221B Lecture Notes
Quantum Field Theory II (Bose Systems)

1 Statistical Mechanics of Bosons

1.1 Partition Function

As discussed in 221A, the path integral with the imaginary time gives you the partition function of the system. Let us consider the partition function of the free Schrödinger field theory, first the bosonic one. This calculation shows non-trivially that the quantized Schrödinger field theory indeed contains multi-body states automatically and is also useful from a practical point of view.

The path integral in the particle quantum mechanics is given by the summation over all possible paths in the configuration space $x_i(t)$. In the field theory, $\psi(\vec{x})$ is the canonical coordinate, and it can follow various "paths" $\psi(\vec{x},t)$. Therefore, the path integral in field theory is a summation over all possible field configurations $\psi(\vec{x},t)$. This discussion defines the path integral

$$\int \mathcal{D}\psi(\vec{x},t)\mathcal{D}\psi^\dagger(\vec{x},t)e^{iS/\hbar}, \tag{1}$$

where the action is that of the field theory, such as

$$S = \int d\vec{x}dt \left(\psi^* i\hbar\dot{\psi} + \psi^* \frac{\hbar^2\Delta}{2m}\psi\right) \tag{2}$$

in the free case.

To calculate the partition function, we go to the imaginary time $t = -i\tau$,

$$Z = \int \mathcal{D}\psi(\vec{x},\tau)\mathcal{D}\psi^\dagger(\vec{x},\tau) \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\vec{x} \left(\psi^*\hbar\dot{\psi} + \psi^*\frac{-\hbar^2\Delta}{2m}\psi\right)\right]. \tag{3}$$

We impose the periodic boundary condition $\psi(\vec{x}, t+\hbar\beta) = \psi(\vec{x})$ for $\beta = 1/kT$.

Because of the periodic boundary condition in τ and also in space due to the box normalization, we can expand in Fourier series both in the imaginary time as well as in space,

$$\psi(\vec{x},\tau) = \frac{1}{L^{3/2}}\sum_{\vec{p},n} z_{\vec{p},n} e^{i\vec{p}\cdot\vec{x}/\hbar} e^{2\pi i n\tau/\hbar\beta} \tag{4}$$

and simiarly for $\psi^\dagger$

$$\psi^\dagger(\vec{x},\tau) = \frac{1}{L^{3/2}} \sum_{\vec{p},n} z^*_{\vec{p},n} e^{-i\vec{p}\cdot\vec{x}/\hbar} e^{-2\pi i n\tau/\hbar\beta}. \tag{5}$$

Then the exponent in the partition function Eq. (3) is

$$-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\vec{x} \left(\psi^*\hbar\dot{\psi} + \psi^*\frac{-\hbar^2\Delta}{2m}\psi\right) = -\sum_{\vec{p},n}\left(2\pi i n + \beta\frac{\vec{p}^2}{2m}\right) z^*_{\vec{p},n} z_{\vec{p},n}. \tag{6}$$

Therefore, the path integral is simply a product of many many Gaussian integrals

$$Z = \prod_{\vec{p},n}\int dz^*_{\vec{p},n} dz_{\vec{p},n} e^{-(2\pi i n + \beta\vec{p}^2/2m) z^*_{\vec{p},n} z_{\vec{p},n}} = \prod_{\vec{p},n} \frac{\pi}{2\pi i n + \beta\vec{p}^2/2m}. \tag{7}$$

Now we use the infinite product representation of the hyperbolic functions

$$\begin{aligned} \prod_{n=1}^{\infty}\left(1 + \frac{x^2}{n^2}\right) &= \frac{\sinh \pi x}{\pi x} \\ \prod_{n=1}^{\infty}\left(1 + \frac{x^2}{(2n-1)^2}\right) &= \cosh\frac{\pi x}{2}. \end{aligned} \tag{8}$$

We use the first identity here. The partition function Eq. (7) can be rewritten as

$$\begin{aligned} Z &= \prod_{\vec{p}} \frac{\pi}{\beta\vec{p}^2/2m} \prod_{n=1}^{\infty} \frac{\pi}{(2\pi n)^2 + (\beta\vec{p}^2/2m)^2} \\ &= \prod_{\vec{p}} \frac{\pi}{\beta\vec{p}^2/2m} \prod_{n=1}^{\infty} \frac{\pi}{(2\pi n)^2} \left(1 + \frac{(\beta\vec{p}^2/2m/2\pi)^2}{n^2}\right)^{-1} \\ &= \prod_{\vec{p}} \left(\prod_{n=1}^{\infty} \frac{\pi}{(2\pi n)^2}\right) \frac{\pi}{\beta\vec{p}^2/2m} \frac{\beta\vec{p}^2/4m}{\sinh\beta\vec{p}^2/4m} \\ &= c\prod_{\vec{p}} \frac{2}{\sinh\beta\vec{p}^2/4m} \\ &= c\prod_{\vec{p}} \frac{e^{-\beta\vec{p}^2/4m}}{1 - e^{-\beta\vec{p}^2/2m}}. \end{aligned} \tag{9}$$

where c is an (infinite) overall constant, which is not important when evaluating various thermally averages quantities. This is a grand partition function which contains summation over all possible number of particles but with no chemical potential. One small difference from the conventional calculation is that the path integral automatically includes the "zero-point energy" $\vec{p}^2/4m$, which results in the exponential factor in the numerator. The reason why there is this zero-point energy is because the Fock space is a collection of (infinite number of) harmonic oscillators and each harmonic oscillator has the zero-point energy. But the zero-point energy does not lead to any physical consequences (while the zero-point fluctuation does) and we can always shift the energy of the system by an infinite constant $\sum_{\vec{p}} \vec{p}^2/4m$ to remove the zero-point energy in the expression.

This simple calculation clearly shows the advantage of the Schrödinger field theory: it sums up states with different number of particles automatically.

The inclusion of the chemical potential is obvious. Because the number operator is $N = \int d\vec{x}\psi^\dagger(\vec{x})\psi\vec{x}$ and the grand canonical emsenble is summed with a factor of $e^{-\beta(E-\mu N)}$, the path integral Eq. (3) is modified to

$$\begin{aligned} Z &= \int \mathcal{D}\psi(\vec{x},\tau)\mathcal{D}\psi^\dagger(\vec{x},\tau) \\ &\quad \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\vec{x}\left(\psi^*\hbar\dot{\psi} + \psi^*\frac{-\hbar^2\Delta}{2m}\psi - \mu\psi^*\psi\right)\right]. \end{aligned} \tag{10}$$

The result of the path integral is then

$$Z = c\prod_{\vec{p}} \frac{e^{-\beta(\vec{p}^2/2m-\mu)/2}}{1-e^{-\beta(\vec{p}^2/2m-\mu)}}. \tag{11}$$

Note that $Z = e^{-\beta\Omega}$ with $\Omega = -pV = F - \mu N$ for the grand partition function.

The thermal average energy is given by the standard formula by the derivative with respect to β (but keeping $\beta\mu$ fixed):

$$\begin{aligned} \langle E\rangle &= -\frac{\partial}{\partial\beta}\ln Z\bigg|_{\beta\mu} \\ &= -\frac{\partial}{\partial\beta}\left[\log c + \sum_{\vec{p}}\left(-\frac{1}{2}\beta\left(\frac{\vec{p}^2}{2m}-\mu\right) - \ln(1-e^{-\beta(\vec{p}^2/2m-\mu)})\right)\right]\Bigg|_{\beta\mu} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{\vec{p}} \frac{\vec{p}^2}{2m}\left(\frac{1}{2}+\frac{e^{-\beta(\vec{p}^2/2m-\mu)}}{1-e^{-\beta(\vec{p}^2/2m-\mu)}}\right) \\
&= \sum_{\vec{p}} \frac{\vec{p}^2}{2m}\left(\frac{1}{2}+\frac{1}{e^{\beta(\vec{p}^2/2m-\mu)}-1}\right). \qquad (12)
\end{aligned}
$$

This must be a famililar expression to you, again except the zero-point energy term that can be dropped without changing physical content.

1.2 Bose–Einstein Condensate

One prime application of Schrödinger field theory is the Bose–Einstein condensate.

The expression for the thermally averaged energy Eq. (12) has a problem when the chemical potential μ is positive. The region of the momentum space $\vec{p}^2/2m < \mu$ does not give meaningful result: it is negative. The explanation you have heard back in college may be that this suggests that there is a macroscopic number of bosons condensed in this momentum region. But what is actually going on?

Let us go back to the partition function Eq. (10), but now with a δ-function repulsive potential term

$$
\begin{aligned}
Z = &\int \mathcal{D}\psi(\vec{x},\tau)\mathcal{D}\psi^\dagger(\vec{x},\tau) \\
&\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\vec{x}\left(\psi^*\hbar\dot{\psi}+\psi^*\frac{-\hbar^2\Delta}{2m}\psi-\mu\psi^*\psi\right)-\frac{1}{2}\lambda\psi^*\psi^*\psi\psi\right].
\end{aligned}
\qquad (13)
$$

(We used to write $\lambda = \hbar^2\gamma$.) The action in the exponent permits the interpretation that the chemical potential is a part of the potential term

$$
V(\psi) = -\mu\psi^*\psi + \frac{1}{2}\lambda\psi^*\psi^*\psi\psi \qquad (14)
$$

Now we can ask the question what happens when $\mu > 0$. The potential for ψ is minimized when it has a finite value:

$$
\psi = \sqrt{\frac{\mu}{\lambda}}e^{i\theta}, \qquad (15)
$$

where θ is an arbitrary phase. The expectation value of the Schrödinger field is the Bose–Einstein condensate. The number density of particles in the condensate is of course

$$\rho = \frac{N}{L^3} = \psi^* \psi = \frac{\mu}{\lambda}, \tag{16}$$

and this is the equation what determines the chemical potential.

When we saw that the quantized Schrödinger field theory gives multi-particle states, we didn't ask the question what Schrödinger field meant *before* the quantization. We were happy that we could successfully obtain the multi-particle quantum mechanics. In the normal situation without a condensate, the expectation value of ψ vanishes. Therefore ψ is definitely not classical and genuinely quantum. The particles are quantum fluctuations around the vanishing expectation value $\langle \psi \rangle = 0$. On the other hand, what we see here is that the *classical* Schrödinger field can exist and describe the Bose–Einstein condensate.

Remember that the field operator ψ is an *annhilation* operator. If it has an expectation value in the ground state, the ground state cannot be an eigenstate of the number operator. This point can be understood by assuming that the only condensate is in the zero-momentum state. The Hamiltonian for the zero-momentum mode with the delta-function potential $V(\vec{x}-\vec{y}) = \lambda\delta(\vec{x}-\vec{y})$ or equivalently $V(\vec{p}-\vec{q}) = \frac{1}{L^3}\lambda$ is

$$H = -\mu a^\dagger(0)a(0) + \frac{\lambda}{2L^3} a^\dagger(0)a^\dagger(0)a(0)a(0). \tag{17}$$

It is difficult to diagonalize this Hamiltonian. However, the following variational method can be used. The coherent state

$$|f\rangle = e^{-f^* f/2} e^{f a^\dagger(0)} |0\rangle, \tag{18}$$

as discussed in 221A, is an eigenstate of the annihilation operator

$$a(0)|f\rangle = f|f\rangle, \tag{19}$$

and the expectation value of the Hamiltonian for this state is

$$\langle f|H|f\rangle = -\mu f^* f + \frac{\lambda}{2L^3} f^* f^* f f. \tag{20}$$

Here, we used the fact that $\langle f|a^\dagger(0) = \langle f|f^*$. Minimizing it with respect to the complex parameter f, the variational method suggests the approximate ground state

$$|f\rangle \qquad \text{with} \qquad f = \sqrt{\frac{\mu L^3}{\lambda}} e^{i\theta}, \qquad E = -\frac{1}{2}\mu f^* f = -\frac{\mu^2 L^3}{2\lambda}. \tag{21}$$

The energy is clearly lower than the "vacuum" $|0\rangle$. This state obviously shows an expectation value for the annihilation operator

$$\langle f|a(0)|f\rangle = \sqrt{\frac{\mu L^3}{\lambda}} e^{i\theta} \tag{22}$$

and hence also for the field operator

$$\langle f|\psi(\vec{x})|f\rangle = \frac{1}{L^{3/2}} \sum_{\vec{p}} \langle f|a(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar}|f\rangle = \sqrt{\frac{\mu}{\lambda}} e^{i\theta}, \tag{23}$$

consitent with Eq. (15). Even though the coherent state is not the true ground state of the Hamiltonian, it is clearly close enough as suggested by the classical minimum of the Schrödinger field.

Note that the condensate could be described in this formalism because it allowed states with different number of particles in the same Hilbert space. This state could never be described in the conventional multi-body Schrödinger wave functions.

1.3 More on Coherent States

How good is the variational method in this case? To see this, let us go back to the Hamiltonian Eq. (17) and act it on the coherent state Eq. (18). We find

$$\begin{aligned} H|f\rangle &= \left(-\mu a^\dagger a + \frac{\lambda}{2L^3} a^\dagger a^\dagger a a)\right)|f\rangle \\ &= \left(-\mu a^\dagger f + \frac{\lambda}{2L^3} a^\dagger a^\dagger f^2)\right)|f\rangle \end{aligned}$$

We dropp the momentum index in this section. What we need to know now is the action of the creation operator on the coherent state.

It is useful to look at the probability distribution in the number of particles in a coherent state.

$$P(n) = |\langle n|f\rangle|^2 = \left|\langle n|e^{-f^*f/2}\frac{f^n}{n!}(a^\dagger)^n|0\rangle\right|^2 = e^{-f^*f}\left|\langle n|\frac{f^n}{\sqrt{n!}}|n\rangle\right|^2 = e^{-f^*f}\frac{(f^*f)^n}{n!}. \tag{24}$$

This is nothing but the Poisson distribution with the averange $\bar{n} = f^* f$. Therefore for a large $N = f^* f$, the fluctuation in the number is $\Delta N = \sqrt{N}$ and hence the number of particles in the coherent state is determined more and more accurately as N increases: $\Delta N/N = 1/\sqrt{N}$. Assuming $N \gg 1$, the number operator $a^\dagger a$ should therefore return the value N up to corrections of order $1/\sqrt{N}$. What it means is that, in the limit of large N, the coherent state is nearly an eigenstate of the creation operator such that

$$N|f\rangle = a^\dagger a|f\rangle = f a^\dagger|f\rangle \simeq f^* f|f\rangle + O(N)^{-1/2}. \tag{25}$$

In this limit, the variational state Eq. (21) becomes exact up to corrections of order $1/\sqrt{N}$.

What is interesting is the emergence of coherence at the expense of uncertainty in the number. This is the reflection of what is called number-phase uncertainty principle. We can define the "phase operator" θ by

$$a = e^{i\theta}\sqrt{N}, \tag{26}$$

which is clearly consistent with the definition of the number operator $N = a^\dagger a$ is the number operator. This definition is singular when $N = 0$, but because we are interested in states with a macroscopic number of particles in the condensate $N \gg 1$, let us ignore the subtlety that happens only when $N = 0$. From the commutation relation $[N, a] = -a$, we find

$$[N, e^{i\theta}] = -e^{i\theta}, \tag{27}$$

which can be rephrased as

$$N = i\frac{\partial}{\partial\theta}. \tag{28}$$

Therefore, we find the commutator

$$[N, \theta] = i. \tag{29}$$

In analogy to the canonical commutation relation $[x, p] = i\hbar$ giving rise to the uncertainty principle $\Delta x \Delta p \geq \hbar/2$, we find the number-phase uncertainty principle

$$\Delta N \Delta\theta \geq \frac{1}{2}. \tag{30}$$

One can construct "eigenstate" of the phase within the cheat we did with the subtlety with the $N = 0$ state. Consider

$$|\phi\rangle \equiv \sum_{n=1}^{\infty} e^{in\phi}|n\rangle. \tag{31}$$

We now act the "phase" operator $e^{i\theta} = a\frac{1}{\sqrt{N}}$ on this state, and find

$$\begin{aligned} e^{i\theta}|\phi\rangle &= \sum_{n=1}^{\infty} e^{in\phi} a \frac{1}{\sqrt{n}}|n\rangle \\ &= \sum_{n=1}^{\infty} e^{in\phi} \frac{1}{\sqrt{n}}\sqrt{n}|n-1\rangle \\ &= e^{i\phi} \sum_{n=0}^{\infty} e^{in\phi}|n\rangle \\ &= e^{i\phi}(|\phi\rangle + |0\rangle). \end{aligned} \tag{32}$$

Up to the subtlety with the state $|0\rangle$, it is an "eigenstate" of the phase operator. Note that in this state, the number is completely uncertain: the states with different numbers are added together with equal weight (unity).

It is useful to picture what the number-phase uncertainty means. In case of a simple harmonic oscillator, one can write $a = (x + ip)/\sqrt{2\hbar}$. On the classical phase space (x, p), the number operator N is the squared radius from the origin (times a half), while the phase operator $e^{i\theta}$ is nothing but the phase on the complex plane $x + ip$. The uncertainty principle tells you that a quantum mechanical state occupies the minimum area of $2\pi\hbar$ on the phase space. The number eigenstate is therefore approximately a "daughnut" with a radius $2\pi\hbar N \leq x^2 + p^2 \leq 2\pi\hbar(N + 1)$. The phase is completely uncertain in this case. On the other hand, the phase eigenstate would correspond to a thin ray emanating from the origin towards infinity. It has a well-defined phase, while the number is completely uncertain. The coherent state is a compromise between the number and phase. The number is uncertain only by $\Delta N = \sqrt{N}$ and hence the relative error is small $\Delta N/N = 1/\sqrt{N}$ for $N \gg 1$. That allows the phase to be also relatively well determined $\Delta\theta \simeq 1/\sqrt{N}$. It can be viewed as a patch around a point on the phase space spread both along the radial and the angular directions.

Note that the coherent state is not a ground state of the Hamiltonian Eq. (17) but we regard it as a variationa ansatz. If this ansatz is better than the number eigenstate has to be studied including the non-zero modes.

1.4 Excitations above Bose–Einstein Condensate

The fascinating aspect of Bose–Einstein condensates is that a macroscopic number of particles behave collectively as a coherent matter wave. Starting from the classical picture of particles, it is definitely a highly quantum mechanical phenomenon. On the other hand, from the point of view of the field theory formulation, the *classical* field describes the coherent matter wave while its quantization gives ordinary particles. Two approaches are therefore the opposite.

Going back to the real-time action

$$S = \int dt d\vec{x} \left[\psi^* i\hbar\dot{\psi} - \psi^* \frac{-\hbar\Delta}{2m}\psi + \mu\psi^*\psi - \frac{\lambda}{2}\psi^*\psi^*\psi\psi \right], \qquad (33)$$

we write down the Euler–Lagrange equation for the *classical* field $\psi(\vec{x}, t)$

$$i\hbar\dot{\psi} - \frac{-\hbar\Delta}{2m}\psi + \mu\psi - \lambda\psi^*\psi\psi = 0. \qquad (34)$$

The expectation value $\psi = \sqrt{\mu/\lambda}$ we discussed already is a solution to this classical equation of motion.

It is instructive to study the fluctuation around the static expectation value from this equation of motion. The field can fluctuate both in the density and the phase. We parameterize them by

$$\psi = \left(\sqrt{\frac{\mu}{\lambda}} + \chi \right) e^{i\theta} \qquad (35)$$

where both χ and θ are real-valued fields. By plugging this parameterization into the equation of motion Eq. (34), we obtain

$$i\hbar\dot{\chi} - \hbar\langle\psi\rangle\dot{\theta} + \frac{\hbar^2}{2m}(\Delta\chi + 2(\vec{\nabla}\chi)\cdot i\vec{\nabla}\theta + (\langle\psi\rangle + \chi)(-(\vec{\nabla}\theta)^2 + i\Delta\theta))$$
$$+\mu(\langle\psi\rangle + \chi) - \lambda(\langle\psi\rangle + \chi)^3 = 0. \qquad (36)$$

This non-linear equation cannot be solved in general. However, if we are interested in small fluctuations, we can linearize the equation, *i.e.*, drop all terms quadratic in the fluctuation or higher. Then the linearized equation is quite simple:

$$i\hbar\dot{\chi} - \hbar\langle\psi\rangle\dot{\theta} + \frac{\hbar^2}{2m}(\Delta\chi + \langle\psi\rangle i\Delta\theta)) - 2\mu\chi = 0. \qquad (37)$$

Since the real and imaginary parts of the equation must both be satisfied, we find two coupled equations

$$\left(2\mu - \frac{\hbar^2\Delta}{2m} \right) \chi + \hbar\langle\psi\rangle\dot{\theta} = 0 \qquad (38)$$

$$\hbar\dot{\chi} + \frac{\hbar^2}{2m}\langle\psi\rangle\Delta\theta = 0. \tag{39}$$

Taking $\hbar(\partial/\partial t)$ of the first equation and substituting it into the second one, we find

$$-\hbar^2\ddot{\theta} + \left(2\mu - \frac{\hbar^2}{2m}\right)\frac{\hbar^2\Delta}{2m}\theta = 0. \tag{40}$$

Now using the Fourier modes $\theta \propto \sin((Et - \vec{p}\cdot\vec{x})/\hbar)$, we find the dispersion relation of the fluctuation

$$E^2 = \left(2\mu + \frac{\vec{p}^2}{2m}\right)\frac{\vec{p}^2}{2m}. \tag{41}$$

For small momentum in Eq. (41), we find that the energy is linear in momentum. We identify this limit as the sound wave. Note that the χ field is fluctuation in the density $\rho = \psi^*\psi = (\langle\psi\rangle + \chi)^2$, and is related to the plane wave of θ by Eq. (38). Therefore the wave is indeed a progation of density fluctuation, which justifies the interpretation. The sound speed is then directly read off from the dispersion relation Eq. (41) for small momentum

$$c_s^2 = \left.\frac{E^2}{\vec{p}^2}\right|_{\vec{p}\to 0} = \frac{\mu}{m}. \tag{42}$$

After quantization, this becomes a quasi-particle (elementary excitation of a collective system) called phonon with the energy $E = c_s|\vec{p}|$.

On the other hand, at large momentum, the dispersion relation Eq. (41) can be approxiimated as

$$E \simeq \frac{\vec{p}^2}{2m} + \mu + O(\vec{p}^2)^{-1} \tag{43}$$

and hence it is the same as the single particle excitation except the offset $\mu = c_s^2 m$. This is called the excitation in the free-particle regime.

In the case of liquid ^{4}He, the interaction is quite strong and the linearized analysis fails. The dispersion relation rises linearly in the phonon-regime but it turns around the develops a minimum called “roton.” On the other hand, recent developement of Bose–Einstein condensate in atomic gas made the comparison of data to perturbation theory possible. A small complication, however, is that the system size is somewhat small ($\sim 10^7$ particles) and the finite-size corrections are important especially for the phonon-regime.

You can read about this in a good review by Dan Stamper-Kurn in our Department (together with Ketterle at MIT) in cond-mat/0005001.

How do we describe the quasi-particle excitation with the operator language? To study this, we write down the Hamiltonian in the momentum space using formulae in the previous lecture note,

$$H = \sum_{\vec{p}} \left(\frac{\vec{p}^2}{2m} - \mu \right) a(\vec{p})^\dagger a(\vec{p}) + \frac{1}{2} \frac{\lambda}{L^3} \sum_{\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4} a^\dagger(\vec{p}_4) a^\dagger(\vec{p}_3) a(\vec{p}_2) a(\vec{p}_1) \delta_{\vec{p}_1 + \vec{p}_2, \vec{p}_3 + \vec{p}_4}. \tag{44}$$

Because we took the coherent state for $a(0) = \sqrt{\mu/\lambda} L^{3/2}$ as the variational ansatz, the Hamiltonian for the non-zero modes is

$$H = \sum_{\vec{p}} \left(\frac{\vec{p}^2}{2m} - \mu \right) a(\vec{p})^\dagger a(\vec{p}) + \frac{1}{2} \lambda \sum_{\vec{p}} \frac{\mu}{\lambda} \left(a(\vec{p}) a(-\vec{p}) + a^\dagger(\vec{p}) a^\dagger(-\vec{p}) + 4 a^\dagger(\vec{p}) a(\vec{p}) \right), \tag{45}$$

where interaction terms proportional to λ among non-zero modes are omitted. Note that the second term does not vanish in the weak-coupling limit $\lambda \to 0$ for fixed μ (*i.e.*, fixed sound speed) because of the condensate μ/λ, while the interaction terms vanish in the same limit. Therefore, it makes sense to retain only the terms above and drop the interaction terms to study the behavior of the non-zero modes. This Hamiltonian is rather peculiar because it has a term with creation operators only or annihilation operators only. In other words, this Hamiltonian no longer conserves the number of particles because of the lack of the phase invariance $a(\vec{p}) \to e^{i\theta} a(\vec{p})$.

Bogoliubov found a way to diagonalize this Hamiltonian. Among creation and annihilation operators, both $a(\vec{p})$ and $a^\dagger(-\vec{p})$ change the momentum of the state by $-\vec{p}$, either by annihilating momentum $\vec{p}$ or creating momentum $-\vec{p}$. Because the number conservation is violated, creation and annihilation operator can now mix, as long as they share the same momentum. Therefore, we can consider the Boliubov transformation

$$b(\vec{p}) = a(\vec{p}) \cosh \eta + a(-\vec{p})^\dagger \sinh \eta, \tag{46}$$

$$b(-\vec{p})^\dagger = a(\vec{p}) \sinh \eta + a(-\vec{p})^\dagger \cosh \eta. \tag{47}$$

The point is that the new operators defined this way also satisfy the same commutation relation $[b(\vec{p}), b^\dagger(\vec{q})] = \delta_{\vec{p},\vec{q}}$ and can be regarded as new creation and annihilation operators. By suitably choosing the parameter η, we can make Hamiltonian Eq. (45) not to have terms bb or $b^\dagger b^\dagger$. Choosing

$$\cosh 2\eta = \frac{\frac{\vec{p}^2}{2m}+\mu}{\sqrt{\frac{\vec{p}^2}{2m}\left(\frac{\vec{p}^2}{2m}+2\mu\right)}}, \qquad \sinh 2\eta = \frac{\mu}{\sqrt{\frac{\vec{p}^2}{2m}\left(\frac{\vec{p}^2}{2m}+2\mu\right)}}, \tag{48}$$

we obtain the Hamiltonian

$$H = \sum_{\vec{p}} \left[\sqrt{\frac{\vec{p}^2}{2m}\left(\frac{\vec{p}^2}{2m}+2\mu\right)} b(\vec{p})^\dagger b(\vec{p}) - \frac{1}{2}\left(\frac{\vec{p}^2}{2m}+\mu\right) + \frac{1}{2}\sqrt{\frac{\vec{p}^2}{2m}\left(\frac{\vec{p}^2}{2m}+2\mu\right)} \right]. \tag{49}$$

We used the fact that the summation over $\vec{p}$ includes $-\vec{p}$ and combined both contributions to simplify the expression. The ground state of this Hamiltonian is clearly the state annihilated by the new annihilation operators $b(\vec{p})$, and excitations are created by $b(\vec{p})^\dagger$. The excitation energy for the creation operator $b(\vec{p})^\dagger$ agrees with that obtained from the classical analysis Eq. (41).

How is the ground state $b(\vec{p})|g\rangle = 0$ related to the original Fock states? It is easy to show that the unitarity operator

$$U(\vec{p}) = e^{(a(\vec{p})a(-\vec{p}) - a(\vec{p})^\dagger a(-\vec{p})^\dagger)\eta} \tag{50}$$

relates two sets of operators

$$U(\vec{p})a(\vec{p})U(\vec{p})^\dagger = b(\vec{p}). \tag{51}$$

Therefore, the state $|g(\vec{p})\rangle$ annihilated by $b(\vec{p})$ is written as

$$|g(\vec{p})\rangle = U(\vec{p})|0\rangle = e^{(a(\vec{p})a(-\vec{p}) - a(\vec{p})^\dagger a(-\vec{p})^\dagger)\eta}|0\rangle. \tag{52}$$

This state is different from the coherent state because it does not give an expectation value of the annihilation operator $a(\vec{p})$, but it has a *pair-wise* condensate $\langle g(\vec{p})|a(\vec{p})a(-\vec{p})|g(\vec{p}\rangle \neq 0$. Therefore, it is fair to say that not only the zero mode is condensed in Bose–Einstein condensate, non-zero modes are also condensed when η is sizable, *i.e.*, $\vec{p}^2/2m \lesssim \mu$. This is precisely the momentum range where the naive formula for the occupation number $n(\vec{p}) = 1/(e^{\beta(\vec{p}^2/2m-\mu)} - 1)$ is ill-defined (negative).

Another interesting point is that there is an additional negative constant in the Hamiltonian Eq. (49). The variational ansatz for the full Hamiltonian is

$$|f\rangle \prod_{\vec{p}} |g(\vec{p})\rangle, \tag{53}$$

where $|f\rangle$ with $f = \sqrt{\mu/\lambda}$ is the coherent for the zero mode and $|g(\vec{p})\rangle$ is the Bogoliubov transformed ground state defined in Eq. (52). The constant term contributes to the expectation value of the full Hamiltonian in the variational method, and makes the variational state have lower energy than the number eigenstate.

Many phenomenological consequences of Bose–Einstein condensate can be worked out from simple classical analyses.