- Bose - Einstein Condensation

Free Boson gas $\quad n_{\vec{k}}(T) = \dfrac{1}{e^{\beta(\varepsilon_{\vec{k}}-\mu)}-1}$

assume $\varepsilon_{\vec{k}} = \dfrac{\hbar^2 k^2}{2m}$

$\Rightarrow$ e.g. $\hat{H} = \sum_{\vec{k}} \left(\dfrac{\hbar^2 k^2}{2m} - \mu\right) \hat{a}_k^{+} \hat{a}_k$ (free theory).

$$\langle \hat{n}_{\vec{k}} \rangle = \frac{Tr(\hat{n}_{\vec{k}}\, e^{-\beta(\hat{H}-\mu\hat{N})})}{Tr(e^{-\beta(\hat{H}-\mu\hat{N})})}.$$

basis : $|n_{\vec{k}}\rangle$ momentum image.

why not number state (same as phonon?)

$\Rightarrow$ For grand canonical ensemble,

· Count the total number $\quad N = \sum_{\vec{k}} n_{\vec{k}}$

$$\Rightarrow n = \lim_{V\to\infty} \frac{N}{V} = \frac{1}{V}\sum_{\vec{k}} n_{\vec{k}} = \frac{1}{(2\pi)^3}\int d^3k \, \frac{1}{e^{\beta(\varepsilon_{\vec{k}}-\mu)}-1}$$

Bosons in free space, no potential, no interaction:

$$U_{k'-k} = g = 0 \;\Longrightarrow\; \hat{H} = \sum_k \left(\frac{k^2}{2m} - \mu\right)\hat{b}_k^\dagger \hat{b}_k = \sum_k \varepsilon_k \hat{b}_k^\dagger \hat{b}_k$$

$$n_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle = \frac{Tr\,\hat{b}_k^\dagger \hat{b}_k e^{-\beta\sum_k(\frac{k'^2}{2m}-\mu)\hat{b}_{k'}^\dagger \hat{b}_{k'}}}{Tr\, e^{-\beta\sum_k(\frac{k'^2}{2m}-\mu)\hat{b}_{k'}^\dagger \hat{b}_{k'}}}$$

$\rightarrow$ use $Tr(\hat{A}e^{-\beta\hat{H}}) = \sum_k \langle n_k | \hat{A} e^{-\beta\hat{H}} | n_k \rangle$

$$= \frac{\sum_{n_k=0,1,2\ldots} n_k e^{-\beta(\frac{k^2}{2m}-\mu)n_k} \prod_{k'\neq k} \sum_{n_{k'}=0,1,2\ldots} e^{-\beta(\frac{k'^2}{2m}-\mu)n_{k'}}}{\prod_{k'} \sum_{n_{k'}=0,1,2\ldots} e^{-\beta(\frac{k'^2}{2m}-\mu)n_{k'}}}$$

$$= \frac{\frac{\partial}{-\partial(\beta\varepsilon_k)}\frac{1}{1-e^{-\beta\varepsilon_k}} \prod_{k'\neq k} \frac{1}{1-e^{-\beta(\frac{k'^2}{2m}-\mu)}}}{\prod_{k'} \frac{1}{1-e^{-\beta(\frac{k'^2}{2m}-\mu)}}}$$

as it must be

$$= \frac{\partial}{-\partial(\beta\varepsilon_k)} \ln\frac{1}{1-e^{-\beta\varepsilon_k}} = \frac{e^{-\beta\varepsilon_k}}{1-e^{-\beta\varepsilon_k}} = \frac{1}{e^{\beta\varepsilon_k}-1} = \frac{1}{e^{\beta(\frac{k^2}{2m}-\mu)}-1}$$

occupation of Fock state in momentum representation

$$\begin{cases} \sum_n e^{-\lambda n} = \dfrac{1}{1-e^{-\lambda}} \\ \sum_n e^{-\lambda n} n = -\dfrac{\partial}{\partial\lambda}\sum_n e^{-\lambda n} = \dfrac{e^{-\lambda}}{(1-e^{-\lambda})^2} \end{cases}$$

$$\Rightarrow \int d^3k \Rightarrow \int 4\pi k^2\, dk, \quad z = \beta\varepsilon_{\vec{k}} = \frac{1}{k_B T}\frac{\hbar^2 k^2}{2m}$$

$$n = \frac{1}{(2\pi)^3}(4\pi)\int dk \, \frac{k_B T m}{\hbar^2 k} k^2 \frac{1}{e^{z-\beta\mu}-1}$$

$$= \frac{(m k_B T)^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\infty \frac{\sqrt{z}\,dz}{e^{z-\beta\mu}-1}$$

(For $n>0$)

$\mu_{max} = 0 = \dfrac{\hbar^2 k^2}{2m}\Big|_{min} = 0$

positive constraint : $\mu(T)$ has upper bond zero.

when $T \le T_c$, $\mu(T) = 0$

To simplify, set $\mu = 0$, then solve the integral.

$$n = 2.612\, \frac{(m k_B T)^{3/2}}{(2\pi\hbar^2)^{3/2}} \qquad \left(\mu = \frac{\partial F}{\partial N}\right)$$

This implies that for a give temperature there is a maximum number of particles that can be accomodated in excited level.

$\Rightarrow \quad N_{max} = n V.$

· now fix particle number and change temperature,

For sufficient high temperature, $\quad N < N_{max}$

low temperature, $\quad N > N_{max} \rightarrow$ the rest particles?

They are on ground state.

the integral miss the case $z=0$ ($k=0$)

why don't consider this for Fermion?:

There are only few (one, two, ...) particles on ground state.

$$\Rightarrow n = n_0 + \frac{1}{(2\pi)^3}\int d^3k \, \frac{1}{e^{\beta\hbar^2k^2/2m}-1}, \quad n_0 = \frac{N_0}{V} \text{ as } V\to\infty$$

N_0: number of particles at ground state.

- Critical temperature of condensation

$$T_c = \frac{2\pi\hbar^2}{mk_B}\left(\frac{N/V}{2.612}\right)^{\frac{2}{3}}$$ ← invert : $n = 2.612 \frac{(mk_BT)^{3/2}}{(2\pi\hbar^2)^{3/2}}$

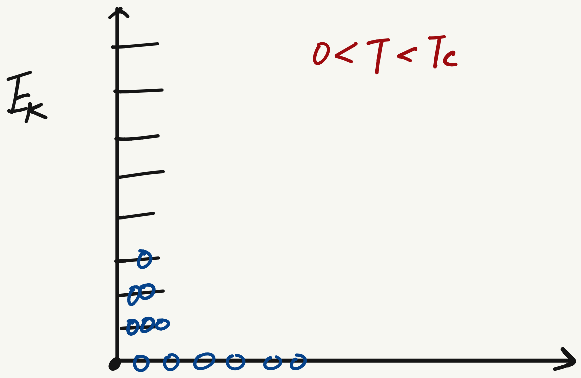
$\begin{cases} T > T_c, \text{ particles start to go to ground state} \\ T < T_c, \text{ excited particle number} \end{cases}$ $\begin{cases} N = N\left(\frac{T}{T_c}\right)^{2/3} & \text{(For excited } (k>0)) \\ N_0 = N\left(1-\left(\frac{T}{T_c}\right)^{2/3}\right) & \text{(ground state)} \end{cases}$

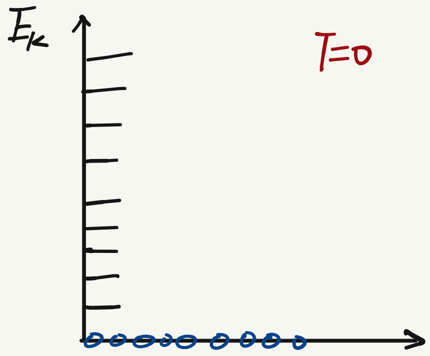
↓ carry zero momentum

→ no pressure and velocity.

$T < T_c$, excited particle number $\begin{cases} N = 1 \\ N_0 = 0. \end{cases}$

(all go to ground state!)





- why can't phonon? :

phonon → canonical ensemble ($\mu = 0$).

virtual

number state is available.

total number isn't conserved!!

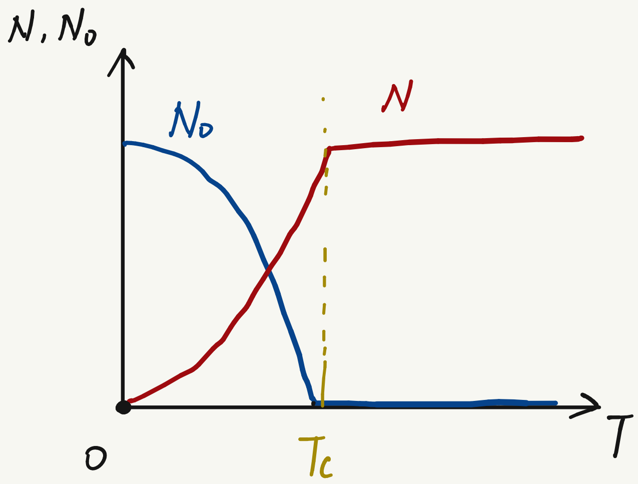
ground state is zero particle :

- BEC → grand canonical ensemble ($\mu \neq 0$).

number is fluctuating,

and the ground state is allowed

for multiple particles (Bosonic).



- For d=1 and d=2,

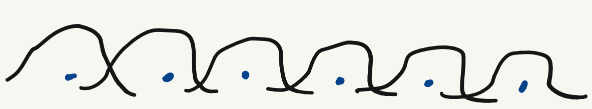
the number of non-condensed particle

is non-convergence.

write T_c in terms of De' Broglie's wavelength,

$$k_BT = \frac{p^2}{2m} \Rightarrow \lambda_D = \frac{h}{p} = 2.44\, n^{-\frac{1}{3}}.$$

BEC:



localized !

wave length ≃ space separation.

Note: $\begin{cases} [\hat{a}_0, \hat{a}_0^+] = 1 \\ \langle \hat{a}_0^+ \hat{a}_0 \rangle = N_0 \end{cases}$

$\Rightarrow \langle \hat{a}_0^+ \rangle = \sqrt{N_0},\ \langle \hat{a}_0 \rangle = \sqrt{N_0}.$

fix the phase θ $\begin{cases} T > T_c, & \varphi = 0 \\ T < T_c, & \varphi \neq 0. \end{cases}$

phase freedom ⇒ Broke U(1) gauge ⟺ XY model.

$$\langle \hat{a}_0^+ \rangle = \sqrt{N_0}\, e^{-i\theta},\ \langle \hat{a}_0 \rangle = \sqrt{N_0}\, e^{i\theta}.$$

⇒ order parameter, $\psi = |\psi| e^{i\theta}$.

many body wavefunction

(strongly coherent)!!!

Spin waves via HP bosons

We use the Holstein-Primakoff boson representation of spin operators

$$S^+ = (\sqrt{2S - n_b})b, \tag{1}$$
$$S^- = b^\dagger(\sqrt{2S - n_b}), \tag{2}$$
$$S^z = S - n_b. \tag{3}$$

in order to understand spin waves around both ferromagnetic and antiferromagnetic ground states. For the antiferromagnetic case, these provide a way to expand systematically around the (effectively classical) large-S limit, as will be seen. We follow Auerbach chapter 11 mostly.

First let's do ferromagnetic spin waves again. Our approach is going to be to expand the square roots in the HP relations in powers of $1/S$; this is justified as long as the spin fluctuations are relatively small,

$$\langle n_b \rangle \ll 2S, \tag{4}$$

which in principle we should check at the end of the calculation. This is basically a check to see whether spin waves are so strong that in fact they destroy the long-range order, as indeed happens in 1D for the antiferromagnet.

Suppose that the ordered ground state is in the $\hat{z}$ direction, and expand the Hamiltonian as

$$\begin{aligned} H &= -|J| \sum_{\langle ij \rangle} S_i \cdot S_j & (5) \\ &= -S^2|J|Nz/2 - |J| \sum_{\langle ij \rangle} \left[S b_i^\dagger \sqrt{1 - n_i/2S}\sqrt{1 - n_j/2S} b_j - \frac{1}{2} S(n_i + n_j) + \frac{1}{2} n_i n_j \right]. & (6) \end{aligned}$$

Here z is the coordination number. We now expand the square roots and keep terms proportional to S^2, S, and S^0, but not S^{-1}. This gives

$$H \approx -S^2|J|Nz/2 + H_1 + H_2 + O(1/S) \tag{7}$$

$$H_1 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \tag{8}$$

$$H_2 = |J|/4 \sum_{\langle ij \rangle} \left] b^\dagger_i b^\dagger_j (b_i - b_j)^2 + (b^\dagger_i - b^\dagger_j)^2 b_i b_j \right] . \tag{9}$$

We are not going to do anything with the quartic terms in H_2, since these are smaller than those in H_1 if the boson occupancy is small. Here the bosonic spin wave operators are

$$b_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}_i} b_i \tag{10}$$

and their energies are

$$\omega_{\mathbf{k}} = S|J|z \left(1 - z^{-1} \sum_{j,\langle ij \rangle} e^{i(\mathbf{x}_j - \mathbf{x}_i)\cdot\mathbf{k}} \right) . \tag{11}$$

Here the sum is over all the z nearest neighbors of one particular site, just as in a single-band tight-binding model. For the cubic lattice, for example, this just becomes

$$\omega_{\mathbf{k}} = S|J|(6 - 2\cos(k_x a) - 2\cos(k_y a) - 2\cos(k_z a)). \tag{12}$$

In Auerbach's notation the above is written as (for the cubic lattice $z = 6$)

$$\omega_{\mathbf{k}} = S|J|z(1 - \gamma_{\mathbf{k}}). \tag{13}$$

Again, this is what we would get for a tight-binding model, but with an offset so that zero k corresponds to zero energy. For the cubic lattice, we have at small $\mathbf{k}$

$$\omega_{\mathbf{k}} \approx S|J|a^2k^2. \tag{14}$$

This soft mode is the Goldstone boson corresponding to broken spin rotational invariance. We will see that the antiferromagnetic spin wave is rather different: it has multiple zero-energy points for the cubic lattice, rather than just the single point $\mathbf{k} = 0$, and also has a linear dispersion relation near these points, rather than a quadratic one.

Before moving on to the antiferromagnet, let's look at how the ferromagnetic order is reduced by spin-wave excitations for $T > 0$. The change in the magnetization per site at finite temperature is given by

$$\Delta m_0 = \frac{1}{N}\langle S^z_{tot} \rangle - S = -\langle n_i \rangle = -\frac{1}{N}\sum_{\mathbf{k}} n_{\mathbf{k}}. \tag{15}$$

The occupation number $n_{\mathbf{k}}$ is just given by Bose-Einstein statistics,

$$n_{\mathbf{k}} = \frac{1}{e^{\omega_{\mathbf{k}}/T} - 1}. \tag{16}$$

In order to understand the effect of temperature, let k_0 be an "infrared cutoff": some small momentum that we will keep as a lower bound when converting the sum over spin-wave modes to an integral. The important physics will be that the behavior under removing this cutoff is strongly dimensionality-dependent, which tells us something about the destruction of order at finite temperature. We also introduce a larger momentum $\bar{k} > k_0$, with the idea that below this momentum the quadratic form $\omega_{\mathbf{k}} \approx S|J|a^2k^2$ is valid.
The sum then becomes

$$\Delta m_0 = -\int_{k_0}^{\bar{k}} \frac{dk\, k^{d-1}}{(2\pi)^d} \frac{T}{JSk^2} - N^{-1} \sum_{|k|>\bar{k}} \frac{1}{e^{\omega_{\mathbf{k}}/T} - 1}. \tag{17}$$

The second part is independent of k_0 and finite, so we ignore it. We want instead to focus on the asymptotic behavior of the first part for small k_0. In one dimension it diverges as $-T/k_0 JS$, while in two dimensions it diverges as $T(\log k_0)/JS$.

These divergences mean obviously that the spin-wave approximation (which required that the expectations be relatively small perturbations to the original ordered state) is not justified at finite temperature in 1D and 2D, since even at low temperature the reduction of magnetization is divergent. The physical interpretation of this is that at finite temperature there is no long-range order in the Heisenberg model in 1D and 2D, as a consequence of the Mermin-Wagner theorem (cf. Phys 212). You can show that the reduction of the moment in 3D is proportional to $T^{3/2}$, so that the magnetic order is stable up to some nonzero temperature.

Now we consider the antiferromagnetic case. We assume a bipartite lattice: a lattice that can be divided into two sublattices A and B so that every bond connects one site from A and one site from B. Then the classical ground state is just all spins up on A and all down on B, modulo a global rotation. It is useful to rotate the spin quantization axis between sublattices, so that zero bosons at every site corresponds to this classical N\'eel state: then on sublattice B we have

$$\tilde{S}_j^z = -S_j^z, \quad \tilde{S}_j^x = S_j^x, \quad \tilde{S}_j^y = -S_j^y. \tag{18}$$

These satisfy the same commutation relation as the original spin operators and therefore can be represented by HP bosons. In this new representation, the Hamiltonian is

$$H = -|J| \sum_{\langle ij \rangle} S_i^z \tilde{S}_j^z + \frac{|J|}{2} \sum_{\langle ij \rangle} (S_i^+ \tilde{S}_j^+ + S_i^- \tilde{S}_j^-). \tag{19}$$

(Because of the rotation on one sublattice, the above has $++$ and $--$ terms instead of combinations of one raising and one lowering operator.) Consider one pair of sites: substituting HP bosons and ignoring quartic and $O(1/S)$ terms leaves

$$-|J|S_i^z\tilde{S}_j^z + \frac{|J|}{2}(S_i^+\tilde{S}_j^+ + S_i^-\tilde{S}_j^-) \approx -|J|S^2 + |J|S(n_i+n_j) + \frac{|J|}{2}S(b_ib_j + b_i^\dagger b_j^\dagger). \tag{20}$$

We can rewrite these in terms of $b_{\mathbf{k}}$ operators as before: note that the sum of n_i will be equal to the sum over all k (Parseval's theorem), and that the bb and $b^\dagger b^\dagger$ terms are just like what we had before.

$$H = -S^2JNz/2 + H_1 \tag{21}$$

$$H_1 = JSz\sum_{\mathbf{k}}\left[b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{\gamma_{\mathbf{k}}}{2}(b_{\mathbf{k}}b_{-\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}^{\dagger})\right]. \tag{22}$$

Cooper pair – like term!

Here we see that H_1 is a bit more complicated: it is still just quadratic in the bosonic operators, but has some terms that change the overall number of bosons. Does this remind you of anything? We use the same Bogoliubov transformation to diagonalize this Hamiltonian that we used to get the γ operators in superconductivity, with the difference being that now we are dealing with bosonic operators. The basis change we want is to new spin-wave operators $\alpha_{\mathbf{k}}$:

$$\alpha_{\mathbf{k}} = \cosh\theta_{\mathbf{k}} b_{\mathbf{k}} - \sinh\theta_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \tag{23}$$

$$b_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}\alpha_{\mathbf{k}} + \sinh\theta_{\mathbf{k}}\alpha_{-\mathbf{k}}^\dagger. \tag{24}$$

The operators α are still bosonic: for example,

$$[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}}^\dagger] = \cosh^2\theta_{\mathbf{k}}[b_{\mathbf{k}}, b_{\mathbf{k}}^\dagger] + \sinh^2\theta_{\mathbf{k}}[b_{-\mathbf{k}}^\dagger, b_{-\mathbf{k}}] = 1. \tag{25}$$

and the $[\alpha,\alpha]$ and $[\alpha^\dagger,\alpha^\dagger]$ commutators vanish.

In terms of the new α operators, we have

$$H_1 = |J|Sz\sum_{\mathbf{k}}\Big[(\cosh 2\theta_{\mathbf{k}} + \gamma_{\mathbf{k}}\sinh 2\theta_{\mathbf{k}})\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} \tag{26}$$

$$+\frac{1}{2}(\sinh 2\theta_{\mathbf{k}} + \gamma_k\cosh 2\theta_{\mathbf{k}})(\alpha_{\mathbf{k}}^\dagger\alpha_{-\mathbf{k}}^\dagger + \alpha_{\mathbf{k}}\alpha_{-\mathbf{k}}) + \sinh^2\theta_{\mathbf{k}} + \frac{\gamma_k}{2}\sinh 2\theta_{\mathbf{k}}\Big]. \tag{27}$$

We can now choose the $\theta_{\mathbf{k}}$ to make the non-boson-number-conserving terms vanish:

$$\tanh 2\theta_{\mathbf{k}} = -\gamma_k, \tag{28}$$

so

$$H_1 = \sum_{\mathbf{k}}\omega_{\mathbf{k}}(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \frac{1}{2}) - \frac{JSzN}{2}, \tag{29}$$

$$\omega_{\mathbf{k}} = |J|Sz\sqrt{1-\gamma_{\mathbf{k}}^2}. \tag{30}$$

This is different from the ferromagnet in two important ways: the function $\omega_{\mathbf{k}}$ is linear near its minima rather than quadratic, and quantum fluctuations cause a reduction in the ground state energy of order S:

$$\Delta E = \frac{1}{2} \sum_{\mathbf{k}} |J| S z (\sqrt{1 - \gamma_{\mathbf{k}}{}^2} - 1). \tag{31}$$

For the d-cubic lattice, near $\mathbf{k} = (0, 0, \ldots)$ and $\mathbf{k} = (\pi, \pi, \pi)$ the spin-wave spectrum looks like $\omega_{\mathbf{k}} \sim JS\sqrt{2z}|\mathbf{k} - \mathbf{k}_{min}|$, so there are two minima with the same spin-wave velocity near each. This prediction has been strikingly confirmed via neutron scattering on antiferromagnets.

A somewhat unsatisfactory way to explain the difference between $\omega \sim |k|$ and $\omega \sim k^2$ is to argue that the ferromagnet breaks time-reversal symmetry "more strongly" than the antiferromagnet, since on long length scales the antiferromagnet's mean magnetization is zero. If time-reversal symmetry were preserved, then a relation like $\omega \sim k^2$ would be impossible because the two sides of the equation transform differently under the time-reversal operator. The problem with this argument, of course, is that the antiferromagnet also breaks time-reversal, but at least the heuristic argument is good for remembering which dispersion relation goes with which magnet.

Note that in the case of both the ferromagnet and antiferromagnet the fundamental excitations carried integer spin (we showed this in an earlier lecture for the ferromagnet). An active area, which you can read more about in Auerbach and also the textbook of Fradkin, is how some "spin liquids" can have deconfined spin-half excitations known as *spinons*.

- Magnon and spin wave.

Imagine a magnetic system with time-reversal symmetry: → apply time-reversal operator, the Hamiltonian remains the same.

$\uparrow\ \uparrow\ \uparrow\ \uparrow\ /\ \uparrow \downarrow \uparrow \downarrow$

examine the low temperature excitation

under following Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad \text{(classical Heisenberg model)}$$

(nearest neighbor)

1D: $\mathcal{H} = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$

Consider an effective field:

$$-J\, \vec{S}_j \cdot (\vec{S}_{j-1} + \vec{S}_{j+1}) = -\vec{S}_j \cdot \vec{H}_j$$

→ like a magnetic field!!

E.O.M: (classical angular momentum)

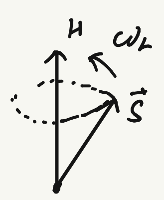
$$\frac{d\vec{S}}{dt} = \vec{S} \times \vec{H}$$

→ for single spin, this leads to a precession around $\vec{H}$. → Lamor precession

e.g.: $\vec{H} = H\hat{z}$, $\frac{dS^z}{dt} = 0$, $\frac{dS^x}{dt} = -HS^y$, $\frac{dS^y}{dt} = HS^x$.

$S^+ = S^x + iS^y$, $S = S^x - iS^y$

then $\frac{dS^+}{dt} = i\omega_L S^+$, $S^+(t) = S^+(0)e^{i\omega_L t}$ (ω_L: Lamor frequency) Here $\omega_L = H$



} single spin.

Consider Heisenberg spin chain:

$$\frac{d\vec{S}_j}{dt} = \vec{S}_j \times J(\vec{S}_{j-1} + \vec{S}_{j+1})$$

assume: only keep first order term.

$$\frac{dS_j^z}{dt} = 0, \quad \frac{dS_j^x}{dt} = -\omega_0 (S_{j-1}^y + S_{j+1}^y - 2S_j^y)$$

$$\frac{dS_j^y}{dt} = \omega_0 (S_{j-1}^x + S_{j+1}^x - 2S_j^x)$$

define $S_j^+ = S_j^x + iS_j^y$

normal mode:

$$\begin{cases} \frac{dS_j^+}{dt} = \omega_0 (S_{j+1}^+ + S_{j-1}^+ - 2S_j^+) \\ S_j^+(t) = S^+(0)\, e^{i(kx_j - \omega(k)t)} \end{cases}$$

⇒ decoupled case:

$\omega(k) = 2\omega_0(1 - \cos ka)$ (dispersion) ← lattice constant.

Small k, $\cos ka = 1 - \frac{1}{2}k^2a^2$, $\omega(k) = \omega_0 k^2 a^2 \propto k^2$.

- In Quantum mechanic,

recall $(\hat{\vec{S}}\cdot\hat{\vec{S}})|s,m_s\rangle = \hat{S}^2|s,m_s\rangle = s(s+1)|s,m_s\rangle$

describe the deviation of $\vec{s}$ from $\hat{z}$,

Construct Bosonic operator.

$$\left.\begin{aligned} S_i^z = S - n_i, \quad \hat{S}_i^+ &= \sqrt{2S}\sqrt{1-\frac{n_i}{2S}}\,\hat{a}_i \\ \hat{S}_i^- &= \sqrt{2S}\sqrt{1-\frac{n_i}{2S}}\,\hat{a}_i^+ \end{aligned}\right\}$$

here only consider linear term.

- HP Bosons

- number of Boson n_i gives the deviation of spin from z direction

Consider a lattice of N spins -

a running wave of spin "deviation" $\Rightarrow$ normal mode

$$a_k = \frac{1}{\sqrt{N}}\sum_j e^{i\vec{k}\cdot\vec{r}_j}\hat{a}_j, \quad \hat{a}_j = \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}\cdot\vec{r}_j}\hat{a}_k$$

Fourier transform and rewrite the Hamiltonian,

(in $\boxed{\text{linear approximation}}$)

$$\begin{cases} \hat{S}_j^+ = \sqrt{\frac{2S}{N}}\sum_k e^{-i\vec{k}\cdot\vec{r}_j}\hat{a}_k, \quad \hat{S}_j^- = \sqrt{\frac{2S}{N}}\sum_k e^{i\vec{k}\cdot\vec{r}_j}\hat{a}_k^+ \\ \hat{S}_j^z = S - \frac{1}{N}\sum_{\vec{k},\vec{q}} e^{-i(\vec{k}-\vec{q})\cdot\vec{r}_j}\hat{a}_{\vec{k}}^+\hat{a}_{\vec{q}} \end{cases}$$

order parameter $\langle m_{s_i}\rangle = \sum_i S_i^z (-1)^{x_i+y_i}$ (2D)

Consider $\hat{H} = -J\sum_{j,\delta}\vec{S}_j\cdot\vec{S}_{j+\delta}$ (Ferromagnetic state) $\longrightarrow$ anti Ferro : <u>Bogoliubov TR.</u>

(Neel state)

$$\begin{matrix} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \end{matrix}$$

simple cubic :

$$\begin{cases} \hat{H} = -JNz\hat{S}^2 + 2Jz\hat{S}\sum_k(1-\gamma_k)\hat{a}_k^+\hat{a}_k \\ \gamma_k = \frac{1}{z}\sum_\delta e^{i\vec{k}\cdot\vec{\delta}} = \frac{1}{z}\sum_\delta \cos(\vec{k}\cdot\vec{\delta}) \end{cases}$$

$(\sin(-k) = -\sin k)$

$$\Rightarrow \hat{H} = \sum_k \hbar\omega_k\left(\hat{a}_k^+\hat{a}_k + \tfrac{1}{2}\right)$$

$$\omega_k = 2JzS\left(1-\frac{1}{z}\sum_\delta\cos(\vec{k}\cdot\vec{\delta})\right)$$

- Thermal effects

- magnetic contribution to the internal energy (of Ferro magnetic)

$$U = \sum_{\vec{k}} \hbar\omega_{\vec{k}} \langle n_{\vec{k}} \rangle + U_{eq}$$

$$U = \sum_{\vec{k}} \frac{\hbar\omega_{\vec{k}}}{e^{\beta\hbar\omega_{\vec{k}}}-1}, \quad C_v = \frac{\partial}{\partial T}\sum_{\vec{k}} \frac{\hbar\omega_{\vec{k}}}{e^{\beta\hbar\omega_{\vec{k}}}-1} \to V\frac{\partial}{\partial T}\int\frac{d^3k}{(2\pi)^3}\frac{\hbar\omega_{\vec{k}}}{e^{\beta\hbar\omega_{\vec{k}}}-1}$$

Set $\omega_{\vec{k}} = Dk^2$ ($\propto k^2$ when k is small)

$$C_v = V\frac{\partial}{\partial T}\int\frac{4\pi k^2 dk}{(2\pi)^3}\frac{\hbar Dk^2}{e^{\beta\hbar Dk^2}-1}$$

set $y^2 = \beta\hbar Dk^2 \Rightarrow C_v = \frac{V}{2\pi^2}\frac{\partial}{\partial T}\frac{(k_BT)^{5/2}}{(\hbar D)^{3/2}}\int_0^\infty \frac{y^4}{e^{y^2}-1}dy$

$\Rightarrow C_v \propto T^{3/2}$. (For FM magnon)

- magnetization :

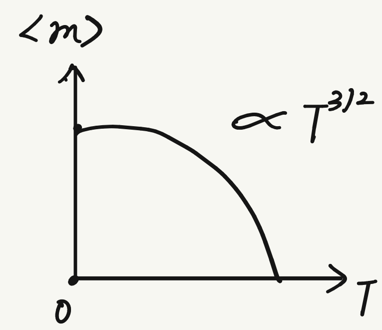
each magnon excited decreases the magnetization.

$$\hat{M} = \sum_i \hat{S}_i^z = N\hat{S} - \sum_{\vec{k}} \hat{a}_k^\dagger \hat{a}_k$$

$$\langle \hat{M}(T=0)\rangle - \langle \hat{M}(T)\rangle = \sum_k \langle \hat{a}_k^\dagger \hat{a}_k \rangle$$

$$\Delta\langle M\rangle = \sum_{\vec{k}}\langle \hat{a}_k^\dagger \hat{a}_k \rangle = \frac{V}{(2\pi)^3}\left(\frac{k_BT}{\hbar D}\right)^{3/2}\int_0^\infty \frac{y^2}{e^{y^2}-1}dy \propto T^{3/2}$$ (Bloch law)

widely used!!!!



- Fermi gas

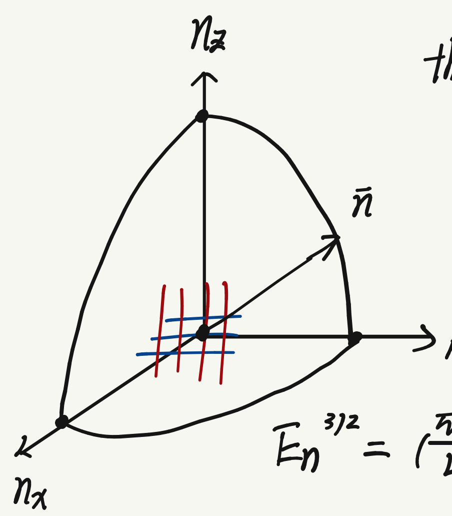
- Pauli exclusion and consider Fermions in 3D box

$$\begin{cases} \psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}y\right)\sin\left(\frac{n_z\pi}{L}z\right) \\ E_n = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2+n_y^2+n_z^2) \end{cases}$$

each energy level is degenerate,

$|n_x, n_y, n_z, m_s\rangle$, degeneracy 2 (Pauli exclusion)

Take large V, energy space is small.



For large n,

the total number of states

is the volume of this sphere

$$N_s = \frac{1}{8}\cdot\frac{4}{3}\pi n^3 \times \underset{\text{spin!}}{2}$$

$$= \frac{1}{3}\pi n^3$$

$$E_n^{3/2} = \left(\frac{\pi\hbar}{L}\right)^3 \frac{1}{(2m)^{3/2}} n^3$$

$$N_s = \frac{1}{3}\pi n^3 = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{3/2}$$

Call the highest filled level — Fermi energy.

$$N_s = \frac{1}{3\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E_F^{3/2}$$

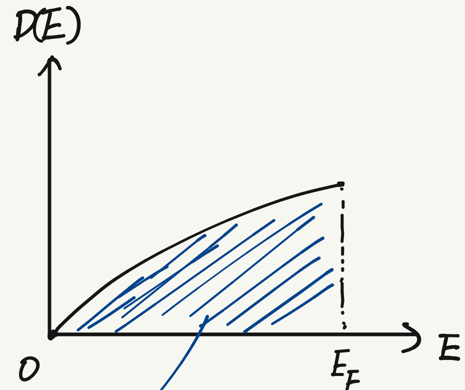
$\Rightarrow$ For big N_s, the density of particle is $\rho = \frac{N_s}{V}$

$$\Rightarrow E_F = \frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3} \Rightarrow k_F = (3\pi^2\rho)^{1/3},\ E_F = \frac{\hbar^2 k_F^2}{2m}.$$

· Density of states : $D(E)$

the number of particle quantum states in an energy regime $(E, E+dE)$ $\Rightarrow D(E)dE$

$$D(E) = \frac{dN_s}{dE} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{1/2}.$$



occupied states at $T=0$!!

· Total energy

$$E_{tot} = \int_0^{E_F} E\, D(E)\, dE = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V \int_0^{E_F} E^{3/2} dE = \frac{1}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E_F = \frac{3}{5} N E_F$$

$$N = \frac{1}{3\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E_F^{3/2}$$

$\downarrow$

average particle energy at $T=0$,

$$\bar{E} = \frac{E_{tot}}{N} = \frac{3}{5} E_F$$

· Thermal properties — Fermi gas

- no periodic structure
- ignore interaction

· specific heat

In equilibrium, same energy for each degree of freedom, it is $\frac{1}{2}k_B T$

· classical equipartition

$$U = k_B T\left(\frac{3}{2}N\right) \Rightarrow C_V = \frac{3}{2} N k_B$$

(like high temperature for phonon)

(For one particle, it has 3 translational degree of freedom)

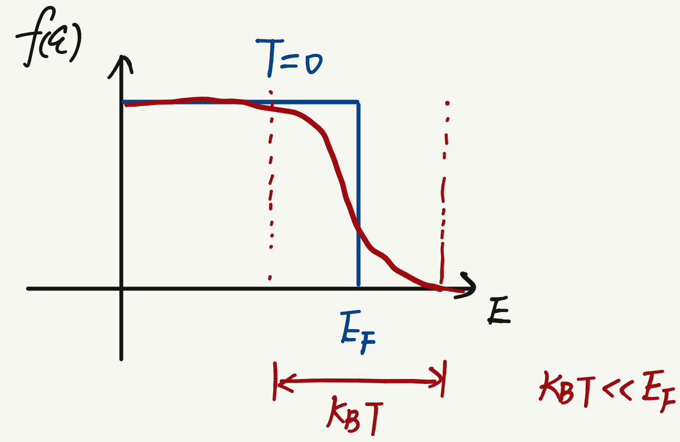
$\downarrow$

In fact, the real specific heat is much lower.

- Quantum :

Pauli exclusion.

Fermi- Dirac distribution. $\langle n_j \rangle_T = f(\varepsilon_i) = \dfrac{1}{e^{\beta(\varepsilon_j-\mu)}+1}$



$\downarrow$ · The effective number is much less than large N!!

when we heat up the metal. only the "k_BT" range electrons move outside the Fermi surface.

$$\begin{cases} N_{eff} \approx \underbrace{k_B T}_{\text{energy domain}} \, D(E_F) \rightarrow \text{density of states.} \\ D(E_F) = \frac{3}{2} N / E_F \Rightarrow N_{eff} \approx k_B T \, \frac{3}{2} \frac{N}{E_F}. \end{cases}$$

$$U \approx k_B T \, \frac{3}{2} N_{eff} = \frac{3N}{2E_F} (k_B T)^2 \Rightarrow C_V = 3k_B^2 \frac{N}{E_F} T.$$

- Full calculation,

$$U(T) = \int_0^\infty E \, D(E) \, f(E) \, dE \quad (\text{Sommefield integral})$$

$$C_V = \frac{\pi^2 N k_B}{2} \frac{k_B T}{E_F}$$