Advanced Quantum Mechanics

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Lecture #14

Quantum Mechanics of Many Particles

Recap of Last Class

Multi Electron Atoms: The Case of Carbon

Occupation No. and Fock space

Creation Annihilation Operators

Writing Many Body States with creation annihilation operators

Writing Many Body Operators with creation annihilation operators

Operators in 2nd Quantized Notation

1 particle operators $\hat{A} = \sum_i \hat{A}_i$

Generic 1-particle operator: $\hat{A}_i = \sum_{\alpha\beta} A_{\alpha\beta} |\alpha\rangle_i \; _i\langle\beta|$

where α and β are single particle states.

Let $\hat{A}_i = |\alpha\rangle_i \; _i\langle\beta|$

$$\hat{A}|\beta_1, ...\beta_i, ...\beta_N\} = \sum_i |\beta_1, ...\alpha_i....\beta_N\} = a^\dagger_\alpha a_\beta |\beta_1, ...\beta_i, ...\beta_N\}$$

So, for the generic case

$$\boxed{\hat{A} = \sum_{\alpha\beta} A_{\alpha\beta} a^\dagger_\alpha a_\beta}$$

Some Important examples:

Identity Operator $A_{\alpha\beta} = \delta_{\alpha\beta}$ → $\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha$ Total Number Operator

Real Space Density $\delta(x - x_i)\delta(x_i - x'_i)$ → $\hat{\rho}(x) = a^\dagger_x a_x$

Kinetic Energy: $\sum_p \frac{p^2}{2m} a^\dagger_p a_p$

External Potential: $\sum_x U(x) a^\dagger_x a_x = \sum_x U(x) \hat{\rho}(x)$

Operators in 2nd Quantized Notation

Hamiltonian of a non-interacting many particle system, each moving in an external potential

$$\hat{H} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \sum_x U(x) a_x^\dagger a_x$$

How does the creation/annihilation operators change with change in the SP basis?

Work with $\hat{A} = \sum_{\alpha\beta} A_{\alpha\beta} a_\alpha^\dagger a_\beta$

Change basis from {| α >} to {|m>} $\hat{A}_i = \sum_{\alpha\beta} A_{\alpha\beta} |\alpha\rangle_i \, {}_i\langle\beta| = \sum_{mn} \sum_{\alpha\beta} A_{\alpha\beta} \langle m|\alpha\rangle_i \langle\beta|n\rangle_i |m\rangle_i \, {}_i\langle n|$

$$\hat{A} = \sum_{mn} a_m^\dagger a_n \sum_{\alpha\beta} A_{\alpha\beta} \langle m|\alpha\rangle\langle\beta|n\rangle$$

Let $A_{\alpha\beta} = 1$

$$\hat{A} = \sum_\alpha a_\alpha^\dagger \sum_\beta a_\beta = \sum_\alpha \sum_m a_m^\dagger \langle m|\alpha\rangle \sum_\beta \sum_n a_n \langle\beta|n\rangle$$

So $a_\alpha^\dagger = \sum_m a_m^\dagger \langle m|\alpha\rangle$

Operators in 2nd Quantized Notation

$$a_\alpha^\dagger = \sum_m a_m^\dagger \langle m|\alpha\rangle \qquad a_p^\dagger = \sum_x a_x^\dagger \langle x|p\rangle = \sum_x a_x^\dagger e^{ip\cdot x}$$

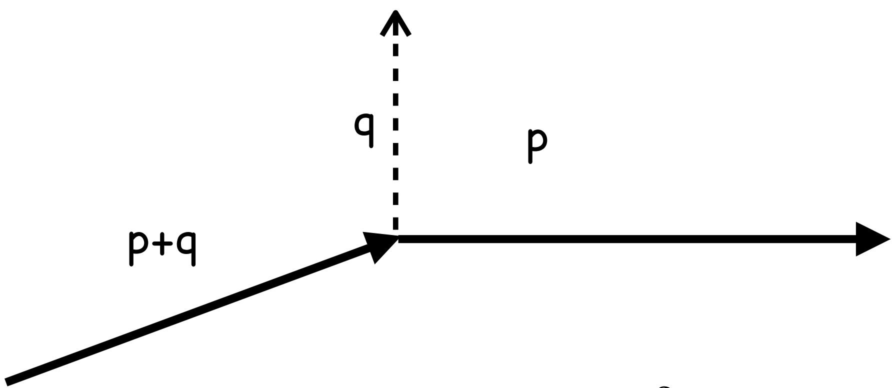
Hamiltonian of a non-interacting many particle system, each moving in an external potential

$$\hat{H} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \sum_x U(x) a_x^\dagger a_x$$

Momentum is not conserved !!

2nd term in H: $$\sum_x U(x) a_x^\dagger a_x = \sum_{pp'} a_p^\dagger a_{p'} \sum_x U(x) e^{i(p'-p)x} = \sum_{pq} U(q) a_p^\dagger a_{p+q}$$

Potential scatters a particle from momentum state p+q to momentum state p with amplitude U(q)



So, $$\hat{H} = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \sum_{pq} U(q) a_p^\dagger a_{p+q}$$

Operators in 2nd Quantized Notation

2-particle operators in 1st Quantized notation

$$\hat{B} = \sum_{i \neq j} \hat{B}_{ij} \qquad \hat{B}_{ij} = \sum_{\alpha\beta\gamma\delta} B^{\alpha\beta}_{\gamma\delta} |\alpha\rangle_i |\beta\rangle_j \; {}_j\langle\gamma|_i\langle\delta|$$

Using arguments similar to 1 part. operators:

$$\hat{B} = \sum_{\alpha\beta\gamma\delta} B^{\alpha\beta}_{\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta$$

Example: pairwise interaction between particles

$$\hat{V} = \sum_{xx'} V(x - x') a^\dagger_x a^\dagger_{x'} a_{x'} a_x$$

Interaction between particles with internal states

$$\hat{V} = \sum_{\alpha\beta\gamma\delta} \sum_{xx'} V^{\alpha\beta}_{\gamma\delta}(x - x') a^\dagger_{x\alpha} a^\dagger_{x'\beta} a_{x'\gamma} a_{x\delta}$$

Example: Coulomb Interaction between spinful Fermions

$$\hat{V} = \frac{e^2}{4\pi\varepsilon_0} \sum_{xx'\sigma\sigma'} \frac{1}{|x - x'|} a^\dagger_{x\sigma} a^\dagger_{x'\sigma'} a_{x'\sigma'} a_{x\sigma}$$

A bit of Stat Mech

Where does this separation occur ?

If all the eigenstates and eigenenergies of the many-body Hamiltonian are known

construct the thermal density matrix $\hat{\rho}(T) = \sum_n e^{-\beta E_n} |n\rangle\langle n|$ β = 1/T

Beyond QM expectation, avg. over thermal ensemble with the Boltzmann weight

$$\langle \hat{A} \rangle_T = Tr \hat{\rho}(T) \hat{A} = \sum_n e^{-\beta E_n} \langle n|\hat{A}|n\rangle$$

This is different from QM, where you add amplitudes of different terms

T = 0 ⟶ only contribution from the ground state

low T ⟶ only contribution from low energy excitations (E ~ T)

high T ⟶ system behaves classically

density $\rho = \frac{N}{V} \rightarrow l = n^{-1/d}$

inter-particle distance

A quantum particle confined within l has a kinetic energy $E_Q = \frac{\hbar^2}{2ml^2}$

$$k_B T_Q = \frac{\hbar^2 n^{2/d}}{2m}$$

QM is important to describe the system for $T < T_Q$

A bit of Thermodynamics

Internal Energy U $$U = \langle H \rangle_T = \sum_n E_n e^{-\beta E_n}$$

At T=0, U is just the energy of the ground state.

$$dU = TdS - pdV \qquad p = -\left(\frac{\partial U}{\partial V}\right)_N = -\left(\frac{\partial U}{\partial \rho}\right)_N \left(\frac{\partial \rho}{\partial V}\right)_N = \rho^2 \left(\frac{\partial (U/N)}{\partial \rho}\right)_N$$

So, at T=0, we can calculate pressure of the gas if GS energy is known for all densities

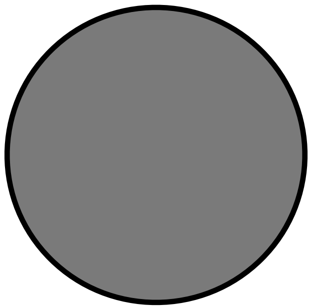
Inverse Compressibility $$B = \frac{1}{K} = -V\left(\frac{\partial P}{\partial V}\right)_N = \rho \left(\frac{\partial P}{\partial \rho}\right)_N$$

Chemical Potential $$\mu = \left(\frac{\partial U}{\partial N}\right)_V = \left(\frac{\partial (U/V)}{\partial \rho}\right)_V$$

At finite T, $$C_V = \left(\frac{\partial (U/V)}{\partial T}\right)_V$$

Non-interacting Fermions

$$H = \sum_{k\sigma} \frac{k^2}{2m} c^\dagger_{k\sigma} c_{k\sigma}$$



Ground State of N non-interacting free Fermions

Filled Fermi Sea $\quad |\psi\rangle = \prod_{\sigma,|k|<k_F} c^\dagger_{k\sigma}|0\rangle \qquad k_F^3 = 3\pi^2 \frac{N}{V}$

Fermi Surface: Surface separating the filled states from empty states

Fermi Energy: Energy of the states at the Fermi surface, or highest energy of filled state

$$\epsilon_F = \frac{k_F^2}{2m}$$

Ground State Energy: $\quad E = \sum_k \frac{k^2}{2m} \langle\psi|c^\dagger_{k\sigma} c_{k\sigma}|\psi\rangle$ $\qquad$ Consider 3D

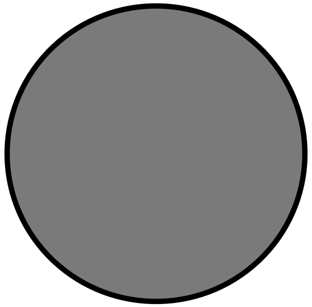
$$\frac{U}{V} = 2\int \frac{d^3k}{(2\pi)^3} \Theta(k_F - |k|) \frac{k^2}{2m} = \frac{1}{\pi^2}\int_0^{k_F} dk k^2 \frac{k^2}{2m} = \frac{k_F^5}{10\pi^2 m}$$

$$= \frac{(3\pi^2\rho)^{5/3}}{10\pi^2 m}$$

$$\frac{U}{N} = \frac{3}{10m}(3\pi^2\rho)^{2/3}$$

Non-interacting Fermions

$$H = \sum_{k\sigma} \frac{k^2}{2m} c^\dagger_{k\sigma} c_{k\sigma}$$



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Filled Fermi Sea $\quad |\psi\rangle = \prod_{\sigma, |k|<k_F} c^\dagger_{k\sigma} |0\rangle \qquad k_F^3 = 3\pi^2 \frac{N}{V}$

$$\frac{U}{N} = \frac{3}{10m}(3\pi^2\rho)^{2/3} = \frac{3}{5}\epsilon_F$$

$$P = \rho^2 \left(\frac{\partial (U/N)}{\partial \rho} \right)_N = \frac{3}{10m}\frac{2}{3}(3\pi^2)^{2/3}\rho^2\rho^{-1/3}$$

$$P = \frac{1}{5m}(3\pi^2)^{2/3}\rho^{5/3} = \frac{2}{5}\rho\epsilon_F$$

Fermi degeneracy pressure --> increases with density

Finite pressure at T=0 ——> compare with ideal classical gas PV = nkT

Bulk modulus $\quad B = \frac{2}{3}\rho\epsilon_F$

$$\frac{U}{V} = \frac{(3\pi^2\rho)^{5/3}}{10\pi^2 m}$$

Chemical potential $\quad \mu = \epsilon_F$

Non Interacting Bosons: BEC

For Bosons at temp T, the occupation probability of a state with energy E is $n_B(E) = \frac{1}{e^{E/T} - 1}$

For a dispersion E(k), the total occupation of non-zero k modes is $N_{ex} = \sum_k n_B(E_k) = \int dE g(E) n_B(E)$

For a Density of state $g(E) = AE^\alpha$ $\quad N_{ex} = AT^{\alpha+1}\zeta(\alpha+1)\Gamma(\alpha+1)$ for $\alpha > 0$

If the total number of particles is larger than this value, the rest goes to E=0 state.

This macroscopic occupation of E=0 state is called BEC.

This implies that we can fix the total number of particles independent of temperature etc.

Examples (not necessarily non-interacting):

- BEC of Cold Alkali gases (Nobel Prize -- 2001)
- BEC in Superfluid He4 (Nobel Prize -- 1962)

Examples of Bosonic systems which do not condense:

Blackbody radiation

Phonons (Lattice vibrations)

In these systems, total no. of bosons are not conserved and vary with temp. So the basic argument of BEC fails.

Non Interacting Bosons: BEC at T=0

ground state for non-interacting Bosons: $|\psi\rangle = \frac{\left(a_0^\dagger\right)^N}{\sqrt{N!}}|0\rangle$

$$H = \sum_k \frac{k^2}{2m} a_k^\dagger a_k$$

U=0 for arbitrary densities

P=0

μ =0

$$\frac{U}{V}(T) = \int d^3k \frac{k^2}{2m} n_B(k^2/2m) = \int d\epsilon g(\epsilon)\epsilon n_B(\epsilon)$$

$$g(\epsilon) = \frac{m}{2\pi^2}\sqrt{2m}\epsilon^{1/2}$$

$$\frac{U}{V}(T) = T^{5/2}\int dx g(x) x n_B(x)$$

x = ε /T

$$C_V \sim T^{3/2}$$