Quantum Field Theory in Condensed Matter Physics

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Description: an introduction to quantum field theory and quantum entanglement for macroscopic quantum phenomena: superfluidity in ultracold atomic gases and liquid helium and superconductivity in metals.

First part (Salasnich, 12 hours)

- Von Neuman entropy and entanglement for bipartite systems. Interacting bosons in a double-well potential: coherence visibility, Fisher information and entanglement entropy.
Second part (Dell’Anna, 12 hours)

- BCS theory of metals by functional integration. Hubbard-Stratonovich transformation and the bosonic field of pairing.
- Saddle point approximation: gap equation and critical temperature. Ginzburg-Landau theory from the BCS effective action.
- Gaussian fluctuations: Goldstone mode, Meissner effect and Higgs mechanism.
N. Nagaosa, Quantum Field Theory in Condensed Matter Physics (Springer, 1999).

A. Altland and B. Simons, Condensed Matter Field Theory (Cambridge Univ. Press, 2006).

M. Le Bellac, A Short Introduction to Quantum Information and Quantum Computation (Cambridge Univ. Press, 2006).

1.1 Partition function of bosons (I)

Let us consider a gas of non-interacting bosons in thermal equilibrium with a bath at the temperature $T$. The relevant quantity to calculate all thermodynamical properties of the system is the grand-canonical partition function $Z$, given by

$$Z = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}]$$

(1)

where $\beta = 1/(k_B T)$ with $k_B$ the Boltzmann constant,

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha} \hat{N}_{\alpha},$$

(2)

is the quantum Hamiltonian,

$$\hat{N} = \sum_{\alpha} \hat{N}_{\alpha}$$

(3)

is total number operator, and $\mu$ is the chemical potential, fixed by the conservation of the average particle number. Here $\alpha$ represents the set of single-particle quantum numbers.
1.1 Partition function of bosons (II)

Figure: Ground-state of non-interacting bosons (a) and fermions (b) is a harmonic trap. Horizontal lines describe single-particle energies $\epsilon_\alpha$.

The single-particle-state number operator $\hat{N}_\alpha$ is given by

$$\hat{N}_\alpha = \hat{c}_\alpha^+ \hat{c}_\alpha ,$$

(4)

where the operators $\hat{c}_\alpha$ and $\hat{c}_\alpha^+$ act in the Fock space of the identical bosons. A generic state of this Fock space is given by

$$|\{n_\alpha\}\rangle = |... n_\alpha ... n_\beta ...\rangle ,$$

(5)

meaning that there are $n_\alpha$ bosons in the single-particle state $|\alpha\rangle$, $n_\beta$ bosons in the single-particle state $|\beta\rangle$, et cetera.
The operators $\hat{c}_\alpha$ and $\hat{c}_\alpha^+$ are called annihilation and creation operators because they respectively destroy and create one boson in the single-particle state $|\alpha\rangle$, namely

$$\hat{c}_\alpha |... n\alpha ...\rangle = \sqrt{n\alpha} |... n\alpha - 1 ...\rangle, \quad (6)$$

$$\hat{c}_\alpha^+ |... n\alpha ...\rangle = \sqrt{n\alpha + 1} |... n\alpha + 1 ...\rangle. \quad (7)$$

Note that these properties follow directly from the commutation relations

$$[\hat{c}_\alpha, \hat{c}_\beta^+] = \delta_{\alpha,\beta}, \quad [\hat{c}_\alpha, \hat{c}_\beta] = [\hat{c}_\alpha^+, \hat{c}_\beta^+] = 0, \quad (8)$$

where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. 

1.1 Partition function of bosons (III)
The vacuum state, where there are no particles, can be written as

\[ |0\rangle = |\{0\}\rangle = |...0...0...\rangle , \]  
(9)

and

\[ \hat{c}_\alpha |0\rangle = 0 , \quad \hat{c}_\alpha^+ |0\rangle = |1_\alpha\rangle = |\alpha\rangle , \]  
(10)

where \( |\alpha\rangle \) is such that

\[ \langle r |\alpha\rangle = \phi_\alpha (r) . \]  
(11)

From Eqs. (6) and (7) it follows immediately that \( \hat{N}_\alpha \) counts the number of bosons in the single-particle state \( |\alpha\rangle \), i.e.

\[ \hat{N}_\alpha |... n_\alpha ...\rangle = n_\alpha |... n_\alpha ...\rangle . \]  
(12)
1.1 Partition function of bosons (V)

Taking into account the properties of Fock state, from the definition

\[ Z = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] \]  

(13)

of the grand-canonical partition function we find

\[
Z = \sum_{\{n_{\alpha}\}} \langle\{n_{\alpha}\}| e^{-\beta(\hat{H} - \mu \hat{N})}|\{n_{\alpha}\}\rangle = \sum_{\{n_{\alpha}\}} \langle\{n_{\alpha}\}| e^{-\beta \sum_{\alpha}(\epsilon_{\alpha} - \mu) \hat{N}_{\alpha}}|\{n_{\alpha}\}\rangle \\
= \sum_{\{n_{\alpha}\}} e^{-\beta \sum_{\alpha}(\epsilon_{\alpha} - \mu) n_{\alpha}} = \prod_{\{n_{\alpha}\}} \sum_{\alpha} e^{-\beta(\epsilon_{\alpha} - \mu) n_{\alpha}} \\
= \prod_{\alpha} \sum_{n_{\alpha}} e^{-\beta(\epsilon_{\alpha} - \mu) n_{\alpha}} = \prod_{\alpha} \sum_{n=0}^{\infty} \left(e^{-\beta(\epsilon_{\alpha} - \mu)}\right)^n 
\]

(14)

and finally

\[
Z = \prod_{\alpha} \frac{1}{1 - e^{-\beta(\epsilon_{\alpha} - \mu)}}. 
\]

(15)
1.1 Partition function of bosons (VI)

Quantum statistical mechanics dictates that the thermal average of any operator \( \hat{A} \) is obtained as

\[
\langle \hat{A} \rangle = \frac{1}{Z} \text{Tr}[\hat{A} e^{-\beta(\hat{H} - \mu \hat{N})}] . \tag{16}
\]

It is then quite easy to show that

\[
\langle \hat{H}' \rangle = \frac{1}{Z} \text{Tr}[(\hat{H} - \mu \hat{N}) e^{-\beta(\hat{H} - \mu \hat{N})}] = -\frac{\partial}{\partial \beta} \ln \left( \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] \right) = -\frac{\partial}{\partial \beta} \ln(Z) . \tag{17}
\]

By using Eq. (15) we immediately obtain

\[
\ln(Z) = \sum_{\alpha} \ln \left( 1 - e^{-\beta(\epsilon_{\alpha} - \mu)} \right) , \tag{18}
\]

and finally from Eq. (17) we get

\[
\langle \hat{H} \rangle = \sum_{\alpha} \frac{\epsilon_{\alpha}}{e^{\beta(\epsilon_{\alpha} - \mu)} - 1} \quad \text{and also} \quad \langle \hat{N} \rangle = \sum_{\alpha} \frac{1}{e^{\beta(\epsilon_{\alpha} - \mu)} - 1} . \tag{19}
\]
1.2 Bosonic fields (I)

Introducing the bosonic field operator

\[ \hat{\psi}(r) = \sum_{\alpha} \hat{c}_{\alpha} \phi_{\alpha}(r) , \]  

(20)

one immediately finds

\[ \hat{H} = \int d^3r \, \hat{\psi}^+(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \hat{\psi}(r) = \sum_{\alpha} \epsilon_{\alpha} \hat{c}_{\alpha}^+ \hat{c}_{\alpha} , \]

(21)

where \( U(r) \) is the external trapping potential of bosons and \( \phi_{\alpha}(r) \) are the orthonormalized single-particle eigenfunctions of the single-particle stationary Schrödinger equation

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \phi_{\alpha}(r) = \epsilon_{\alpha} \phi_{\alpha}(r) \]

(22)

with single-particle eigenvalues \( \epsilon_{\alpha} \). Again \( \alpha \) represents the set of single-particle quantum numbers.
1.2 Bosonic fields (II)

A remarkable property of the adjoint field operator

\[ \hat{\psi}^+(r) = \sum_\alpha \hat{c}_\alpha^+ \phi^*_\alpha(r) , \]  

is the following:

\[ \hat{\psi}^+(r) |0\rangle = |r\rangle . \]  

That is the operator \( \hat{\psi}^+(r) \) creates a particle in the state \( |r\rangle \) from the vacuum state \( |0\rangle \). In fact,

\[ \hat{\psi}^+(r) |0\rangle = \sum_\alpha \hat{c}_\alpha^+ \phi^*_\alpha(r) |0\rangle = \sum_\alpha \hat{c}_\alpha^+ \langle \alpha |r\rangle |0\rangle \]

\[ = \sum_\alpha \hat{c}_\alpha^+ |0\rangle \langle \alpha |r\rangle = \sum_\alpha |\alpha\rangle \langle \alpha |r\rangle = |r\rangle , \]

because of the completeness relation (closure)

\[ \sum_\alpha |\alpha\rangle \langle \alpha | = 1 . \]
It is straightforward to show that the bosonic field operators satisfies the following commutation rules

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}').$$  \hspace{1cm} (26)

and also

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = [\hat{\psi}^+(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')] = 0.$$  \hspace{1cm} (27)

Let us prove Eq. (26). By using the expansion of the field operators one finds

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^+(\mathbf{r}')] = \sum_{\alpha,\beta} \phi_\alpha(\mathbf{r}) \phi^*_\beta(\mathbf{r}') \hat{c}_\alpha \hat{c}^+_\beta$$

$$= \sum_{\alpha,\beta} \phi_\alpha(\mathbf{r}) \phi^*_\beta(\mathbf{r}') \delta_{\alpha,\beta} = \sum_{\alpha} \phi_\alpha(\mathbf{r}) \phi^*_\alpha(\mathbf{r}')$$

$$= \sum_{\alpha} \langle \mathbf{r} | \alpha \rangle \langle \alpha | \mathbf{r}' \rangle = \langle \mathbf{r} | \sum_{\alpha} | \alpha \rangle \langle \alpha | \mathbf{r}' \rangle$$

$$= \langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}').$$
1.3 Bosonic coherent states (I)

It is interesting to observe that

$$\langle n_\alpha | \hat{c}_\alpha | n_\alpha \rangle = \langle n_\alpha | \hat{c}^+_\alpha | n_\alpha \rangle = 0. \tag{28}$$

This result is due to the fact that the expectation value is performed with the Fock state $|n_\alpha\rangle$, which simply means that the number of bosons in the single-particle state $\alpha$ is fixed because

$$\hat{N}_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle, \tag{29}$$

with $\hat{N}_\alpha = \hat{c}^+_\alpha \hat{c}_\alpha$. In some cases the number of bosons is not fixed, in other words the system is not in a pure Fock state. For example, the radiation field of a well-stabilized laser device operating in a single mode $|\alpha\rangle$ is described by a coherent state $|c_\alpha\rangle$, such that

$$\hat{c}_\alpha |c_\alpha\rangle = c_\alpha |c_\alpha\rangle. \tag{30}$$

The coherent state $|c_\alpha\rangle$, introduced in 1963 by Roy Glauber, is thus the eigenstate of the annihilation operator $\hat{c}_\alpha$ with complex eigenvalue $c_\alpha = |c_\alpha| e^{i\theta_\alpha}$. 
The coherent state $|c_\alpha\rangle$ does not have a fixed number of photons, i.e. it is not an eigenstate of the number operator $\hat{N}_\alpha$, and it is not difficult to show that $|c_\alpha\rangle$ can be expanded in terms of number (Fock) states $|n_\alpha\rangle$ as follows

$$|c_\alpha\rangle = e^{-|c_\alpha|^2/2} \sum_{n_\alpha=0}^{\infty} \frac{c_{n_\alpha}}{\sqrt{n_\alpha!}} |n_\alpha\rangle = e^{-|c_\alpha|^2/2} e^{c_\alpha \hat{c}_\alpha^+} |0\rangle,$$  

(31)

taking into account the normalization to one, i.e.

$$\langle c_\alpha | c_\alpha \rangle = 1.$$  

(32)

From Eq. (30) one immediately finds

$$\bar{N}_\alpha = \langle c_\alpha | \hat{N}_\alpha | c_\alpha \rangle = |c_\alpha|^2,$$  

(33)

and it is natural to set

$$c_\alpha = \sqrt{\bar{N}_\alpha} e^{i\theta_\alpha},$$  

(34)

where $\bar{N}_\alpha$ is the average number of photons in the coherent state, while $\theta_\alpha$ is the phase of the coherent state.
1.3 Bosonic coherent states (III)

We observe that

\[ \langle c_\alpha | \hat{N}_\alpha^2 | c_\alpha \rangle = |c_\alpha|^2 + |c_\alpha|^4 = \bar{N}_\alpha + \bar{N}_\alpha^2 \]  

\[ \text{(35)} \]

and consequently

\[ \langle c_\alpha | \hat{N}_\alpha^2 | c_\alpha \rangle - \langle c_\alpha | \hat{N}_\alpha | c_\alpha \rangle^2 = \bar{N}_\alpha \ , \]  

\[ \text{(36)} \]

while for the Fock states

\[ \langle n_\alpha | \hat{N}_\alpha^2 | n_\alpha \rangle = n_\alpha^2 \text{ and consequently } \langle n_\alpha | \hat{N}_\alpha^2 | n_\alpha \rangle - \langle n_\alpha | \hat{N}_\alpha | n_\alpha \rangle^2 = 0 \ . \]  

\[ \text{(37)} \]
1.3 Bosonic coherent states (IV)

The coherent state $|c_\alpha\rangle$ satisfies the remarkable completeness relation

$$\int \frac{dc_\alpha^* dc_\alpha}{2\pi i} |c_\alpha\rangle \langle c_\alpha| = 1 .$$

(38)

Let us suppose that $|c_\alpha\rangle$ is the coherent state of the single-particle state $|\alpha\rangle$ and $|c_\beta\rangle$ is the coherent state of the single-particle state $|\beta\rangle$. It is quite easy to prove that they are not orthogonal:

$$\langle c_\alpha| c_\beta \rangle = e^{-\frac{1}{2}(|c_\alpha|^2 + |c_\beta|^2 - 2c_\alpha^* c_\beta)} .$$

(39)

In fact,

$$\langle c_\alpha| c_\beta \rangle = \langle c_\alpha| \sum_{n_\beta=0}^{\infty} e^{-|c_\beta|^2/2} \frac{c_\beta^{n_\beta}}{\sqrt{n_\beta}!} |n_\beta\rangle$$

$$= \sum_{n_\alpha=0}^{\infty} \sum_{n_\beta=0}^{\infty} e^{-|c_\alpha|^2/2} e^{-|c_\beta|^2/2} (c_\alpha^*)^{n_\alpha} \frac{n_\alpha!}{\sqrt{n_\alpha}!} \frac{c_\beta^{n_\beta}}{\sqrt{n_\beta}!} \langle n_\alpha| n_\beta\rangle$$

$$= e^{-(|c_\beta|^2 + |c_\alpha|^2)/2} \sum_{n_\alpha=0}^{\infty} \frac{(c_\alpha^* c_\beta)^{n_\alpha}}{n_\alpha!} = e^{-(|c_\beta|^2 + |c_\alpha|^2)/2} e^{c_\alpha^* c_\beta} .$$
1.3 Bosonic coherent states (V)

We can now introduce the general coherent state

$$|\psi\rangle = \prod_{\alpha} |c_{\alpha}\rangle = e^{-\sum_{\alpha}|c_{\alpha}|^2/2} e^{\sum_{\alpha} c_{\alpha} \hat{c}_{\alpha}^+} |0\rangle,$$

such that

$$\hat{c}_{\alpha}|\psi\rangle = c_{\alpha}|\psi\rangle \quad \text{for any } \alpha.$$  \hspace{1cm} (41)

Notice that $|\psi\rangle$ is the tensor product of all coherent states $|c_{\alpha}\rangle$ taking into account their normalization to one. As a consequence, we get

$$\langle \psi | \psi \rangle = 1.$$  \hspace{1cm} (42)

The overlap between two general coherent states $|\psi\rangle$ and $|\tilde{\psi}\rangle$ is instead given by

$$\langle \psi | \tilde{\psi} \rangle = e^{-\frac{1}{2} \sum_{\alpha} [c_{\alpha}^*(c_{\alpha} - \tilde{c}_{\alpha}) - (c_{\alpha}^*-\tilde{c}_{\alpha}^*)\tilde{c}_{\alpha}]}.$$  \hspace{1cm} (43)
Moreover, it is possible to prove that the set of coherent states \( \{ |c_\alpha\rangle \} \) obtained by varying \( \alpha \) is (over)complete and the generalized coherent state \( |\psi\rangle \) satisfies the completeness relation

\[
\int d[\psi^*, \psi] |\psi\rangle \langle \psi| = 1 ,
\]

where the integration measure is defined by

\[
\int d[\psi^*, \psi] = \prod_\alpha \int \frac{dc^*_\alpha dc_{\alpha}}{2\pi i} .
\]
1.3 Bosonic coherent states (VII)

Given the field operator

$$\hat{\psi}(r) = \sum_{\alpha} \hat{c}_\alpha \phi_\alpha(r)$$  \hspace{1cm} (46)

one immediately finds that the generalized coherent state $|\psi\rangle$ is eigenstate of the field operator $\hat{\psi}(r)$, namely

$$\hat{\psi}(r)|\psi\rangle = \psi(r)|\psi\rangle,$$  \hspace{1cm} (47)

where

$$\psi(r) = \sum_{\alpha} c_\alpha \phi_\alpha(r)$$  \hspace{1cm} (48)

is the “classical” complex field associated to the field operator $\hat{\psi}(r)$. Notice that $c_\alpha$ and $\psi(r)$ represent the same complex field in reciprocal spaces, and the integration measure can also be written as

$$\int d[\psi^*, \psi] = \prod_r \int \frac{d\psi^*(r)d\psi(r)}{2\pi i}. \hspace{1cm} (49)$$
1.4 Functional integration of bosonic fields (I)

The partition function

\[ Z = \text{Tr}[e^{-\beta(\hat{H} - \mu\hat{N})}] \] (50)

of interacting bosons cannot be calculated exactly. In general, the quantum-field-theory Hamiltonian is given by

\[
\hat{H} = \int d^3r \ \hat{\psi}^+(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \hat{\psi}(r) + \frac{1}{2} \int d^3r \ d^3r' \ \hat{\psi}^+(r) \hat{\psi}^+(r') V(r, r') \hat{\psi}(r') \hat{\psi}(r), \] (51)

where \( V(r, r') \) is the inter-particle interaction, while the number operator reads

\[ \hat{N} = \int d^3r \ \hat{\psi}^+(r)\hat{\psi}(r). \] (52)
By expanding the field operator \( \hat{\psi}(r) \) as

\[
\hat{\psi}(r) = \sum_{\alpha} \hat{c}_\alpha \phi_\alpha(r)
\]

(53)

where \( \phi_\alpha(r) \) are the orthonormal eigenfunctions of the non-interacting problem with single-particle energies \( \epsilon_\alpha \), one finds

\[
\hat{H} = \sum_{\alpha} \epsilon_\alpha \hat{c}_\alpha^+ \hat{c}_\alpha + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \hat{c}_\alpha^+ \hat{c}_\beta^+ \hat{c}_\delta \hat{c}_\gamma
\]

(54)

where

\[
V_{\alpha\beta\delta\gamma} = \int d^3r \ d^3r' \ \phi_\alpha^*(r) \ \phi_\beta^*(r') \ V(r, r') \ \phi_\delta(r') \ \phi_\gamma(r)
\]

(55)

and also

\[
\hat{N} = \sum_{\alpha} \hat{c}_\alpha^+ \hat{c}_\alpha
\]

(56)
The partition function $\mathcal{Z}$ can be expressed as a functional integral taking into account that the trace of an operator can be performed by using any complete set of basis states, and in particular the basis of generalized coherent states. Thus, we write

$$\mathcal{Z} = \text{Tr}[e^{-\beta(\hat{H} - \mu \hat{N})}] = \int d[\psi^*, \psi] \langle \psi | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi \rangle,$$

(57)

where $|\psi\rangle$ is the generalized coherent state and

$$\int d[\psi^*, \psi] = \prod_\alpha \int \frac{dc'^* \cdot dc_\alpha}{2\pi i} = \prod_r \int \frac{d\psi^*(r) \cdot d\psi(r)}{2\pi i}.$$ 

(58)

Moreover, we observe that

$$\langle \psi | \tilde{\psi} \rangle = e^{-\frac{1}{2} \sum_\alpha [c^*_\alpha (c_\alpha - \tilde{c}_\alpha) - (c^*_\alpha - \tilde{c}^*_\alpha) \tilde{c}_\alpha]}$$

$$= e^{-\frac{1}{2} \int d^3r [\psi^*(r) (\psi(r) - \tilde{\psi}(r)) - (\psi^*(r) - \tilde{\psi}^*(r)) \tilde{\psi}(r)]}.$$ 

(59)
The main problem in the functional representation of the partition function $\mathcal{Z}$ is the calculation of
\[
\langle \psi | e^{-\beta (\hat{H} - \mu \hat{N})} | \psi \rangle .
\] (60)

The simple semiclassical approximation
\[
\langle \psi | e^{-\beta (\hat{H} - \mu \hat{N})} | \psi \rangle \simeq e^{-\beta \langle \psi | (\hat{H} - \mu \hat{N}) | \psi \rangle}
\] (61)
gives
\[
\mathcal{Z} = \int d[\psi^*, \psi] e^{-\beta (E[\psi^*, \psi] - \mu N[\psi^*, \psi])}
\] (62)
where
\[
E[\psi^*, \psi] = \int d^3r \psi^*(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \psi(r)
+ \frac{1}{2} \int d^3r d^3r' |\psi(r)|^2 V(r, r') |\psi'(r')|^2 ,
\] (63)
and
\[
N[\psi^*, \psi] = \int d^3r \psi^*(r) \psi(r) .
\] (64)
1.4 Functional integration of bosonic fields (V)

To better treat the expectation value

\[ \langle \psi | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi \rangle \]  

(65)

we write \( |\psi_0\rangle \) instead of \( |\psi\rangle \) and also (with \( M \to \infty \))

\[ \Delta \tau = \frac{\hbar \beta}{M}. \]  

(66)

In this way

\[ \langle \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi_0 \rangle = \langle \psi_0 | e^{-M \Delta \tau (\hat{H} - \mu \hat{N})/\hbar} | \psi_0 \rangle \]

\[ = \langle \psi_0 | \left( e^{-\Delta \tau (\hat{H} - \mu \hat{N})/\hbar} \right)^M | \psi_0 \rangle \]

\[ = \langle \psi_0 | e^{-\Delta \tau (\hat{H} - \mu \hat{N})/\hbar} ... e^{-\Delta \tau (\hat{H} - \mu \hat{N})/\hbar} | \psi_0 \rangle. \]  

(67)

Then we insert \( M - 1 \) completeness relations for the general coherent state \( |\psi_j\rangle \) \( (j = 1, ..., M - 1) \)

\[ \int d[\psi^*_j, \psi_j] |\psi_j\rangle \langle \psi_j| = 1 \]  

(68)
and obtain

\[ \langle \psi_0 | e^{-\beta (\hat{H} - \mu \hat{N})} | \psi_0 \rangle = \int \left( \prod_{j=1}^{M-1} d[\psi^*_j, \psi_j] \right) \prod_{j=1}^{M} \langle \psi_j | e^{-\Delta \tau (\hat{H} - \mu \hat{N}) / \hbar} | \psi_{j-1} \rangle \]

imposing that \( |\psi_0\rangle = |\psi_M\rangle \). In the limit \( M \to \infty \) one has \( \Delta \tau \to 0 \) and also

\[ \langle \psi_j | e^{-\Delta \tau (\hat{H} - \mu \hat{N}) / \hbar} | \psi_{j-1} \rangle = \langle \psi_j | \psi_{j-1} \rangle e^{-\Delta \tau (E[\psi^*_j, \psi_j] - \mu N[\psi^*_j, \psi_j]) / \hbar} \]  

Moreover, the overlap between two general coherent states reads

\[ \langle \psi_j | \psi_{j-1} \rangle = e^{-\Delta \tau / 2} \int d^3 r \left( \psi^*_j(r) \frac{[\psi_j(r) - \psi_{j-1}(r)]}{\Delta \tau} - \psi_j(r) \frac{[\psi^*_j(r) - \psi^*_{j-1}(r)]}{\Delta \tau} \right) . \]

Finally, setting \( \tau = j \Delta \tau \), \( \psi(r, \tau) = \psi_j(r) \) and

\[ \frac{\partial}{\partial \tau} \psi(r, \tau) = \frac{[\psi_j(r) - \psi_{j-1}(r)]}{\Delta \tau} \]
we obtain for the partition function $Z$ the elegant result

$$Z = \int D[\psi, \psi^*] \exp \left\{ - \frac{S[\psi, \psi^*]}{\hbar} \right\}, \quad (73)$$

where

$$S[\psi, \psi^*] = \int_0^{\hbar \beta} d\tau \int d^3r \, L(\psi^*, \psi) \quad (74)$$

is the Euclidean action of Lagrangian density

$$L(\psi^*, \psi) = \frac{\hbar}{2} \left( \psi^*(r, \tau) \frac{\partial}{\partial \tau} \psi(r, \tau) - \psi(r, \tau) \frac{\partial}{\partial \tau} \psi^*(r, \tau) \right)$$

$$+ \psi^*(r, \tau) \left( - \frac{\hbar^2}{2m} \nabla^2 + U(r) - \mu \right) \psi(r, \tau)$$

$$+ \frac{1}{2} \int d^3r' \, |\psi(r', \tau)|^2 \, V(r, r') \, |\psi(r, \tau)|^2 \quad (75)$$

with $\psi(r, 0) = \psi(r, \hbar \beta)$ and

$$\int D[\psi, \psi^*] = \prod_{(r, \tau)} \int \frac{d\psi^*(r, \tau) \, d\psi(r, \tau)}{2\pi i}. \quad (76)$$
We consider a D-dimensional \((D = 1, 2, 3)\) Bose gas of ultracold and dilute neutral atoms either noninteracting or with a contact interaction, namely

\[
V(r - r') = g \delta(r - r') ,
\]

where \(\delta(x)\) is the Dirac delta function and \(g\) the strength of the interaction. We adopt the path integral formalism, where the atomic bosons are described by the complex field \(\psi(r, \tau)\).

The Euclidean Lagrangian density of the free system in a D-dimensional box of volume \(L^D\) and with chemical potential \(\mu\) is given by

\[
\mathcal{L} = \psi^* \left[ \frac{\hbar}{2m} \nabla^2 - \mu \right] \psi + \frac{1}{2} g |\psi|^4 ,
\]

where \(g\) is the strength of the contact inter-atomic coupling.
We have seen that the partition function $Z$ of the system at temperature $T$ can then be written as

$$Z = \int \mathcal{D}[\psi, \psi^*] \exp \left\{ - \frac{S[\psi, \psi^*]}{\hbar} \right\},$$

(79)

where

$$S[\psi, \psi^*] = \int_0^{\hbar \beta} d\tau \int_{L^D} d^D r \mathcal{L}(\psi, \psi^*)$$

(80)

is the Euclidean action and $\beta \equiv 1/(k_B T)$ with $k_B$ being Boltzmann’s constant.

The grand potential $\Omega$ of the system, which is a function of $\mu$, $T$ and $g$, is then obtained as

$$\Omega = -\frac{1}{\beta} \ln Z.$$  

(81)
2.1 Broken symmetry and ideal Bose gas (III)

We work in the superfluid phase where the global U(1) gauge symmetry of the system is spontaneously broken. For this reason we set

\[ \psi(\mathbf{r}, \tau) = \psi_0 + \eta(\mathbf{r}, \tau), \quad (82) \]

where \( \eta(\mathbf{r}, \tau) \) is the complex field of bosonic fluctuations around the order parameter \( \psi_0 \) (condensate in 3D or quasi-condensate in 1D and 2D) of the system. We suppose that \( \psi_0 \) is constant in time, uniform in space and real.

First we analyze the case with \( g = 0 \), where exact analytical results can be obtained in any spatial dimension \( D \). In this case the Lagrangian density reads

\[ \mathcal{L} = -\mu \psi_0^2 + \eta^*(\mathbf{r}, \tau) \left[ \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \eta(\mathbf{r}, \tau). \quad (83) \]
The Euclidean action of the ideal Bose gas can be written in a diagonal form as

\[ S[\psi, \psi^*] = -\mu \psi_0^2 \hbar \beta L^D + \sum_Q \hbar \lambda_Q \eta_Q^* \eta_Q \]  

(84)

where \( Q = (q, i\omega_n) \) is the \( D + 1 \) vector denoting the momenta \( q \) and bosonic Matsubara frequencies \( \omega_n = 2\pi n/(\beta \hbar) \), and

\[ \lambda_Q = \beta (-i\hbar \omega_n + \frac{\hbar^2 q^2}{2m} - \mu) . \]  

(85)

Here \( \eta_Q = \eta_q, i\omega_n = \eta_q, n \) is the Fourier transform of \( \eta(r, \tau) \) and the quantization of frequencies \( \omega_n \) is a consequence of the periodicity \( \eta(r, \tau + \hbar \beta) = \eta(r, \tau) \).
2.1 Broken symmetry and ideal Bose gas (V)

Taking into account that

$$\int \mathcal{D}[\eta, \eta^*] \exp \left\{ - \sum_Q \lambda_Q \eta^*_Q \eta_Q \right\} = \frac{1}{\prod_Q \lambda_Q} \quad (86)$$

and

$$\sum_{n=-\infty}^{+\infty} \ln (-i n + a) = \frac{1}{2} \sum_{n=-\infty}^{+\infty} \ln (n^2 + a^2), \quad (87)$$

one finds the grand potential

$$\Omega = -\mu \psi_0^2 L^D + \frac{1}{\beta} \sum_Q \ln (\lambda_Q)$$

$$= -\mu \psi_0^2 L^D + \frac{1}{2\beta} \sum_q \sum_{n=-\infty}^{+\infty} \ln [\beta^2 (\hbar^2 \omega_n^2 + \xi_q^2)] \quad (88)$$

where $\xi_q$ is the shifted free-particle spectrum, i.e.

$$\xi_q = \frac{\hbar^2 q^2}{2m} - \mu. \quad (89)$$
The sum over bosonic Matsubara frequencies gives

\[ \frac{1}{2\beta} \sum_{n=-\infty}^{+\infty} \ln \left[ \beta^2 (\hbar^2 \omega_n^2 + \xi_q^2) \right] = \frac{\xi_q}{2} + \frac{1}{\beta} \ln \left( 1 - e^{-\beta \xi_q} \right). \quad (90) \]

In fact, the derivative with respect to \( \xi_q \) of Eq. (90) reads

\[ \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} \frac{\xi_q}{\omega_n^2 + \xi_q^2} = \frac{1}{2} + \frac{1}{e^{\beta \xi_q} - 1} = \frac{1}{2} \coth \left( \frac{\beta \xi_q}{2} \right), \quad (91) \]

and this formula is a straightforward consequence of the exact result

\[ \sum_{n=-\infty}^{+\infty} \frac{1}{n^2 + a^2} = \frac{\pi}{a} \coth (\pi a) \quad (92) \]

remembering that the Matsubara frequencies are given by \( \omega_n = 2\pi n/\beta \).
The grand potential finally reads

\[ \Omega = \Omega_0 + \Omega^{(0)} + \Omega^{(T)}, \]  

(93)

where

\[ \Omega_0 = -\mu \psi_0^2 L^D \]  

(94)

is the grand potential of the order parameter,

\[ \Omega^{(0)} = \frac{1}{2} \sum_q \xi_q \]  

(95)

is the zero-point energy of bosonic single-particle excitations, i.e. the zero-temperature contribution of quantum fluctuations, and

\[ \Omega^{(T)} = \frac{1}{\beta} \sum_q \ln (1 - e^{-\beta \xi_q}) \]  

(96)

takes into account thermal fluctuations.
In the continuum limit, where $\sum_q \to L^D \int d^D q/(2\pi)^D$, the zero-point energy

$$\frac{\Omega^{(0)}}{L^D} = \frac{1}{2} \frac{S_D}{(2\pi)^D} \int_0^{+\infty} dq \, q^{D-1} \left( \frac{\hbar^2 q^2}{2m} - \mu \right)$$

(97)

of the ideal Bose gas is clearly ultraviolet divergent at any integer dimension $D$, i.e. for $D = 1, 2, 3$. Here $S_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}$ is the solid angle in $D$ dimensions with $\Gamma(x)$ the Euler gamma function. We shall show that this divergent zero-point energy of the ideal Bose gas is completely eliminated by dimensional regularization. Consequently, the exact grand potential of the ideal Bose gas is given by

$$\frac{\Omega}{L^D} = -\mu \psi_0^2 + \frac{1}{\beta L^D} \sum_q \ln \left( 1 - e^{-\beta \xi_q} \right).$$

(98)
2.1 Broken symmetry and ideal Bose gas (IX)

We notice that $\psi_0$ is not a free parameter but must be determined by minimizing $\Omega_0$, namely

$$
\left( \frac{\partial \Omega_0}{\partial \psi_0} \right)_{\mu, T, L^D} = 0,
$$

(99)

from which one finds that

$$
\psi_0 = \begin{cases} 
0 & \text{if } \mu \neq 0 \\
\text{any value} & \text{if } \mu = 0 
\end{cases}
$$

(100)

The number density $n = N/L^D$ is obtained from the thermodynamic relation

$$
n = -\frac{1}{L^D} \left( \frac{\partial \Omega}{\partial \mu} \right)_{T, L^D, \psi_0},
$$

(101)

which gives:

$$
n = \psi_0^2 + \frac{1}{L^D} \sum_q \frac{1}{e^{\beta \xi_q} - 1}.
$$

(102)
In the continuum limit \( \sum_{\mathbf{q}} \rightarrow L^D \int d^D \mathbf{q}/(2\pi)^D \), by setting \( \mu = 0 \) (condensed phase) from Eq. (102) one gets

\[
n = n_0 + \int \frac{d^D \mathbf{q}}{(2\pi)^D} \frac{1}{e^{\frac{\hbar^2 q^2}{2mk_B T}} - 1},
\]

which gives the condensate density \( n_0 = \psi_0^2 \) as a function of the temperature \( T \).

The critical temperature \( T_c \) is obtained setting \( \psi_0 = 0 \) in the previous equation. In this way one finds

\[
k_B T_c = \begin{cases} 
\text{no solution} & \text{for } D = 1 \\
0 & \text{for } D = 2 \\
\frac{1}{2\pi \zeta(3/2)^{2/3}} \frac{\hbar^2}{m} n^{2/3} & \text{for } D = 3
\end{cases}
\]

where \( \zeta(x) \) is the Riemann zeta function.
2.1 Broken symmetry and ideal Bose gas (XI)

In the three-dimensional case \((D = 3)\) from the equation

\[
n = n_0 + \int \frac{d^3q}{(2\pi)^3} \frac{1}{\frac{h^2q^2}{e^{2mk_B T}} - 1},
\]

we find

\[
n = n_0 + \zeta(3/2) \left(\frac{mk_B T}{2\pi \hbar^2}\right)^{3/2}.
\]

It follows that

\[
\frac{n_0}{n} = 1 - \frac{\zeta(3/2) \left(\frac{mk_B}{2\pi \hbar^2}\right)^{3/2} T^{3/2}}{n} = 1 - \frac{\zeta(3/2) \left(\frac{mk_B}{2\pi \hbar^2}\right)^{3/2} T^{3/2}}{\zeta(3/2) \left(\frac{mk_B}{2\pi \hbar^2}\right)^{3/2} T_c^{3/2}}.
\]

Thus, the condensate fraction reads

\[
\frac{n_0}{n} = 1 - \left(\frac{T}{T_c}\right)^{3/2}.
\]
Let us now consider a system of bosons with a repulsive contact interaction, i.e. let us set $g > 0$ in

$$
\mathcal{L} = \psi^* \left[ \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right] \psi + \frac{1}{2} g |\psi|^4 . \tag{109}
$$

In this case one finds immediately the partition function of the uniform and constant order parameter $\psi_0$ as

$$
\mathcal{Z}_0 = \exp \left\{ - \frac{S_0}{\hbar} \right\} = \exp \left\{ - \beta \Omega_0 \right\} , \tag{110}
$$

where $S_0 = S[\psi_0]$ and the grand potential $\Omega_0$ reads

$$
\frac{\Omega_0}{LD} = -\mu \psi_0^2 + \frac{1}{2} g \psi_0^4 . \tag{111}
$$

See the figure in the next slide.
2.2 Interacting Bose gas (II)

Figure: Mean-field grand potential $\Omega_0$ as a function of the real order parameter $\psi_0$ for an interacting Bose gas, see Eq. (111).
Again, the constant, uniform and real order parameter $\psi_0$ is obtained by minimizing $\Omega_0$ as
\[
\left( \frac{\partial \Omega_0}{\partial \psi_0} \right)_{\mu, T, L^D} = 0 ,
\]
from which one finds the relation between order parameter and chemical potential
\[
\mu = g \psi_0^2 .
\]
showing that in the superfluid broken phase the chemical potential is positive and
\[
\psi_0 = \sqrt{\frac{\mu}{g}} ,
\]
Inserting this relation into Eq. (111) we find
\[
\frac{\Omega_0}{L^D} = -\frac{\mu^2}{2g} .
\]
Clearly, this equation of state is lacking important informations encoded in quantum and thermal fluctuations.
Thus we consider again

$$\psi(r, \tau) = \psi_0 + \eta(r, \tau)$$  \hspace{1cm} (116)

and expand the action $S[\psi, \psi^*]$ around $\psi_0$ up to quadratic (Gaussian) order in $\eta(r, \tau)$ and $\bar{\eta}(r, \tau)$. We find

$$Z = Z_0 \int \mathcal{D}[\eta, \eta^*] \exp \left\{ -\frac{S_g[\eta, \eta^*]}{\hbar} \right\},$$  \hspace{1cm} (117)

where

$$S_g[\eta, \eta^*] = \frac{1}{2} \sum_Q (\eta_Q^*, \eta_{-Q}) \mathbf{M}_Q \begin{pmatrix} \eta_Q \\ \eta_{-Q}^* \end{pmatrix}$$  \hspace{1cm} (118)

is the Gaussian action of fluctuations in reciprocal space with $Q = (q, i\omega_n)$ the $D + 1$ vector denoting the momenta $q$ and bosonic Matsubara frequencies $\omega_n = 2\pi n/(\beta \hbar)$, and
2.2 Interacting Bose gas (V)

\[
\mathbf{M}_Q = \beta \begin{pmatrix}
-i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2 & -g\psi_0^2 \\
-g\psi_0^2 & i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2
\end{pmatrix}
\]

(119)

is the inverse fluctuation propagator.

Integrating over the bosonic fields \(\eta(Q)\) and \(\bar{\eta}(Q)\) in Eq. (117) one finds the Gaussian grand potential

\[
\Omega_g = \frac{1}{2\beta} \sum_Q \ln \det(M_Q)
\]

(120)

where \(E_q\) is given by

\[
E_q = \sqrt{\left(\frac{\hbar^2 q^2}{2m} - \mu + 2g\psi_0^2\right)^2 - g^2\psi_0^4}.
\]

(121)
By using $\psi_0 = \sqrt{\mu/g}$ the spectrum becomes

$$E_q = \sqrt{\frac{\hbar^2 q^2}{2m} \left( \frac{\hbar^2 q^2}{2m} + 2\mu \right)} \approx c_B \hbar q \quad \text{for small } q,$$

which is the familiar Bogoliubov spectrum, with $c_B = \sqrt{\mu/m}$.

Figure: Bogoliubov spectrum, given by Eq. (122), and its low-momentum phonon spectrum $E_q = c_B \hbar q$, where $c_B = \sqrt{\mu/m}$ is the sound velocity. Energy $E_q$ in units of $\mu$ and momentum $q$ in units of $\sqrt{m\mu/\hbar^2}$. 
Again, the sum over bosonic Matsubara frequencies gives

\[
\frac{1}{2\beta} \sum_{n=-\infty}^{+\infty} \ln \left[ \beta^2 \left( \hbar^2 \omega_n^2 + E_q^2 \right) \right] = \frac{E_q}{2} + \frac{1}{\beta} \ln \left( 1 - e^{-\beta E_q} \right). \tag{123}
\]

The total grand potential may then be written as

\[
\Omega = \Omega_0 + \Omega_g^{(0)} + \Omega_g^{(T)}, \tag{124}
\]

where \(\Omega_0\) is given by Eq. (115).

\[
\Omega_g^{(0)} = \frac{1}{2} \sum_{q} E_q \tag{125}
\]

is the zero-point energy of bosonic collective excitations, i.e. the zero-temperature contribution of quantum Gaussian fluctuations, while

\[
\Omega_g^{(T)} = \frac{1}{\beta} \sum_{q} \ln \left( 1 - e^{-\beta E_q} \right) \tag{126}
\]

takes into account thermal Gaussian fluctuations.
We notice that the continuum limit of the zero-point energy for the interacting Bose gas

$$\frac{\Omega^{(0)}_{g}}{L^{D}} = \frac{1}{2} \frac{S_D}{(2\pi)^D} \int_{0}^{+\infty} dq \, q^{D-1} \sqrt{\frac{\hbar^2 q^2}{2m} \left( \frac{\hbar^2 q^2}{2m} + 2\mu \right)}$$  \hspace{1cm} (127)$$

is ultraviolet divergent at any integer dimension $D$.

We may rewrite Eq. (127) for the zero point energy of a repulsive Bose gas in dimension $D$ as:

$$\frac{\Omega^{(0)}_{g}}{L^{D}} = \frac{S_D(2\mu)^{\frac{D}{2}+1}}{4(2\pi)^D} \left( \frac{2m}{\hbar^2} \right)^{\frac{D}{2}} B\left( \frac{D+1}{2}, -\frac{D+2}{2} \right),$$  \hspace{1cm} (128)$$

where $B(x, y)$ is the Euler Beta function

$$B(x, y) = \int_{0}^{+\infty} dt \frac{t^{x-1}}{(1 + t)^{x+y}}, \quad \text{Re}(x), \text{Re}(y) > 0$$ \hspace{1cm} (129)$$

which may be continued to complex values of $x$ and $y$ as

$$B(x, y) = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x + y)}.$$

\hspace{1cm} (130)
We rewrite Eq. (127) using Eq. (130) to get

\[ \frac{\Omega^{(0)}_{g}}{L^{D}} = \frac{S_{D}(2\mu)^{\frac{D+1}{2}}}{4(2\pi)^{D}} \left( \frac{2m}{\hbar^2} \right)^{\frac{D}{2}} \frac{\Gamma(\frac{D+1}{2}) \Gamma(-\frac{D+2}{2})}{\Gamma(-\frac{1}{2})}. \quad (131) \]

This expression is now finite when \( D = 1 \) or \( D = 3 \), while it is still divergent if \( D = 2 \) since \( \Gamma(p) \) diverges for integers \( p \leq 0 \). In particular, setting \( D = 3 \) in Eq. (131) we get

\[ \frac{\Omega^{(0)}_{g}}{L^{3}} = \frac{8}{15\pi^{2}} \left( \frac{m}{\hbar^2} \right)^{3/2} \mu^{5/2}. \quad (132) \]

In conclusion, the total grand potential of the three-dimensional Bose gas is then given by

\[ \frac{\Omega}{L^{3}} = -\frac{\mu^{2}}{2g} + \frac{8}{15\pi^{2}} \left( \frac{m}{\hbar^2} \right)^{3/2} \mu^{5/2} + \frac{1}{\beta L^{3}} \sum_{q} \ln \left( 1 - e^{-\beta E_{q}} \right). \quad (133) \]
Let us consider again a system of bosons with a repulsive contact interaction, i.e. let us set $g > 0$ in

$$
\mathcal{L} = \psi^* \left[ \hbar \partial_{\tau} - \frac{\hbar^2}{2m} \nabla^2 - \mu + U(\mathbf{r}) \right] \psi + \frac{1}{2} g |\psi|^4 ,
$$

where $U(\mathbf{r})$ is the external trapping potential.

In this inhomogeneous case the partition function of the mean-field (saddle-point) order parameter $\psi_0(\mathbf{r}, \tau)$ reads

$$
\mathcal{Z}_0 = \exp \left\{ - \frac{S_0}{\hbar} \right\} = \exp \{ -\beta \Omega_0 \} ,
$$

where

$$
S_0 = S[\psi_0(\mathbf{r}, \tau), \psi_0^*(\mathbf{r}, \tau)] = \int dt \int d^3r \ \mathcal{L}(\psi_0, \psi_0^*)
$$

and $\psi_0(\mathbf{r}, \tau)$ is the field $\psi(\mathbf{r}, \tau)$ which minimizes $S[\psi(\mathbf{r}, \tau)]$, namely

$$
\delta S[\psi(\mathbf{r}, \tau), \psi^*(\mathbf{r}, \tau)] = 0 .
$$
The minimization of the action $S$ gives the Euler-Lagrange equation

\[
\frac{\partial L}{\partial \psi^*} - \frac{\partial \tau}{\partial (\partial_\tau \psi^*)} - \nabla \frac{\partial L}{\partial (\nabla \psi^*)} + \nabla^2 \frac{\partial L}{\partial (\nabla^2 \psi^*)} = 0 \tag{138}
\]

from which we get

\[
\hbar \partial_\tau \psi_0(r, \tau) = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U(r) + g |\psi_0(r, \tau)|^2 \right] \psi_0(r, \tau). \tag{139}
\]

This is the Gross-Pitaevskii equation with imaginary time $\tau$. Moreover, at the mean-field level, the number of bosons reads

\[
N = -\frac{\partial \Omega_0}{\partial \mu} = \int d^3r |\psi_0(r, \tau)|^2. \tag{140}
\]
Going back to real time $t = i\tau$ we obtain

$$i\hbar \partial_t \psi_0(r, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu + U(r) + g |\psi_0(r, t)|^2 \right] \psi_0(r, t), \quad (141)$$

that is the real-time (time-dependent) Gross-Pitaevskii equation, with the normalization condition

$$N = \int d^3r |\psi_0(r, t)|^2. \quad (142)$$

Immediately one deduces the corresponding stationary Gross-Pitaevskii equation

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + g |\psi_0(r)|^2 \right] \psi_0(r) = \mu \psi_0(r). \quad (143)$$