^2}{m} \frac{N^2}{V} \left( 1 + \frac{4\pi a \hbar^2}{V} \sum_{\mathbf{p} \neq 0} \frac{1}{\mathbf{p}^2} \right) \\ &\quad + \frac{2\pi a \hbar^2 N}{m V} \sum_{\mathbf{p} \neq 0} (2a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{\mathbf{p}} a_{-\mathbf{p}}) + \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \end{aligned}$$

# Low lying states of an imperfect Bose gas

- Terms we want:



# Low lying states of an imperfect Bose gas

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- Bogoliubov transformation

$$\Psi_{\mathbf{p}} = \begin{pmatrix} a_{\mathbf{p}} \\ a_{-\mathbf{p}}^\dagger \end{pmatrix} \quad U^\dagger \Psi_{\mathbf{p}} = \begin{pmatrix} b_{\mathbf{p}} \\ b_{-\mathbf{p}}^\dagger \end{pmatrix} \quad \Lambda = U^\dagger H U$$

- Then diagonalize the matrix in the Hamiltonian and we can get the dispersion relation of the quasiparticle.

$$\epsilon(\mathbf{p}) = \sqrt{\left(\frac{\mathbf{p}^2}{2m}\right)^2 + \frac{4\pi a \hbar^2 N}{mV} \frac{\mathbf{p}^2}{m}}$$

$$H = E_0 + \sum_{\mathbf{p} \neq 0} \epsilon(\mathbf{p}) b_{\mathbf{p}}^\dagger b_{\mathbf{p}}$$

- We can also find the ground state of the system. The calculation is trivial but complicated.

$$E_0 = \frac{2\pi a \hbar^2 N^2}{mV} \left[ 1 + \frac{128}{15\pi^{1/2}} (na^3)^{1/2} \right]$$

# Low lying states of an imperfect Bose gas

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- The Ground state of the quasi particle system is defined as

$$b_{\mathbf{p}}|\Phi_0\rangle = 0$$

- So the occupying number of real particle is

$$\sum_{\mathbf{p} \neq 0} \langle \Phi_0 | a_{\mathbf{p}}^\dagger a_{\mathbf{p}} | \Phi_0 \rangle = N \frac{8}{(3\pi)^{1/2}} (na^3)^{1/2}$$

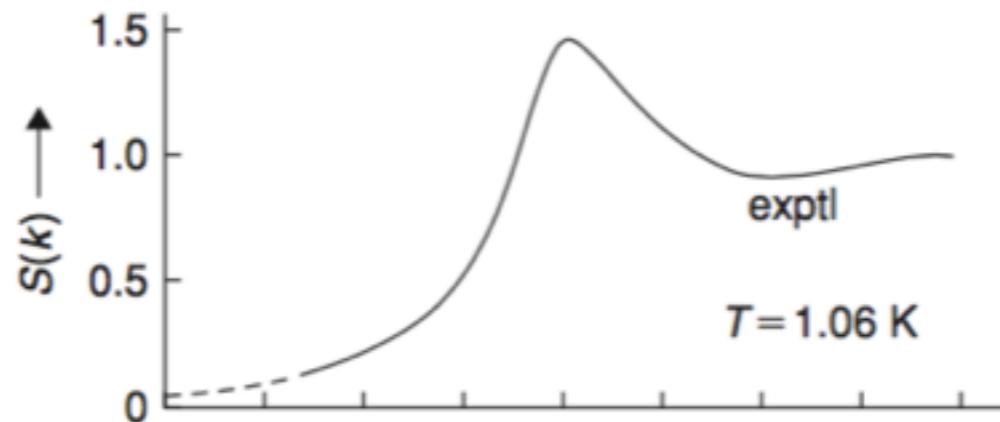
- That means at zero temperature, the occupying number on “excited state” is not zero.

# Spectrum of a Bose liquid

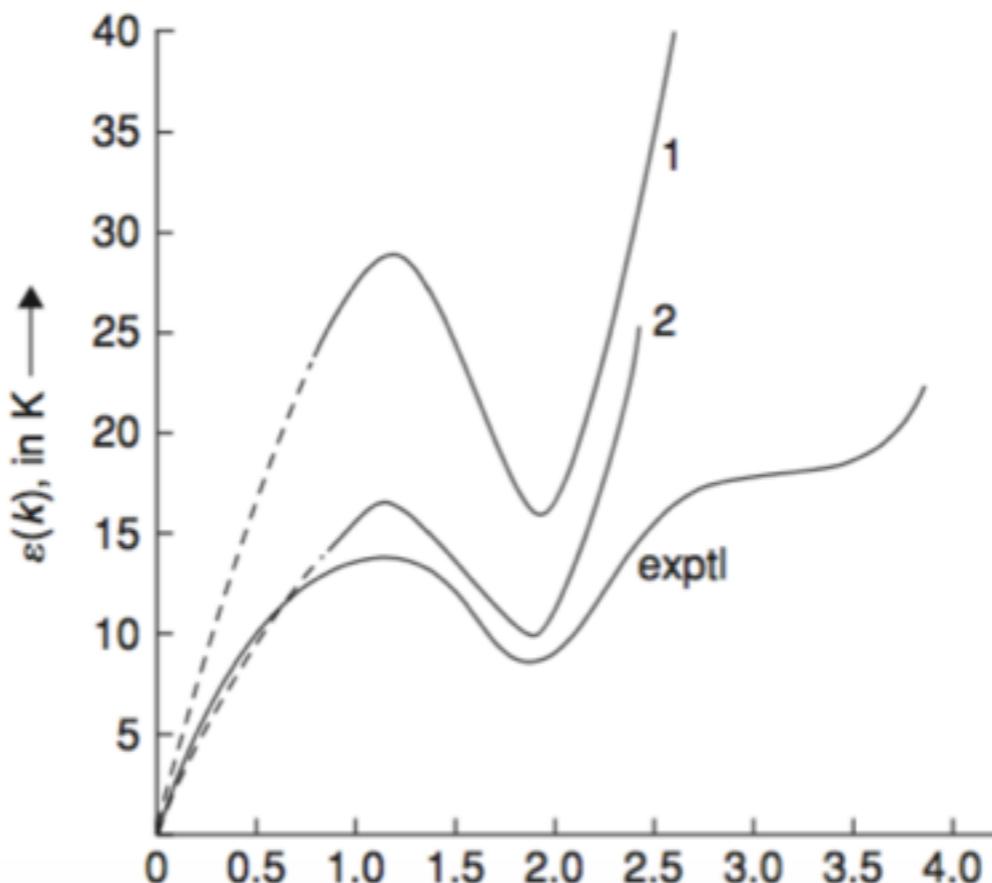
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$$\epsilon(\mathbf{p}) = \sqrt{\left(\frac{\mathbf{p}^2}{2m}\right)^2 + \frac{4\pi a \hbar^2 N}{mV} \frac{\mathbf{p}^2}{m}}$$

- Speed of sound wave
- No roton in the spectrum
- Feynman's approach



$$\epsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2mS(\mathbf{k})}$$



# States with quantized circulation

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- Wave function of uniform liquid Helium-4:

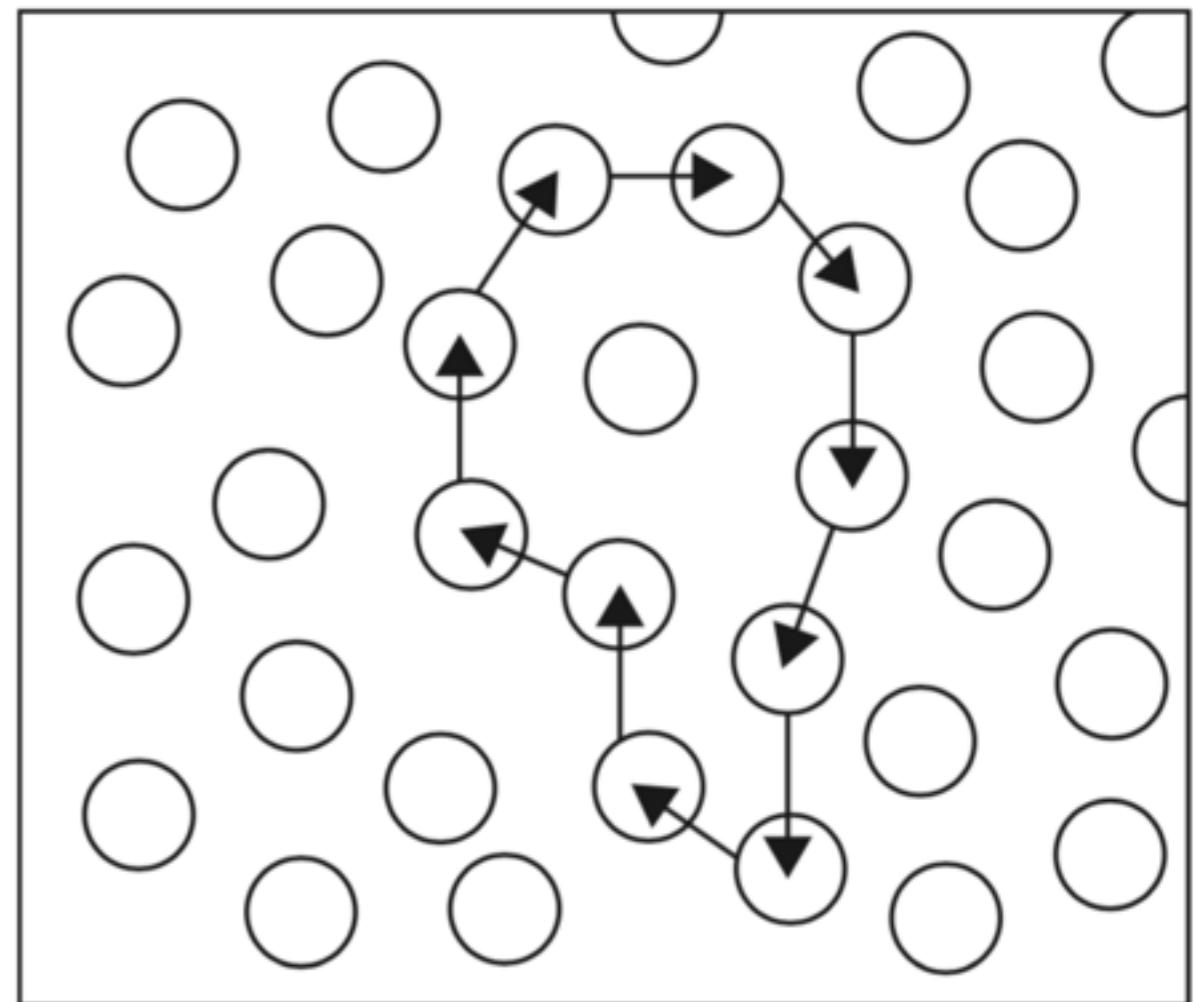
$$\Psi = \Phi e^{i\mathbf{P}_s \cdot \mathbf{R}_s}$$

- If the atoms have a displacement, the phase will change:

$$\Delta\phi = \frac{m}{\hbar} \sum_i \mathbf{v}_i \cdot \Delta\mathbf{r}_i$$

- Take the continuum limit, we get a loop integral. Since the particles are identical, the phase change should be:

$$\frac{m}{\hbar} \oint d\mathbf{r} \cdot \mathbf{v} = 2n\pi$$



- If there is no singularities in the integral loop, we will find that

$$\nabla \times \mathbf{v} = 0$$

# States with quantized circulation

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- Singularities: classical vortex and velocity distribution ( $a$  is the short distance cut-off)

$$\frac{\varepsilon}{L} \sim \frac{n_0 h^2}{4\pi m} \ln \left( \frac{R}{a} \right)$$

- Quantum mechanical case of the vortex:

$$\psi = n^{* \frac{1}{2}} e^{is\phi} f(\rho)$$

- Schrödinger equation

$$\left( -\frac{\hbar^2 \nabla^2}{2m} + u_0 |\psi|^2 \right) \psi = \varepsilon \psi$$

- Solution to the equation:

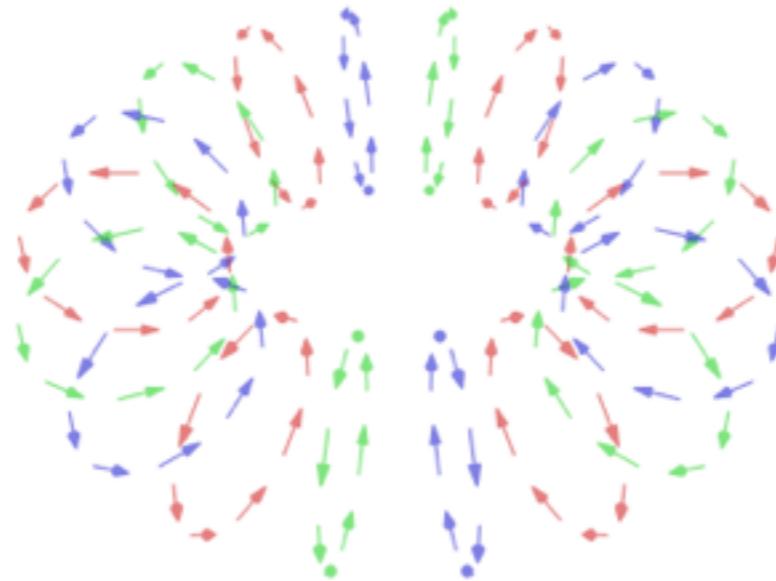
$$f_s(\rho) \sim \rho^s \quad \rho \rightarrow 0$$

$$f_s(\rho) \sim 1 - \frac{s^2}{2\rho'^2} \quad \rho \rightarrow \infty, \rho' = \frac{\rho}{(8\pi a n^*)^{-1/2}} \quad l = (8\pi a n^*)^{-1/2}$$

# Vortex ring and breakdown of superfluidity

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- Vortex lines may not be straight, they may become a ring:



- It moves in the direction perpendicular to the ring plane

$$v \sim \frac{\hbar}{2mr}$$

- The energy of the (classical) vortex ring will be:

$$\varepsilon \sim \frac{n_0 h^2}{2m} r \ln \left( \frac{r}{l} \right)$$

# Vortex ring and breakdown of superfluidity

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- So the velocity-energy relation can be written as:

$$\varepsilon v \sim \frac{n_0 h^3}{8\pi m^2}$$

- If we treat the velocity as the group velocity, the dispersion relation should satisfy:

$$v = \left( \frac{\partial \varepsilon}{\partial p} \right)$$

- So the momentum of the vortex ring is

$$p \sim n_0 h \pi r^2$$

- The critical speed is given by Landau's criterion (See chapter 7)

$$v_c = \left( \frac{\epsilon}{p} \right)_{\min}$$

# Vortex ring and breakdown of superfluidity

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- We can find the critical speed is:

$$v_c = \left( \frac{\epsilon}{p} \right)_{\min} \sim \left[ \frac{\hbar}{mr} \ln \left( \frac{r}{l} \right) \right]_{\min} = \frac{\hbar}{mR} \ln \left( \frac{R}{l} \right)$$

- In chapter 7 we have find that the critical speed we get from the spectrum of phonon is too large, but result we get from the spectrum of vortex ring satisfies good with experimental datas.