The Functional Schrödinger Picture Approach to Many-Particle Systems

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A self-contained pedagogical introduction to the functional Schrödinger picture method of many-body theory is given at a level suitable for graduate students and also for many-body physicists who have not been exposed to the functional Schrödinger picture method previously. Mathematical tools necessary for the functional Schrödinger picture calculation are introduced. The method is first applied to various condensed matter problems including the electron gas, the Hubbard model, the BCS superconductivity, and dilute bose gas within the variational approximation. It is shown that the variational approximation with the Gaussian trial functional invariably leads into the Hartree-Fock results for both zero and finite temperature cases.

In order to go beyond the Gaussian results, concepts of variational and optimized perturbation theories are introduced using simple quantum mechanical languages. Then, the variational perturbation theory in the functional Schrödinger picture is applied to the \( \lambda \phi^4 \) model to yield the effective potential to the third order. The optimized perturbation theory is also applied to the \( \lambda \phi^4 \) model to yield a general expression up to the second order.

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FOREWORD

These notes represent the lectures given at Johannes Kepler Universit"at-Linz, Austria in October and November, 2002 as "Special Topics in Many-Body Theory". The intent of these lectures was to provide a self-contained tutorial introduction to the functional Schrödinger picture approach to many-particle systems.

Condensed matter systems are basically many-particle systems. Whether the system in consideration is a crystalline solid, an amorphous material, or a liquid, one has to deal with substantially large number of particle which often amounts to $10^{23}/\text{cm}^3$. This large number still eludes exact numerical calculation even with ever increasing computational capability of modern day computers.

Many-body theories based on non-relativistic quantum field theories are conceived to deal with almost infinite degrees of freedoms of many-particles in condensed matter systems. Many-body theory closely followed its relativistic brother, quantum field theory in its development. In quantum field theory, there exist basically three alternative approaches, namely operator (Heisenberg), functional integral (path integral), and Schrödinger approaches. Comparing to the former two methods, the last one Schrödinger picture approach was early regarded less convenient and clumsy for development of field theories. However, in 80’s and 90’s, theorists have found that it offers some distinct advantages over others when suitable schemes are employed. Since then the Schrödinger picture has been drawing wide interests and field theories based on the functional Schrödinger picture have been developing rapidly.

In condensed matter physics, so far the Schrödinger picture scheme has been much neglected. Only very recently, efforts to develop the Schrödinger picture method into a useful many-body theoretical tool has started. In this lecture, we present such an effort and try to give a pedagogical overview on this method.

Since these notes are designed for beginning graduate students and newcomers in this field, we tried to make the notes self-contained. In this respect, we tried to limit the number of references to those essential to read these notes. Other relevant references can be found in the references of the papers and books cited in these notes. Although most of essential steps are described in detail to help the readers, some of the derivations are left as problems, so that readers can gain more insights and expertise through exercise.

I. INTRODUCTION

Condensed matter systems are basically many-particle systems with many particles ($\sim 10^{23}$ per cm$^3$). Now, the basic question is whether it is possible to solve the many-particle Schrödinger equation directly?

$$H = \sum_{k=1}^{N} T(x_k) + \frac{1}{2} \sum_{k \neq l=1}^{N} V(x_k, x_l),$$  \hspace{1cm} (1)

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1 \cdots x_N, t) = H \Psi(x_1 \cdots x_N, t).$$  \hspace{1cm} (2)

If we have $\Psi(x_1 \cdots x_N, t)$, then we can calculate all the physical quantities we need. Expansion of $\Psi(x_1 \cdots x_N, t)$ can be written in terms of the single-particle wave function $\psi_{E_k}(x_k)$

$$\Psi(x_1 \cdots x_N, t) = \sum_{E_1' \cdots E_N'} C(E_1' \cdots E_N', t) \psi_{E_1'}(x_1) \cdots \psi_{E_N'}(x_N),$$  \hspace{1cm} (3)

where $E_1' \cdots E_N'$ represent single particle quantum numbers. $C(E_1' \cdots E_N', t)$ is the coefficient for a particular configuration. In general, it is not practical to continue to use $\Psi(x_1 \cdots x_N, t)$ with $N \sim 10^{23}$. Therefore, a suitable scheme to handle the large degree of freedom has to be adopted. Here, we resort to the technique of second quantization.

A. Second Quantization

There are several ways for introducing second quantization to the many-body Schrödinger equation. An explicit and detailed treatise is given in Chapter 1 of Fetter & Walecka (Gen. Ref. 3). However, here, we follow a rather concise but less detailed path to the second quantization commonly adopted by field theory textbooks (Chapt. 2, Gen. Ref. 1 & §12 & 13, Gen. Ref. 4).

The Schrödinger Wave Field of Bose Statistics
(1st quantized) Schrödinger equation is given by

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\vec{x})\Psi = i\hbar \dot{\Psi}. \quad (4) \]

The conjugate complex equation is

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V(\vec{x})\Psi^* = -i\hbar \dot{\Psi}^*. \quad (5) \]

Find a Lagrangian such that the corresponding Euler-Lagrange equation leads back to Schrödinger equation.

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \quad i = 1 \cdots f \quad (6) \]

Such a Lagrangian is given by

\[ L = \int d^3x L = \int \Psi^* \left\{ i\hbar \dot{\Psi} - V(\vec{x})\Psi + \frac{\hbar^2}{2m} \nabla^2 \Psi \right\} d^3x, \quad (7) \]

which leads directly to

\[ \frac{d}{dt} \frac{\delta L}{\delta \dot{\Psi}} - \frac{\delta L}{\delta \Psi} = - \left\{ i\hbar \dot{\Psi} - V(\vec{x})\Psi + \frac{\hbar^2}{2m} \nabla^2 \Psi \right\} = 0. \quad (8) \]

(Note: The above Lagrangian is not Hermitian. We can work with a Hermitian Lagrangian (See Chap. 2, Gen. Ref. 1.) at the expense of slight complications.)

Define the canonically conjugate momentum in the usual way,

\[ \pi = \frac{\delta L}{\delta \dot{\Psi}} = -\frac{\hbar}{i} \Psi^*. \quad (9) \]

The Hamiltonian is given by

\[ H = \int (\pi \dot{\Psi} - L)d^3x = \int \Psi^* \left\{ i\hbar \dot{\Psi} - V(\vec{x})\Psi \right\} d^3x, \]

\[ = \int \left\{ i\hbar \Psi^* \dot{\Psi} - i\hbar \Psi^* \dot{\Psi} - \Psi^* \frac{\hbar^2}{2m} \nabla^2 \Psi + \Psi^* V(\vec{x}) \Psi \right\} d^3x \]

\[ = \int \Psi^*(\vec{x}) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right\} \Psi(\vec{x})d^3x. \quad (10) \]

In the above Hamiltonian, only wave nature appears. In order to restore the particle nature, we expand \( \Psi \) in terms of the 1st quantized eigenfunctions,

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi_\mu = i\hbar \dot{\psi}_\mu, \]

\[ \psi_\mu(\vec{x}, t) = e^{-\frac{i}{\hbar} E_\mu t} \psi_{\mu}(\vec{x}). \quad (11) \]

The expansions are

\[ \Psi(\vec{x}) = \sum_\mu b_\mu(t) \psi_\mu(\vec{x}), \]

\[ \Psi^*(\vec{x}) = \sum_\mu b^*_\mu(t) \psi^*_\mu(\vec{x}), \quad (12) \]

where \( b_\mu(t) = b_\mu(0)e^{-\frac{i}{\hbar} E_\mu t}. \)

With these expressions, we obtain
\[ H = \sum_{\mu} E_{\mu} b_{\mu}^\dagger b_{\mu}. \] (13)

In order to quantize the wave field \( \Psi \), we require
\[
[\pi(x), \Psi(x')] = \frac{\hbar}{i} \delta(x - x') .
\] (14)

(Remember the 1st quantization postulate \([\hat{p}, \hat{x}] = \frac{\hbar}{i}\).)

Thus, we obtain
\[
[\Psi(x'), \Psi^\dagger(x)] = \delta(x - x').
\] (15)

Also we have additional commutation relations
\[
[\Psi(x), \Psi(x')] = 0,
[\Psi^\dagger(x), \Psi^\dagger(x')] = 0.
\] (16)

We find that \( b_{\mu} \) and \( b_{\mu}^\dagger \) satisfy
\[
[b_{\mu}, b_{\nu}^\dagger] = \delta_{\mu\nu}, \quad [b_{\mu}, b_{\nu}] = 0, \quad [b_{\mu}^\dagger, b_{\nu}^\dagger] = 0.
\] (17)

With the new Hamiltonian operator, the ‘Schrödinger equation’ is given by
\[
H \Phi = E \Phi, \quad H = \int \Psi^\dagger(x) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right\} \Psi(x) d^3x \\
\equiv \sum_{\mu} E_{\mu} b_{\mu}^\dagger b_{\mu},
\] (18)

where
\[
\Phi = \prod_{\mu} \frac{1}{\sqrt{n_{\mu}!}} (b_{\mu}^\dagger)^{n_{\mu}} \Phi_0,
E = \sum_{\mu} E_{\mu} n_{\mu} \quad n_{\mu} = 0, 1, 2, \ldots.
\] (19)

A series of energy levels \( E_{\mu} \) are occupied by a definite number \( n_{\mu} \) of quanta. This shows clearly that field quantization guarantees the corpuscular nature of the Schrödinger wave field.

**Expectation Values in the New Formalism**
(How do we relate the new theory to reality?)

- **The particle density operator**
\[
\Psi^\dagger(x, t)\Psi(x, t) \rightarrow \Psi^\dagger(x, t)\Psi(x, t)
\] (1st quantized)  
\[
\Psi^\dagger(x, t)\Psi(x, t)
\] (2nd quantized)

\[
\rho_{op}(x) = \Psi^\dagger(x)\Psi(x) : \text{particle density operator}
\]
\[
\bar{\rho}(x) = \langle \Phi | \Psi^\dagger(x)\Psi(x) | \Phi \rangle
\] (21)

<Problem> Show that the above \( \bar{\rho}(x) \) gives an identical result to the 1st quantized particle density \( \bar{\rho}(x) = \psi^\ast(x)\psi(x) \), when only a single particle is present in state \( k \).

- **The position operator**
In the 1st quantized form, we have
\[ \bar{x} = \int \psi^*(x,t)\psi(x,t) d^3x. \]

The second quantized form is given by

\[ x_{op} = \int \psi^\dagger(x)\psi(x) d^3x, \]
\[ \bar{x} = \langle \Phi | x_{op} | \Phi \rangle \]
\[ = \langle \Phi | \int \psi^\dagger(x)\psi(x) d^3x | \Phi \rangle. \quad (22) \]

- The potential energy operator

\[ V_{op} = \int \psi^\dagger(x)V(x)\psi(x) d^3x. \quad (24) \]

- The interaction energy operator

\[ V(x,x') = V(x-x'). \]

In the first quantized form, it is given by

\[ \frac{1}{2} \int \rho(x,t)V(x,x')\rho(x',t) d^3x d^3x' \]
\[ = \frac{1}{2} \int \Psi^*(x,t)\Psi(x,t)V(x-x')\Psi^*(x',t)\Psi(x',t) d^3x d^3x'. \quad (25) \]

In the second quantized form, the order of the operators is important.
When there is one or zero particle present, the interaction energy is zero.
Thus, we should have \( \Psi \) on the right and \( \Psi^\dagger \) on the left,

\[ \frac{1}{2} \int \Psi^\dagger(x')\Psi^\dagger(x')V(x-x')\Psi(x')\Psi(x) d^3x d^3x'. \quad (26) \]

The expectation value is given by

\[ \langle \Phi | \frac{1}{2} \int \Psi^\dagger(x')\Psi^\dagger(x')V(x-x')\Psi(x')\Psi(x) d^3x d^3x' | \Phi \rangle. \quad (27) \]

**Problem** Calculate the expectation value of the Coulomb interaction energy \( V(x-x') = e^2/|x-x'| \) for \( \Phi = b_{\mu_1}^\dagger \Phi_0 \)
and \( \Phi = b_{\mu_1}^\dagger b_{\mu_2}^\dagger \Phi_0 \).

**Quantization of the Schrödinger Wave Field of Fermi-Dirac Statistics; Fermions**

In reality, electrons which are main constituents of the many-body problems in condensed matter are fermions, which obey F-D statistics.

We expand the wave field into

\[ \Psi(x) = \sum_{\mu} a_{\mu} \psi_{\mu}(x), \]
\[ \Psi^\dagger(x) = \sum_{\mu} a_{\mu}^\dagger \psi_\mu^*(x), \quad (28) \]

where \( \psi_{\mu}(x) \) satisfies

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi_{\mu}(x) = E_{\mu} \psi_{\mu}(x). \]
In order to satisfy the F-D statistics (Pauli exclusion principle), they should obey the following commutation relations.

\[
\{ a_\mu^\dagger, a_\nu^\dagger \} = a_\mu^\dagger a_\nu^\dagger + a_\nu^\dagger a_\mu^\dagger = 0
\]

\[
\{ a_\mu^\dagger, a_\nu \} = \delta_{\mu\nu}
\]

\[
\{ a_\mu, a_\nu^\dagger \} = 0
\]

(29)

Using these relations, we obtain

\[
\{ \Psi^\dagger(x), \Psi(x') \} = \delta(x - x'),
\]

\[
\{ \Psi^\dagger(x), \Psi^\dagger(x') \} = 0,
\]

\[
\{ \Psi(x), \Psi(x') \} = 0.
\]

(30)

**Problem** Derive the above commutation relations using the commutation relations of \( a_\mu^\dagger(x) \) and \( a_\nu(x) \).

The Hamiltonian operator is given by

\[
H = \int \Psi^\dagger(x) \left\{ \frac{\hbar^2}{2m} \nabla^2 + V(x) \right\} \Psi(x) d^3x
\]

\[
\equiv \sum_\mu E_\mu a_\mu^\dagger a_\mu.
\]

(31)

The corresponding Schrödinger equation is

\[
H \Phi = E \Phi.
\]

(32)

We obtain as eigenfunctions

\[
\Phi(n) = \prod_\mu (a_\mu^\dagger)^{n_\mu} \Phi_0,
\]

(33)

with \( N = \sum_\mu N_\mu \) and \( E = \sum_\mu E_\mu n_\mu \).

First consider a one-particle state

\[
\Phi = \sum_\mu c_\mu a_\mu^\dagger \Phi_0
\]

(34)

which is a superposition of one-particle states \( a_\mu^\dagger \Phi_0 \).

We replace \( a_\mu^\dagger \) by \( \Psi^\dagger \) using

\[
\int \psi_\mu(x) \Psi^\dagger(x) d^3x = a_\mu^\dagger.
\]

(35)

\[
\Phi = \int \sum_\mu c_\mu \psi_\mu(x) \Psi^\dagger(x) d^3x \Phi_0
\]

\[
= \int f(x) \Psi^\dagger(x) d^3x \Phi_0
\]

(36)

\( \Phi \) represents a superposition of the single particle, which maybe thought as having been created at different places with a probability amplitude \( f(x) \).

**Problem** Show that \( \Psi^\dagger(x') \) creates a particle at the place \( x' \).

**Sol.** \( \Psi^\dagger(x) \Psi(x') \Psi^\dagger(x') \Phi_0 = \Psi^\dagger(x) \delta(x - x') \Phi_0 = \delta(x - x') \Psi^\dagger(x') \Phi_0. \)

We now have
\[ H \Phi = \int \Psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right) \Psi(x) d^3x \int f(x') \Psi^\dagger(x') d^3x' \Phi_0 \]

\[ = \int \int \Psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right) f(x') \delta(x - x') d^3x d^3x' \Phi_0 \]

\[ = \int \Psi^\dagger(x) \Phi_0 \left( -\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right) f(x) d^3x. \tag{37} \]

Here, we use the relation \( H \Phi = E \Phi = E \int f(x) \Psi^\dagger(x) \Phi_0 d^3x \). This is valid only when

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) f(x) = Ef(x). \tag{38} \]

This one-particle example shows that the second quantization formalism is identical to the usual Schrödinger theory.

- **What about a 2-particle state?**

Consider the most general two-particle state

\[ \Phi = \sum_{\mu_1 \mu_2} c_{\mu_1 \mu_2} a^\dagger_{\mu_1} a^\dagger_{\mu_2} \Phi_0, \tag{39} \]

which can be rearranged

\[ \Phi = \int \left( \sum_{\mu_1 \mu_2} \psi_{\mu_1}(x) \psi_{\mu_2}(x') c_{\mu_1 \mu_2} \right) \Psi^\dagger(x) \Psi^\dagger(x') \Phi_0 d^3x d^3x' \]

\[ = \int f(x, x') \Psi^\dagger(x) \Psi^\dagger(x') \Phi_0 d^3x' d^3x. \tag{40} \]

Now we show that \( f(x, x') \) is antisymmetric. Interchanging \( x \) with \( x' \), we have

\[ \int \int f(x', x) \Psi^\dagger(x') \Psi^\dagger(x) \Phi_0 d^3x' d^3x = - \int \int f(x', x) \Psi^\dagger(x) \Psi^\dagger(x') \Phi_0 d^3x' d^3x. \tag{41} \]

Thus, we note that \( f(x, x') = -f(x', x) \) by comparing to Eq.(40).

Now, we assume the Hamiltonian operator of interacting electrons in second quantization is given by

\[ H = \int \Psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla_x^2 + V(x) \right) \Psi(x) d^3x \]

\[ + \frac{1}{2} \int \int \Psi^\dagger(x) \Psi^\dagger(x') \frac{e^2}{|x - x'|} \Psi(x') \Psi(x) d^3x d^3x'. \tag{42} \]

Combining Eq.(40) with (42), we obtain

\[ \left\{ \frac{\hbar^2}{2m} \nabla^2_{x_1} + V(x_1) - \frac{\hbar^2}{2m} \nabla^2_{x_2} + V(x_2) + \frac{e^2}{|x_1 - x_2|} \right\} f(x_1, x_2) = Ef(x_1, x_2). \tag{43} \]

**Problem** Prove Eq.(43).

- **n-particle state**

If we apply the field Hamiltonian operator to an \( n \)-particle state,

\[ \Phi = \int d^3x_1 \cdots d^3x_n f_n(x_1, \cdots, x_n) \Psi^\dagger(x_1) \cdots \Psi^\dagger(x_n) \Phi_0, \tag{44} \]
we will find the n-body wavefunction must satisfy
\[
\sum_{j=1}^{n} \left( -\frac{\hbar^2}{2m} \nabla_{x_j}^2 + V(x_j) \right) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} \right) f(x_1, \cdots, x_n) = E f(x_1, \cdots, x_n). \tag{45}
\]
In this way, all of the n-body first quantized systems can be contained in the corresponding second quantized theory (quantum field theory). In this sense, ‘many-body theory’ is basically a ‘nonrelativistic quantum field theory’.

For interacting electron systems, the Hamiltonian is given by
\[
H = \int d^3x \Psi^\dagger(x) T \Psi(x) + \frac{1}{2} \int d^3x d^3x' \Psi^\dagger(x) \Psi^\dagger(x') V(x, x') \Psi(x') \Psi(x) \tag{46}
\]
\[
= \sum_{r,s} a_r^\dagger \langle r | T | s \rangle a_s + \frac{1}{2} \sum_{r,s,t,u} a_r^\dagger a_s^\dagger \langle rs | V | tu \rangle a_t a_u. \tag{47}
\]
(Note the order of operators.)

### B. Pictures in Quantum Mechanics

#### Schrödinger Picture

The usual elementary description of quantum mechanics assumes that the state vectors are time dependent, whereas the operators are time independent. The Schrödinger equation in the Schrödinger picture takes the form
\[
i\hbar \frac{\partial}{\partial t} | \Psi_S(t) \rangle = H | \Psi_S(t) \rangle. \tag{48}
\]
A formal solution is given by
\[
| \Psi_S(t) \rangle = e^{-iH(t-t_0)/\hbar} | \Psi_S(t_0) \rangle. \tag{49}
\]
Generally, undergraduate quantum mechanics dwells on the Schrödinger picture formalism, although the Heisenberg picture, which we will discuss shortly, is regarded as a convenient tool for a formal development of quantum mechanics. However, in many-body physics, the situation is completely reversed. It will be shown that the Heisenberg and the interaction pictures naturally lead into perturbative expansions of the physical quantities, which are the basis of the Green’s function formalism.

Therefore, almost all the many-body theoretical schemes are based on the Heisenberg (interaction) picture. Only recently, several quantum field theorists found that the Schrödinger picture provides a convenient scheme to calculate the physical quantities in selected quantum field theoretical problems. Last few years, the authors and their collaborators started to develop a many-body theory based on the Schrödinger picture and have succeeded to provide a general theoretical framework. In this lecture, the many-body theoretical scheme based on the functional Schrödinger picture will be introduced.

#### Heisenberg Picture

In the Heisenberg picture, we pass the burden of the time-dependency from the wavefunction to the operator. The state vector (wavefunction) in the Heisenberg picture is defined as
\[
| \Psi_H(t) \rangle \equiv e^{iHt/\hbar} | \Psi_S(t) \rangle. \tag{50}
\]
Combining Eq.(49) with \( t_0 = 0 \), we obtain
\[
| \Psi_H(t) \rangle = | \Psi_S(t = 0) \rangle \tag{51}
\]
which is independent of \( t \).

Considering the fact that the expectation value should remain same in both pictures,
we obtain

\[ O_H(t) = e^{iHt/\hbar}O_Se^{-iHt/\hbar}. \]  

(53)

We observe that the state vector in the Heisenberg picture is now independent on \( t \), whereas the time-dependency is now carried by the operator. This fact is summarized as follows

| Schrödinger picture | Heisenberg picture |
|---------------------|--------------------|
| State               | Ket                 |
| T-dep.              | T-ind.              |
| Operator            | T-ind.              |
|                     | T-dep.              |

The time derivative of Eq.(53) yields the Heisenberg equation of motion,

\[ i\hbar \frac{\partial}{\partial t} O_H(t) = [O_H(t), H]. \]  

(54)

**Problem** Prove Eq.(54).

This result determines the equation of motion for any operators in the Heisenberg picture. In particular, if \( OS \) commutes with \( H \), then \( O_H \) is a constant of the motion.

**Interaction Picture**

When the Hamiltonian can be expressed as

\[ H = H_0 + H_I, \]  

(55)

where \( H_0 \) yields a soluble problem, we can introduce the interaction picture, which is convenient for perturbative treatment of many-particle systems.

Define the interaction state vector in the following way

\[ |\Psi_I(t)\rangle \equiv e^{iH_0t/\hbar}|\Psi_S(t)\rangle \]  

(56)

(* Note that in the exponent, it is not \( H \) but \( H_0 \).) Then

\[ i\hbar \frac{\partial}{\partial t} |\Psi_I(t)\rangle = -H_0e^{iH_0t/\hbar}|\Psi_S(t)\rangle + e^{iH_0t/\hbar}i\hbar \frac{\partial}{\partial t} |\Psi_S(t)\rangle \]

\[ = e^{iH_0t/\hbar}[-H_0 + H]e^{-iH_0t/\hbar}|\Psi_I(t)\rangle \]

\[ = e^{iH_0t/\hbar}H_Ie^{-iH_0t/\hbar}|\Psi_I(t)\rangle. \]

We, therefore, obtain the following equations.

\[ i\hbar \frac{\partial}{\partial t} |\Psi_I(t)\rangle = H_I(t)|\Psi_I(t)\rangle \]  

(57)

\[ H_I(t) = e^{iH_0t/\hbar}H_Ie^{-iH_0t/\hbar} \]  

(58)

For any operators,

\[ \langle \Psi_S(t)|O_S|\Psi_S(t)\rangle \]

\[ = \langle \Psi_I(t)|e^{iH_0t/\hbar}O_Se^{-iH_0t/\hbar}|\Psi_I(t)\rangle. \]  

(59)

Thus, we have

\[ O_I(t) \equiv e^{iH_0t/\hbar}O_Se^{-iH_0t/\hbar}. \]  

(60)

Differentiating the above equation with respect to time, one obtains
Thus, we obtain
\[ i\hbar \frac{\partial}{\partial t} O_I(t) = e^{iH_0 t/\hbar} (O_S H_0 - H_0 O_S) e^{-iH_0 t/\hbar} = [O_I(t), H_0]. \] (61)

We now solve the equation of motion in the interaction picture. Define a unitary operator that determines the state vector at time \( t \) in terms of the state vector at the time \( t_0 \)
\[ |\Psi_I(t)\rangle = U(t, t_0) |\Psi_I(t_0)\rangle. \] (62)

\( U \) satisfies
\[ U(t_0, t_0) = 1. \] (63)

Using the Schrödinger picture Eq.(49),
\[ |\Psi_I(t)\rangle = e^{iH_0 t/\hbar} |\Psi_S(t)\rangle = e^{iH_0 t/\hbar} e^{-iH(t-t_0)/\hbar} |\Psi_S(t_0)\rangle = e^{iH_0 t/\hbar} e^{-iH(t-t_0)/\hbar} e^{-iH_0 t_0/\hbar} |\Psi_I(t_0)\rangle, \] (64)
which identifies
\[ U(t, t_0) = e^{iH_0 t/\hbar} e^{-iH(t-t_0)/\hbar} e^{-iH_0 t_0/\hbar}. \] (65)

We can immediately show that
1. \( U^\dagger(t, t_0) U(t, t_0) = U(t, t_0) U^\dagger(t, t_0) = 1 \)
   which implies \( U \) is unitary
   \[ U^\dagger(t, t_0) = U^{-1}(t, t_0). \] (66)
2. \( U(t_1, t_2) U(t_2, t_3) = U(t_1, t_3). \) (67)
3. \( U(t, t_0) U(t_0, t) = 1. \) (68)

Although Eq.(65) is the formal solution of Eq.(62), it is not very useful.
From Eq.(57), one can write
\[ i\hbar \frac{\partial}{\partial t} U(t, t_0) |\Psi_I(t_0)\rangle = H_I(t) U(t, t_0) |\Psi_I(t_0)\rangle, \]
which is true for arbitrary \( |\Psi_I(t_0)\rangle \).
Thus, we obtain
\[ i\hbar \frac{\partial}{\partial t} U(t, t_0) = H_I(t) U(t, t_0). \] (69)

Integrating this equation from \( t_0 \) to \( t \), it is shown
\[ U(t, t_0) - U(t_0, t_0) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' H_I(t') U(t', t_0), \]
which gives the relation,
\[ U(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' H_I(t') U(t', t_0). \] (70)

Thus, we arrived at an integral equation for the unitary operator \( U(t, t_0) \).
The above equation is solved by iteration.
\[ U(t, t_0) = 1 + \left( \frac{-i}{\hbar} \right) \int_{t_0}^{t} dt' H_I(t') + \left( \frac{-i}{\hbar} \right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' H_I(t') H_I(t'') + \cdots \] (71)
Consider the third term in this expansion. It may be written as

\[
\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') \quad = \quad \frac{1}{2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') + \frac{1}{2} \int_{t_0}^{t} dt' \int_{t}^{t'} dt'' H_1(t') H_1(t'').
\]  

(72)

Now the second term becomes (with \(t' \leftrightarrow t''\))

\[
\frac{1}{2} \int_{t_0}^{t} dt'' \int_{t_0}^{t} dt' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^{t} dt' \int_{t}^{t'} dt'' H_1(t') H_1(t'').
\]

Thus, we have altogether

\[
\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^{t} dt' \int_{t}^{t'} dt''[H_1(t') H_1(t'') \theta(t' - t'') + H_1(t'') H_1(t') \theta(t'' - t')],
\]

(73)

where \(\theta(t)\) is the step function. We note that the operator containing the latest time stands farthest to the left. We call this a time-ordered product of operators, denoted by the symbol \(T\). Thus the above expression can be rewritten

\[
\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_1(t') H_1(t'') = \frac{1}{2} \int_{t_0}^{t} dt' \int_{t}^{t'} dt'' T[H_1(t') H_1(t'')].
\]

(74)

Finally, a general expression for \(U\) is obtained,

\[
U(t, t_0) = \sum_{n=0}^{\infty} \left( -\frac{i}{\hbar} \right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n T[H_1(t_1) \cdots H_1(t_n)].
\]

(75)

Now, a Heisenberg operator can be related to an interaction operator using \(U\).

\[
O_H(t) = e^{i\mathcal{H}t/\hbar} O_S e^{-i\mathcal{H}t/\hbar}
\]

\[
= e^{i\mathcal{H}t/\hbar} e^{-i\mathcal{H}_0 t/\hbar} O \left( e^{i\mathcal{H}_0 t/\hbar} e^{-i\mathcal{H}t/\hbar} \right).
\]

(76)

Eq.(65) yields

\[
O_H(t) = U(0, t) O_S(t) U(t, 0).
\]

(77)

In addition
\[ |\Psi_H\rangle = |\Psi_S(0)\rangle = |\Psi_I(0)\rangle, \quad O_S = O_H(0) = O_I(0), \] (78)

so that all three pictures coincide at time \( t = 0 \).

These relations provide a formal way to obtain the exact eigenstates of the interacting system from the noninteracting ones.

Since \( |\Psi_H\rangle \) is independent of time, it satisfies the time-independent form of the Schrödinger equation

\[ H|\Psi_H\rangle = E|\Psi_H\rangle. \] (79)

These state vectors are therefore the exact eigenstates of the system and are naturally very complicated for an interacting system. This can be expressed

\[ |\Psi_H\rangle = |\Psi_I(0)\rangle = U(0, t_0)|\Psi_I(t_0)\rangle. \] (80)

If we choose \( |\Psi_I(t_0)\rangle = |\Psi_I(-\infty)\rangle \) and \( H = H_0 + e^{-\epsilon t} H_I \) and use the concept of "adiabatic switching on", we can express an exact eigenstate of the interacting system in terms of an eigenstate of \( H_0 \).

\[ |\Psi_H\rangle = |\Psi_I(0)\rangle = U_\epsilon(0, -\infty)|\Psi_0\rangle, \] (81)

\[ H_0|\Psi_0\rangle = E_0|\Psi_0\rangle. \] (82)

(For details, see Chapt. 3 of Gen. Ref. 3.)

The above relation allows a convenient and systematic calculation of physical quantities using Green’s function method in the Heisenberg picture.

C. Green’s Function Method

Zero-Temperature Formalism

The concept of a Green’s function (or propagator) plays a fundamental role in the many-particle theory. The single particle Green’s function is defined by

\[ iG_{\alpha\beta}(x,t,x',t') = \frac{\langle \Psi_0 | T[\psi_{H\alpha}(x,t)\psi_{H\beta}^\dagger(x',t')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \] (83)

where \( |\Psi_0\rangle \) is the Heisenberg ground state of the interacting system satisfying

\[ H|\Psi_0\rangle = E|\Psi_0\rangle \] (84)

and \( \psi_{H\alpha}(x,t) \) is a Heisenberg operator,

\[ \psi_{H\alpha}(x,t) = e^{iHt/\hbar} \psi_\alpha(x)e^{-iHt/\hbar}. \] (85)

Here, the indices \( \alpha \) and \( \beta \) label the components of the field operators; \( \alpha \) and \( \beta \) may represent two values for spin \( \frac{1}{2} \) fermions, whereas there are no indices for spin zero bosons.

The \( T \) product represents the time ordering,

\[ T[\psi_{H\alpha}(x,t)\psi_{H\beta}^\dagger(x',t')] = \psi_{H\alpha}(x,t)\psi_{H\beta}^\dagger(x',t') \quad t > t', \]
\[ \pm\psi_{H\beta}^\dagger(x',t')\psi_{H\alpha}(x,t) \quad t' > t, \] (86)

where the upper (lower) sign refers to bosons (fermions).

Here, we ask why the Green’s function is so useful. The answers are as follows:

1. The Green’s function offers a convenient basis for the perturbation expansion in combination with the Feynman rules.
2. Although the ground-state expectation value implies the loss of much detailed information about the ground state, still the single-particle Green’s function contains the observable properties of great interest:

(a) The expectation value of any single-particle operator in the ground state of the system.
(b) The ground-state energy of the system.
(c) The excitation spectrum of the system.

The single-particle operator is expressed as

\[ J = \int d^3x J(x), \quad (87) \]

where

\[ J(x) = \sum_{\alpha\beta} \psi_\beta^\dagger(x) J_{\beta\alpha}(x) \psi_\alpha(x). \quad (88) \]

\( J_{\beta\alpha}(x) \) is the first-quantized operator.

The ground-state expectation value of the operator density is given by

\[ \langle J(x) \rangle \equiv \frac{\langle \Psi_0 | J(x) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \lim_{x' \to x} \sum_{\alpha\beta} J_{\beta\alpha}(x) \frac{\langle \Psi_0 | \psi_\beta^\dagger(x') \psi_\alpha(x) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \]

\[ = \pm i \lim_{t' \to t^+} \lim_{x' \to x} \sum_{\alpha\beta} J_{\beta\alpha}(x) G_{\alpha\beta}(x,t,x') \]

\[ = \pm i \lim_{t' \to t^+} \lim_{x' \to x} \text{tr}[J(x)G(x,t',x')]. \quad (89) \]

For example, the number density operator, \( n(x) = \psi^\dagger(x) \psi(x) \), becomes

\[ \langle n(x) \rangle = \pm i \text{tr} G(x,t^+). \quad (90) \]

The kinetic energy \( \langle T \rangle \) is

\[ \langle T \rangle = \pm i \int d^3x \lim_{x' \to x} \left[ -\frac{\hbar^2}{2m} \nabla^2 \text{tr} G(x,t,x') \right] \]

and the potential energy is

\[ \langle V \rangle = \pm \frac{1}{2} i \int d^3x \lim_{t' \to t^+} \lim_{x' \to x} \sum_{\alpha} \left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \nabla^2}{2m} \right] G_{\alpha\alpha}(x,t,x'). \quad (92) \]

<Problem> Prove Eq.(92).

The total ground state energy is solely given in terms of the single-particle Green’s function.

\[ E = \langle T + V \rangle = \langle H \rangle \]

\[ = \pm \frac{1}{2} i \int d^3x \lim_{t' \to t^+} \lim_{x' \to x} \left[ i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \nabla^2}{2m} \right] \text{tr} G(x,t^+,x'). \quad (93) \]

In addition to the above useful quantities, we can also obtain information on the excitation spectrum of the system [Section 7, Gen. Ref. 3.].

Now the usefulness of the above relations boils down to the point that how accurately we can calculate the Green’s function. In this lecture, it is not intended to explain the Green’s function method. Here, we only mention that the Green’s function method leads into a perturbative expansion without proof.
The exact Green’s function may be written as
\[
iG_{\alpha\beta}(x,y) = \sum_{\nu=0}^{\infty} \left( -\frac{i}{\hbar} \right)^\nu \frac{1}{\nu!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_\nu \times \frac{\langle \Psi_0 | T[ H_1(t_1) \cdots H_1(t_\nu) \psi_{\alpha}(x) \psi_{\beta}^\dagger(y)] | \Psi_0 \rangle}{\langle \Psi_0 | S | \Psi_0 \rangle}.
\]
(94)

Here, \( S = U_e(\infty, -\infty) \). The above expression clearly shows that we can calculate the Green’s function order by order of the perturbation, \( H_1 \), up to the desired order. This is greatly facilitated by the Feynman diagram method.

**Dyson’s equation**

The concept of the Green’s function method can be beautifully represented by the Dyson’s equation pictorially.

\[
G = G_0 + G_0 \Sigma G_0,
\]
(95)

where \( \Sigma \) represents the self-energy due to the interaction and \( G_0 \) the free particle Green’s function. This equation is graphically represented.

Using the concept of the proper self-energy, this expression can be modified as

\[
G = G_0 + G_0 \Sigma^* G,
\]
(96)

which is graphically given

A proper self-energy is the self-energy insertion that can not be separated into two pieces by cutting a single particle line.

Eq.(96) and its graphic representation clearly shows the perturbative nature of the formal solution as follows

\[
G = G_0 + G_0 \Sigma^* G_0 + G_0 \Sigma^* G_0 \Sigma^* G_0 + \cdots.
\]
(97)

This perturbation expansion allows one to calculate the Green’s function and consequently associated physical observables as accurately as possible when the perturbation (or the mutual interaction) is weak.

**Finite-Temperature Formalism**

At finite temperatures, it is necessary to separate the calculation into two parts. The first step is the introduction of a temperature Green’s function \( \mathcal{G} \). This function has a simple perturbation expansion similar to that for \( G \) at \( T = 0 \) and also enable us to evaluate the equilibrium thermodynamic properties of the system. The second step then relates \( \mathcal{G} \) to a time-dependent Green’s function that describes the linear response of the system to an external perturbation and provides the excitation energies of the system containing one more or one less particle.

At finite temperature, it is most convenient to use the grand canonical ensemble, whose grand Hamiltonian is given by

\[
K = H - \mu N.
\]
(98)

The grand partition function is written as
\[ Z_G = \sum_N \sum_j e^{-\beta(E_j - \mu N)} \]
\[ = \sum_N \sum_j \langle N_j | e^{-\beta(H - \mu N)} | N_j \rangle \]
\[ = \text{Tr} \left( e^{-\beta(H - \mu N)} \right) \]
\[ = \text{Tr} \left( e^{-\beta K} \right). \] (99)

The thermodynamic potential is given by
\[ \Omega(T, V, \mu) = -k_B T \ln Z_G. \] (100)

The statistical operator \( \rho_G \) is given by
\[ \rho_G = Z_G^{-1} e^{-\beta(H - \mu N)} \]
\[ = e^{\beta(\Omega - K)}. \] (101)

For any operator, the ensemble average \( \langle O \rangle \) is obtained with the prescription
\[ \langle O \rangle = \text{Tr} \left( \rho_G O \right) = \text{Tr} \left( e^{\beta(\Omega - K)} O \right) \]
\[ = \frac{\text{Tr} \left( e^{-\beta K} O \right)}{\text{Tr} e^{-\beta K}}. \] (102)

We introduce the modified Heisenberg picture operator
\[ O_K(x, t) = e^{K \tau / \hbar} O_S(x) e^{-K \tau / \hbar}. \] (103)

In particular, the field operators assume the form
\[ \psi_{K\alpha}(x, \tau) = e^{K \tau / \hbar} \psi_\alpha(x) e^{-K \tau / \hbar}, \]
\[ \psi_{K\alpha}^\dagger(x, \tau) = e^{K \tau / \hbar} \psi_\alpha^\dagger(x) e^{-K \tau / \hbar}. \] (104)

Note that \( \psi_{K\alpha}^\dagger(x, \tau) \) is not the adjoint of \( \psi_{K\alpha}(x, \tau) \) as long as \( \tau \) is real.

The single-particle temperature Green’s function is defined as
\[ G_{\alpha\beta}(x\tau, x'\tau') \equiv \text{Tr} \left\{ \rho_G [\psi_{K\alpha}(x, \tau) \psi_{K\beta}^\dagger(x', \tau')] \right\}. \] (105)

Here the symbol \( T_\tau \) orders the operators with smaller \( \tau \) at the right.

The temperature Green’s function is useful because it enables us to calculate the thermodynamic behavior of the system. If \( H \) is time independent, then \( G \) depends only on the combination \( \tau - \tau' \) and not on \( \tau \) and \( \tau' \) separately.

By definition,
\[ \text{tr} G(x\tau, x\tau^+) = \mp \sum_\alpha \text{Tr} \left[ \rho_G \psi_{K\alpha}^\dagger(x, \tau) \psi_{K\alpha}(x, \tau) \right] \]
\[ = \mp e^{\beta \Omega} \sum_\alpha \text{Tr} \left[ e^{-\beta K} e^{K \tau / \hbar} \psi_\alpha^\dagger(x) \psi_\alpha(x) e^{-K \tau / \hbar} \right] \]
\[ = \mp e^{\beta \Omega} \sum_\alpha \text{Tr} \left[ e^{-\beta K} \psi_\alpha^\dagger(x) \psi_\alpha(x) \right] \]
\[ = \mp \langle n(x) \rangle. \] (106)

A single-particle operator can be written
\[ \langle J \rangle = \text{Tr}(\rho_G J) \]
\[ = \sum_{\alpha\beta} \int d^3 x \lim_{\tau' \to \tau} \lim_{\tau \to \tau^+} J_{\beta\alpha}(x) G_{\alpha\beta}(x\tau, x'\tau') \]
\[ = \mp \int d^3 x \lim_{\tau' \to \tau} \lim_{\tau \to \tau^+} \text{tr} [J(x) G(x\tau, x'\tau')]. \] (107)
Particular examples of interest are

\[ \langle \sigma \rangle = \mp \int d^3x \text{tr} [\sigma \mathcal{G}(x\tau, x\tau^+)], \]

\[ \langle T \rangle = \mp \int d^3x \lim_{x' \to x} \frac{-\hbar^2\nabla^2}{2m} \text{tr} \mathcal{G}(x\tau, x'\tau^+). \]

The ensemble average of two body operators usually requires a two-particle temperature Green’s function. However, the mean potential energy of two-body interactions can be solely expressed in terms of \( \mathcal{G} \) as in the zero-temperature case. The expression is given by

\[ \langle V \rangle = \frac{1}{2} \int d^3x \int d^3x' V(x - x') \text{Tr} \left[ \beta \mathcal{G} \psi_{\alpha}^\dagger(x) \psi_{\gamma}^\dagger(x') \psi_{\gamma}(x') \psi_{\alpha}(x) \right] \]

\[ = \mp \frac{1}{2} \int d^3x \lim_{x' \to x, \tau' \to \tau} \left[ -\hbar \frac{\partial}{\partial \tau} + \frac{\hbar^2\nabla^2}{2m} + \mu \right] \text{tr} \mathcal{G}(x\tau, x'\tau'). \]  

<Problem> Starting from the Heisenberg equation of motion on \( \psi_{K\alpha}(x\tau) \), prove Eq.(110).

The internal energy is given by

\[ E = \langle H \rangle = \langle T + V \rangle \]

\[ = \mp \frac{1}{2} \int d^3x \lim_{x' \to x, \tau' \to \tau} \left[ -\hbar \frac{\partial}{\partial \tau} + \frac{\hbar^2\nabla^2}{2m} + \mu \right] \text{tr} \mathcal{G}(x\tau, x'\tau'). \]

Here, we give the expression for the thermodynamic potential in terms of the single-particle Green’s function without proof (For details see Section 23, Gen. Ref. 3).

\[ \Omega(T, V, \mu) = \Omega_0(T, V, \mu) \mp \int_0^1 \lambda^{-1}d\lambda \int d^3x \lim_{x' \to x, \tau' \to \tau} \frac{1}{2} \left[ -\hbar \frac{\partial}{\partial \tau} + \frac{\hbar^2\nabla^2}{2m} + \mu \right] \text{tr} \mathcal{G}^\lambda(x\tau, x'\tau'), \]

where the Hamiltonian is written as

\[ H(\lambda) = H_0 + \lambda H_1. \]

Again, here we observe that the problem of obtaining useful physical quantities boils down to the point how one can obtain exact Green’s function.

We end this section without going into the Green’s function formalism. Instead, we just give the expression for the Green’s function which shows the perturbative nature of the formalism.

\[ \text{tr} \mathcal{G}_{\alpha\beta}(x\tau, x'\tau') = -\text{Tr} \left\{ e^{-\beta K_0} \sum_{n=0}^{\infty} \frac{(-\hbar)^{-n}}{n!} \int_0^{\beta\hbar} d\tau_1 \cdots \int_0^{\beta\hbar} d\tau_n T_\tau \left[ K_1(\tau_1) \cdots K_1(\tau_n) \psi_{I\alpha}(x\tau) \psi_{I\beta}(x'\tau') \right] \right\} \]

\[ / \text{Tr} \left\{ e^{-\beta K_0} \sum_{n=0}^{\infty} \frac{(-\hbar)^{-n}}{n!} \int_0^{\beta\hbar} d\tau_1 \cdots \int_0^{\beta\hbar} d\tau_n T_\tau \left[ K_1(\tau_1) \cdots K_1(\tau_n) \right] \right\}. \]

The denominator is just the perturbation expansion of \( e^{-\beta \Omega} \). It serves to eliminate all disconnected diagrams in the numerator. It should be reminded that the Dyson’s equations in the zero-temperature are equally valid in the finite temperature formalism.

In this section, we showed that the Green’s functions in the zero and finite temperature formalism naturally lead into perturbative expansions. The perturbative calculations are greatly facilitated by the Feynman diagram rules.
As will be shown later in this lecture, in general, perturbation theory yields an asymptotic rather than convergent series. Under appropriate circumstances, it may yield a useful physical approximation but it cannot be applied to arbitrary precision. Therefore, when the perturbation, which often represents interactions between particles is large, then the outcome of the Green’s function method is in doubt. It should be noted that many of challenging problems in condensed matter physics originate from strongly correlated systems. In order to handle such strongly correlated systems, various non-perturbative schemes have been developed. However, in many cases, the approaches lack systematic means of improvement beyond the first obtained result. In later chapters, we address this problem and present a method, which provides a systematic improvement scheme beyond the mean field results for strongly correlated systems.

II. SCHRÖDINGER PICTURE IN MANY-BODY THEORY

The Schrödinger picture for many-body (field) theory is a natural extension of one- or few-body quantum mechanics.

For ordinary quantum mechanics, we start with a Hamiltonian operator and canonically quantize by postulating commutation relations between coordinate of position operators and their conjugate momenta. We reach the coordinate Schrödinger picture representation by representing the diagonal position operator with its eigenvalues, and use a differential representation of the commutators by replacing the conjugate momenta with derivatives. Coordinate representation of state vectors are called wavefunctions. The Schrödinger equation becomes a differential equation.

For many-body (field) theory in the Schrödinger picture, wavefunction should carry infinite number of degrees of freedom. This can be accomplished by substituting ‘function’ by ‘functional’. Differential representations of the canonical commutators are obtained by replacing conjugate momenta with functional derivatives. Coordinate representations of state vectors or elements of Fock space are wavefunctionals. The Schrödinger equation is a functional differential equation, whose solutions, the eigenfunctionals of the Hamiltonian functional differential operator, represent possible states of the system.

In addition to the functional Schrödinger picture method, the path integral formulation of many-body theory also requires functional calculus. In this connection, this approach is called functional integral method of many-particle (field) theory. In this lecture, we will not treat functional integral method. Instead, we refer to Gen. Ref. 2.

First, we learn about functional and its calculus.

A. Functional Calculus

Functional

A functional space is an infinite-dimensional space where each point in the space is a function on space-time. That is, each point in the function space is a mapping of space-time into the real or complex numbers. A particular point in a function space will map points in space-time to scalars, spinors or vectors.

A mapping of the points in the function space to numbers is called a functional. Thus, a functional associates a number with each function on space-time.

For example, let \( a \) be a point in a scalar function space \( A \). \( a \) is a scalar function on space-time, \( a = a(x) \in \mathbb{C} \) or \( \mathbb{R} \). Let \( F \) be a functional on \( A \). \( F \) maps points in \( A \) into numbers. \( F = F[a] \in \mathbb{C} \) or \( \mathbb{R} \). A simple example of a functional is \( F[a] = \int a(x)dx \).

Functional Derivatives

The functional derivative is formally defined by

\[
\frac{\delta F[a]}{\delta a} = \lim_{\epsilon \to 0} \frac{F[a + \epsilon \delta] - F[a]}{\epsilon},
\]

(116)

where \( \delta \) is the Dirac \( \delta \)-function distribution. Similarly, we can define a functional directional derivative in the direction of the function \( \lambda(x) \) as

\[
\frac{\delta \lambda F[a]}{\delta \lambda a} = \lim_{\epsilon \to 0} \frac{F[a + \epsilon \lambda] - F[a]}{\epsilon}.
\]

(117)
Fig. II.1 (i) \(a\) is a function on space-time. It maps points in space-time to real or complex numbers. (ii) \(a\) is a point in function space \(A\). The functional \(F[a]\) maps points in the function space \(A\) to real or complex numbers. The functional \(F[a]\) turns functions into numbers.

Also by \(\delta F[a]/\delta a(x)\), we mean the change in \(F\) with respect to a change in the function \(a\) at the point \(x\) only. Formally

\[
\frac{\delta F[a]}{\delta a(x)} = \lim_{\epsilon \to 0} \frac{F[\hat{a}] - F[a]}{\epsilon}.
\]  

(118)

Here, \(\hat{a}\) is equal to \(a\) except at the point \(x\) where \(\hat{a} = a + \epsilon\). For example, if \(F[a] = \int a(z)\delta(z - y)dz = a(y)\), then \(F[\hat{a}] = \int (a(z) + \epsilon\delta(x - z))\delta(z - y)dz = a(y) + \epsilon\delta(x - y)\).

From above, we observe that

\[
\frac{\delta a(y)}{\delta a(x)} = \lim_{\epsilon \to 0} \frac{a(y) + \epsilon\delta(x - y) - a(y)}{\epsilon} = \delta(x - y).
\]  

(119)

Similarly,

\[
\frac{\delta \lambda a(y)}{\delta \lambda a(x)} = \lambda(x - y).
\]  

(120)

Important examples include the action functional \(S = \int L(q, \dot{q}, t)dt\), the Lagrangian functional \(L = \int \mathcal{L}(\phi, \nabla \phi, \dot{\phi}, t)d^3x\) and the Hamiltonian functional \(H = \int (\pi(x, t) \cdot \partial_t \phi(x, t) - \mathcal{L})d^3x\). In fact, in deriving Eq.(8) from Eq.(7) we have implicitly used the functional calculus.

As an exercise, we consider the action for the \(\lambda \phi^4\) model in the scalar field theory (We use the scalar field theory as a prototype to develop the functional Schrödinger theory.). The action is given by

\[
S[\phi] = \int dt \int d^3y \mathcal{L}(x)
= \int d^4y \left[ \frac{1}{2} (\partial_\mu \phi \partial^\mu \phi - m^2_\phi \phi^2) - \frac{\lambda}{4!} \phi^4 \right].
\]  

(121)
Here the notation
\[ ds^2 = dx^\mu dx_\mu = dt^2 - (dx^2 + dy^2 + dz^2) \] (122)
is used with \( c = 1 \). We used
\[ x^\mu = (x^0, x^1, x^2, x^3) = (ct, x, y, z), \]
\[ x_\mu = (x_0, x_1, x_2, x_3) = (c, -x, -y, -z). \] (123)

Also, the differential operators are defined
\[
\partial_\mu = \frac{\partial}{\partial x^\mu} = (\partial_0, \partial_1, \partial_2, \partial_3) = \left( \frac{1}{c} \frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)
\]
\[ = \left( \frac{1}{c} \frac{\partial}{\partial t}, -\nabla \right), \]
\[ \partial^\mu = \frac{\partial}{\partial x_\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t}, -\nabla \right). \] (124)

For future reference, we also list
\[
\Box = \partial^\mu \partial_\mu = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)
\]
\[ = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2, \] (125)
called the d’Alembertian operator.

The energy-momentum 4-vector of a particle is
\[ p^\mu = \left( \frac{E}{c}, \vec{p} \right), \quad p_\mu = \left( \frac{E}{c}, -\vec{p} \right) \] (126)
given the invariant
\[ p^2 = p^\mu p_\mu = \frac{E^2}{c^2} - \vec{p} \cdot \vec{p} = m^2 c^2 \] (127)
or, when \( c = 1 \)
\[ p^2 = E^2 - \vec{p}^2 = m^2. \] (128)

Often \( p \cdot x \) is used for \( p_\mu x^\mu \)
\[ p \cdot x = p_\mu x^\mu = Et - \vec{p} \cdot \vec{r}. \] (129)

From Eq.(121), we have
\[
\frac{\delta}{\delta \phi(x)} \int d^4 y \frac{1}{2} (\partial^\mu \phi \partial_\mu \phi) = -\frac{\delta}{\delta \phi(x)} \int d^4 y \frac{1}{2} (\phi \partial^\mu \partial_\mu \phi)
\]
\[ = -\int d^4 y \delta^4(x - y) \partial^\mu \partial_\mu \phi(y) = -\partial^\mu \partial_\mu \phi(x), \] (130)
and
\[
\frac{\delta}{\delta \phi(y)} \int d^4 y \phi^n(y) = n \int d^4 y \phi^{n-1}(y) \delta^4(x - y)
\]
\[ = n \phi^{n-1}(x). \] (131)

Thus
\[
\frac{\delta S[\phi]}{\delta \phi(x)} = -\left( \partial_\mu \partial^\mu \phi(x) + m_0^2 \phi(x) + \frac{\lambda_0}{3!} \phi^3(x) \right) = 0, \] (132)

19
which is the Klein-Gordon equation with the $\phi^4$ interaction.

**Functional Differential Equations**

In the Schrödinger picture of many-body theory, the Schrödinger equation is a functional differential equation. For an action $S[\psi]$, the field equations are

$$\frac{\delta S[\psi]}{\delta \psi(x)} = 0.$$  

(133)

A functional differential equation can be thought of as an infinite set of coupled partial differential equations or a partial differential equation on an infinite-dimensional vector space.

For example, consider

$$\int dy \left( \frac{\delta}{\delta a(y)} \frac{\delta}{\delta a(y)} - b(y) \right) F[a] = 0.$$  

(134)

This equation is satisfied by

$$F[a] = \eta \exp(\pm \int dx \sqrt{b(x)a(x)}).$$  

(135)

<Problem> Show that the above $F[a]$ satisfies Eq.(134).

A more realistic form which may appear in the real problem is given by

$$\int dy \frac{\delta}{\delta a(y)} \frac{\delta}{\delta a(y)} F[a] + \int dxdy f(x,y)a(x)a(y)F[a] = \mu F[a].$$  

(136)

Assume $f(x, y)$ is symmetric in $x$ and $y$.

First we substitute

$$F[a] = \eta \exp(G[a]),$$  

(137)

and solve the resulting equation for $G[a]$.

$$\int dy \left( \frac{\delta}{\delta a(y)} \frac{\delta}{\delta a(y)} G[a] + \left( \frac{\delta}{\delta a(y)} G[a] \right)^2 \right) = \mu - \int dxdy f(x,y)a(x)a(y).$$  

(138)

To proceed, we must match the power of $a(y)$ for both sides. Thus, we write

$$G[a] = \frac{1}{2} \int dxdyg(x,y)a(x)a(y).$$  

(139)

$G[a]$ will be a solution provided the symmetric $g(x,y)$ satisfies

$$\mu = \int dyg(y,y) \text{ and } f(x,y) = \int dzg(x,z)g(y,z).$$  

(140)

This technique of comparing the powers of both sides is called the 'power counting' method.

**Functional Integrals - Bosonic Variables**

Functional integrals are integrals of functionals over function spaces and, in general, are not well defined. There are only two types that can be done exactly. The first type is the $\delta$-functional, $\delta[a - \xi]$.

$$\int Da \delta[a - \xi] = 1.$$  

(141)
\( D \) in the measure indicates that the integral is over the function space containing \( a(\vec{x}) \), which can be expressed
\[
Da = \prod_{\vec{x}} da(\vec{x}).
\]  
(142)

Correspondingly,
\[
\delta[a - \xi] = \prod_{\vec{x}} \delta(a(\vec{x}) - \xi(\vec{x})).
\]  
(143)

Thus the integral in Eq.(141) is an infinite product of independent integrals, one for each \( \vec{x} \). Thus, we have
\[
\int Da F[a] \delta[a - \xi] \approx \prod_{\vec{x}} \int da(\vec{x}) \delta(a(\vec{x}) - \xi(\vec{x})) F[a]
\]
\[
= \prod_{\vec{x}} \int da(\vec{x}) \delta(a(\vec{x}) - \xi(\vec{x})) F[a]
\]
\[
= F[\xi].
\]  
(144)

Often it helps to think of the functions, such as \( a(x) \), as infinite dimensional (column) vectors where \( x \) plays the role of an index. With this view, a functional integral looks like the natural infinite-dimensional limit of ordinary finite-dimensional integrals. The second type of functional that we can integrate exactly is the Gaussian functional.
\[
\int Dae^{-F[a]}, \quad \text{where } F[a] = \int dxa^2(x)
\]  
(145)

We have
\[
\int Dae^{-\int dxa^2(x)} = \int \prod_x da(x) e^{-\sum_x a^2(x)}
\]
\[
= \prod_x \int da(x) e^{-a^2(x)} = \prod_x \sqrt{\pi},
\]  
(146)

where we used \( \int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \).

Following the same steps, we have
\[
\int Dae^{-\int df(x)a^2(x)} = \prod_x \sqrt{\frac{\pi}{f(x)}}
\]  
(147)

We regard \( f(x) \) as an infinite-dimensional diagonal matrix
\[
f(x, y) = f(x) \delta(x - y).
\]

\( f(x) \) also represents the diagonal elements of the diagonal matrix. They are also the eigenvalues of the matrix. The product of the eigenvalues is the determinant of the matrix, hence
\[
\prod_x \sqrt{\frac{\pi}{f(x)}} \rightarrow (\sqrt{\pi})^\infty \prod_x \frac{1}{\sqrt{f(x)}} = (\sqrt{\pi})^\infty \sqrt{\det f}
\]
\[
= \det^{-1/2} \left( \frac{f}{\pi} \right),
\]  
(148)

so
\[
\int Dae^{-\int df(x)a^2(x)} = \det^{-1/2} \left( \frac{f}{\pi} \right).
\]  
(149)

If the operator is not diagonal, the result is still the same.
\[
\int Dae^{-\int dx dy g(x,y)a(y)} = \frac{(\sqrt{\pi})^\infty}{\sqrt{\det g}}
\]  
(150)
Finally, consider
\[ \int Dae^{F[a,J]}, \tag{151} \]
where
\[ F[a,J] = \int dxdya(x)g(x,y)a(y) + \int dxJ(x)a(x) \tag{152} \]
is the Gaussian functional with the addition of a source term.

For the 1-dimensional case
\[ \int_{-\infty}^{\infty} dx e^{-\alpha x^2 + bx} = \int_{-\infty}^{\infty} dx e^{-\alpha(x-b/2)^2} e^{1/4(b/\alpha)} \]
\[ = e^{1/4(b/\alpha)} \int dx e^{-\alpha x^2} = e^{1/4(b/\alpha)} \frac{\sqrt{\pi}}{\alpha}. \tag{153} \]

Thus,
\[ \int Dae^{-F[a,J]} = \exp \left( \frac{1}{4} \int dxdyJ(x)g^{-1}(x-y)J(y) \right) \left( \frac{\sqrt{\pi}}{\sqrt{\det g}} \right) \tag{154} \]
where \( g^{-1}(x-y) \) is the inverse operator (matrix) of \( g(x-y) \),
\[ \int dzg^{-1}(x-z)g(z-y) = \delta(x-y). \tag{155} \]

The source term in the Gaussian allows us to easily compute the functional integral of any moment of the Gaussian. Namely,
\[ \int Da(a(1) \cdots a(x_n)exp(-\int dxdya(x,y)a(y)) \]
\[ = \frac{\delta}{\delta J(x_1)} \cdots \frac{\delta}{\delta J(x_n)} \left. \int Dae^{-F[a,J]} \right|_{J=0}. \tag{156} \]

Using the above relation, we obtain
\[ \int Da(a(1)exp(-\int dxdya(x,y)a(y) = 0. \tag{157} \]
and
\[ \int Da(a(1)a(x_2)exp(-\int dxdya(x,y)a(y)) \]
\[ = \frac{1}{2}g^{-1}(x_1-x_2) \left( \frac{\sqrt{\pi}}{\sqrt{\det g}} \right) \tag{158} \]

In fact, any odd moment vanishes. Here, we note that the potentially bothersome infinite number in the numerator is often absorbed in or canceled by a normalization.

**Fermionic Variables - Grassmann Algebra**

Since fermionic operators anticommute, we must introduce anticommuting numbers and functions, which are called 'Grassmann variables'. Consider an eigenvalue problem for the fermion field operator,
\[ \psi(\vec{x})|\phi\rangle = \phi(\vec{x})|\phi\rangle. \tag{159} \]

For two such operators, a naive calculation shows
\[ \psi_1\psi_2|\phi\rangle = \psi_1\phi_2|\phi\rangle = \phi_1\phi_2|\phi\rangle \]
\[ = -\psi_2\psi_1|\phi\rangle = -\psi_2\phi_1|\phi\rangle = -\phi_2\phi_1|\phi\rangle, \]
which gives \( \phi_1\phi_2 = -\phi_2\phi_1 \). Also we note that \( \phi^2 = 0 \) following the Pauli exclusion principle.

Let \( \eta \) be such an anticommuting variable. This means that

\[
\{ \eta, \eta \} = 0,
\]

thus \( \eta^2 = 0 \). Let us define the derivative operator for an anticommuting variable in an analogous way to the bosonic case,

\[
\left\{ \frac{d}{d\eta}, \eta \right\} = 1.
\]

For any \( f(\eta) \), the power series expansion of \( f \) must be of the form

\[
f(\eta) = a + b\eta,
\]

since \( \eta^2 = 0 \). Therefore, \( d^2 f / d\eta^2 = 0 \), so

\[
\left\{ \frac{d}{d\eta}, \frac{d}{d\eta} \right\} = 0.
\]

When \( a \) and \( b \) are anticommuting numbers, then

\[
\frac{df}{d\eta} = -b.
\]

We introduce integration by defining two following integrals :

\[
\int d\eta \equiv 0,
\]

\[
\int d\eta \eta \equiv 1.
\]

This definition is chosen so that \( \int d\eta \) is translationally invariant and linear. It is not the inverse operation of \( d/d\eta \); in fact, integration acts like differentiation. For example, if \( \eta_1 \) and \( \eta_2 \) are two anticommuting variables, then

\[
\int d\eta_1 d\eta_2 \eta_1 \eta_2 = -\int d\eta_1 d\eta_2 \eta_2 \eta_1
\]

\[
= -\int d\eta_2 d\eta_1 \eta_1 \eta_2
\]

\[
= -1.
\]

Let’s consider a space of anticommuting functions, \( \eta(x) \), namely

\[
\left\{ \frac{\delta}{\delta\eta(x)}, \eta(y) \right\} = \delta(x - y).
\]

We carry out the functional integrals as in the bosonic case. From the definition of integration, Eq.(165), we see that the \( \delta \)-functional \( \delta[\eta] \) is

\[
\delta[\eta] = \prod_x \eta(x),
\]

so that

\[
\int D\eta \delta[\eta] = 1.
\]

Here, we choose the ordering of the \( d\eta(x) \)'s in \( D\eta = \prod_x d\eta(x) \) to be the opposite of the ordering in the functional so that no extra minus signs are introduced in doing the integrals. Similarly

\[
\delta[\eta - \sigma] = \prod_x (\eta(x) - \sigma(x)),
\]
then,
\[ \int D\eta \delta[\eta - \sigma] F[\eta] = \int \prod_x d\eta(x) \prod_x (\eta(x) - \sigma(x)) F[\eta] = F[\sigma]. \] (171)

Note that \( F[\eta] \) is placed on the right side of the delta function (See p.28, Gen. Ref. 2.) not to spoil the ordering convention discussed above.

\textbf{<Problem> Prove the above equation using one component delta function} \( \delta[\eta - \sigma] = \eta - \sigma \).

Now consider the Gaussian integral,
\[ \int D\eta \exp(-\int dx dy \eta(x)g(x,y)\eta(y)). \] (172)

\( g(x, y) = -g(y, x) \) in order to get a non-vanishing result. For the 2-dimensional integral, we have \( \eta_1 \) and \( \eta_2 \) so that
\[ \int d\eta_1 d\eta_2 e^{-\eta_1 g_{12} \eta_2 - \eta_2 g_{12} \eta_1} = \int d\eta_1 d\eta_2 e^{-2\eta_1 g_{12} \eta_2} \] (173)

where we used \( \eta_2 g_{21} \eta_1 = -\eta_1 g_{21} \eta_2 = \eta_1 g_{12} \eta_2 \).

Expand the exponential in a power series,
\[ e^{-2\eta_1 g_{12} \eta_2} = 1 - 2\eta_1 g_{12} \eta_2 + 2(\eta_1 g_{12} \eta_2)^2 + \cdots = 1 - 2\eta_1 g_{12} \eta_2. \] (174)

Finally, we obtain
\[ \int d\eta_1 d\eta_2 e^{-2\eta_1 g_{12} \eta_2} = \int d\eta_1 d\eta_2 (1 - 2\eta_1 g_{12} \eta_2) = 2g_{12}. \] (175)

Since for an antisymmetric \( 2 \times 2 \) matrix, \( \det g = -g_{12}g_{21} = (g_{12})^2 \), we rewrite
\[ \int d\eta_1 d\eta_2 e^{-2\eta_1 g_{12} \eta_2} = 2\sqrt{\det g}. \] (176)

\textbf{<Problem> Show that for the 4-dimensional case},
\[ \int d\eta_1 \cdots d\eta_4 e^{-2(\eta_1 g_{12} \eta_2 + \cdots + \eta_3 g_{34} \eta_4)} \]
\[ = \frac{2^3}{2!}(g_{12}g_{34} - g_{13}g_{24} + g_{14}g_{23}) = 4\sqrt{\det g}. \] (177)

We can show by induction
\[ \int d\eta_1 \cdots d\eta_N e^{-2(\eta_1 g_{12} \eta_2 + \cdots + \eta_{N-1} g_{N-1,N} \eta_N)} \]
\[ = (2)^{N/2} \sqrt{\det g}. \] (178)

We assert that in the \( N \to \infty \) limit
\[ \int D\eta \exp(-\int dx dy \eta(x)g(x,y)\eta(y)) = (\sqrt{2})^\infty \sqrt{\det g}. \] (179)
Often, it is necessary to consider the fields to be complex. For bosonic functional integrals, the generalization is straightforward. Let \( a(x) \) be an ordinary complex function with \( a(x) = (a_1(x) + ia_2(x))/\sqrt{2} \) where \( a_1(x) \) and \( a_2(x) \) are real valued.

If we switch variables from \((a^*, a)\) to \((a_1, ia_2)\), the Gaussian integral can be readily performed to be

\[
\int D\eta D\eta^* \exp\left(-\int dx dy \eta^*(x)f(x, y)a(y)\right)
= \int D\eta_1 D(ia_2) \exp\left(-\int dx dy (a_1(x) - ia_2(x))f(x, y)(a_1(y) + ia_2(y))\right)
= \frac{(i\pi)^{\infty}}{\det f}. \tag{180}
\]

In the second step, \( f(x, y) \) is assumed symmetric and can be diagonalized so that the integral gives two copies of Eq. (150).

The fermionic Gaussian functional integral over complex anticommuting functions requires a little more attention. Let \( \eta \) be a complex anticommuting variable and write \( \eta = (\xi_1 + i\xi_2)/\sqrt{2} \) where \( \xi_1 \) and \( \xi_2 \) are real-valued. Then \( \eta^* = (\xi_1 - i\xi_2)/\sqrt{2} \).

Let

\[
\int d\eta = 1, \quad \int d\eta^* = 1,
\int d\eta = \int d\eta^* = \int d\eta^* = 0. \tag{181}
\]

This means that \( d\eta = (d\xi_1 - id\xi_2)/\sqrt{2} \) and \( d\eta^* = (d\xi_1 + id\xi_2)/\sqrt{2} \).

**<Problem>** Show that using Eq. (181), \( d\eta = (d\xi_1 - id\xi_2)/\sqrt{2} \) and \( d\eta^* = (d\xi_1 + id\xi_2)/\sqrt{2} \).

Thus, we have \( d\eta^* d\eta = -id\xi_1 d\xi_2 \). The 1-dimensional Gaussian integral is simply ( \( m = \) an ordinary commuting number)

\[
\int d\eta^* d\eta \exp(-\eta^* m\eta) = \int d\eta^* d\eta (1 - \eta^* m\eta) = m. \tag{182}
\]

The 2-dimensional Gaussian integral is

\[
\int d\eta_1^* d\eta_2^* d\eta_1 d\eta_2 \exp\left(-\sum_{ij=1}^2 \eta_i^* m_{ij} \eta_j\right)
= \int d\eta_1^* d\eta_2^* d\eta_1 d\eta_2 \left[ 1 - (\eta_1^* m_{11} \eta_1 + \eta_1^* m_{12} \eta_2 + \eta_2^* m_{21} \eta_1 + \eta_2^* m_{22} \eta_2)ight]
+ \frac{1}{2!}(\ldots)^2 + \ldots
= \int d\eta_1^* d\eta_2^* d\eta_1 d\eta_2 \left( \eta_1^* \eta_2^* \eta_1 \eta_2 (m_{11} m_{22} - m_{12} m_{21})\right)
= -\det m_{ij}. \tag{183}
\]

In order to avoid the annoying sign problem, we define

\[
D\eta^* D\eta = \prod_x d\eta^* (x) d\eta(x). \tag{184}
\]

Therefore, we should order \( d\eta_1^* d\eta_1 d\eta_2^* d\eta_2 \cdots d\eta_N^* d\eta_N \). Then, we have

\[
\int D\eta^* D\eta \exp \left( -\int dx dy \eta^*(x) g(x, y) \eta(y) \right) = \det g. \tag{185}
\]

The hyperbolic fermionic Gaussian integral \( \int D\eta^* D\eta \exp \left( +\int dx dy \eta^*(x) g(x, y) \eta(y) \right) \) has no well-defined bosonic analogue. In order to get a well-defined limit, we should reverse the order, so that \( D\eta^* D\eta = \prod_x (d\eta(x) d\eta^*(x)) \). Thus,
\[ \int D\eta^* D\eta \exp \left( + \int dx dy \eta^* (x) g(x, y) \eta(y) \right) = \text{det} g. \tag{186} \]

Functional integral techniques using the above results have emerged in last two decades as a powerful tool for study of many-particle systems. Unfortunately, this topic is out of the scope of this lecture. Instead, we refer to Gen. Ref. 2 for a detailed treatment on this topic.

B. Functional Schrödinger Picture -Schrödinger Picture in The Second Quantized Formalism

We have learned that the Heisenberg picture method provides a convenient tool to study the many-particle system through Green’s function. However, when the mutual interaction is strong, perturbative approaches are known less than reliable. Also when one studies systems such as nonequilibrium many-particle systems and evolution of a system in which time variation is important, Green’s function method may not be a good starting point.

In this connection, field theorists have been studying the functional Schrödinger picture field theory to provide an alternative theory to the Green’s functions formalism.

In quantum mechanics (first quantized system), coordinate and conjugate momentum are represented by \( q_i(t) \) and \( p_i(t) \). In second quantized system, the field \( \psi(\vec{x}, t) \) and its conjugate momentum are used to represent the infinite degrees of freedom.

**Bosonic Theory**

We now work in a coordinate Schrödinger picture but with an infinite degree of freedom. In analogy to \( \hat{x}|x\rangle = x|x\rangle \) in quantum mechanics, we consider

\[ \psi(\vec{x})|\phi\rangle = \phi(\vec{x})|\phi\rangle, \tag{187} \]

where \( \phi(\vec{x}) \) is the eigenvalue function corresponding to the field operator \( \psi(\vec{x}) \). \(|\phi\rangle\) represents an eigenstate. The coordinate representation of the state \(|\Psi\rangle\), now time dependent, is the wave functional, \( \Psi[\phi] \).

\[ \Psi[\phi] = \langle \phi|\Psi \rangle \tag{188} \]

In analogy to the quantum mechanical commutation relation \([q_i, p_j] = i\hbar\delta_{ij}\), we require

\[ [\phi(\vec{x}), \pi(\vec{x}')] = i\hbar\delta(\vec{x} - \vec{x}'). \tag{189} \]

This requirement is easily satisfied by

\[ \pi(\vec{x}) = \hbar \frac{\delta}{\delta \phi(\vec{x})}. \tag{190} \]

Compare this expression with the corresponding quantum mechanical one \( p = \hbar \frac{\partial}{\partial x} \).

In terms of the coordinate basis,

\[ \langle \phi'|\pi(\vec{x})|\phi\rangle = \hbar \frac{\delta}{\delta \phi(\vec{x})} \delta[\phi - \phi']. \tag{191} \]

With this prescription, the Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H|\Psi\rangle \tag{192} \]

turns into a functional differential equation

\[ i\hbar \frac{\partial}{\partial t} \Psi[\phi, t] = H[\phi, \frac{\hbar}{i} \frac{\delta}{\delta \phi}] \Psi[\phi, t]. \tag{193} \]

In a time-independent case,

\[ H[\phi, \frac{\hbar}{i} \frac{\delta}{\delta \phi}] \Psi[\phi] = E \Psi[\phi], \tag{194} \]
with $\Psi[\phi, t] = e^{-iEt/\hbar}\check{\Psi}[\phi]$.

As an example of the bosonic formalism developed above, the free scalar theory will be studied. As it is a convention in the field theory, we set $\hbar = c = 1$. The action for the free scalar theory is given (See Eq.(121).)

$$S[\psi] = \frac{1}{2} \int d^3 x L(x)$$
$$= \frac{1}{2} \int d^3 x (\partial^\mu \phi(x) \partial_\mu \phi(x) - m^2 \phi^2(x)).$$ (195)

The corresponding Hamiltonian is defined by the Legendre transform of the Lagrangian

$$H = \int d^3 x (\pi(x, t) \cdot \partial_t \phi(x, t) - L).$$ (196)

Compare this with the quantum mechanical relation $H(q, p, t) = \sum_i q_i p_i - L(q, p, t)$. Here, we note that the field momentum conjugate to $\phi$ is

$$\pi(x) = \frac{\partial L}{\partial (\partial_t \phi(x))} = \dot{\phi}(x).$$ (197)

Using these relations, the Hamiltonian is written as

$$H = \frac{1}{2} \int d^3 x (\pi^2 + |\nabla \phi|^2 + m^2 \phi^2).$$ (198)

Using Eq.(190) for $\pi(x)$, the time-independent Schrödinger functional equation is expressed as

$$\frac{1}{2} \int d^3 x \left( -\frac{\delta^2 \Psi[\phi]}{\delta \phi^2(x)} + (|\nabla \phi|^2 + m^2 \phi^2)\Psi[\phi] \right) = E\Psi[\phi].$$ (199)

This equation can be solved exactly since there is no coupling term.

**<Problem>** Solve the functional differential equation (199) using a trial functional for the ground state, $\Psi[0][\phi] = \eta \exp(-G[\phi]).$ Show that the ground state energy is given by $E_0 = \frac{1}{2} \int d^3 k \omega_k \delta^3(0).$ (See Chapt. 10, Gen. Ref. 1.).

**Fermionic Theory**

The functional Schrödinger picture for fermionic many-particles is more complicated than the bosonic case because we should handle anticommuting Grassmann variables.

In order to deal with the situation, we examine the nature of the fermionic field theory which provides the anti-commutivity of the field operators. In the fermionic field theory, one can use either hermitian or non-hermitian field operators (For a somewhat deeper discussion, see Appendix A.).

It should be noted that for neutral (chargeless) Majorana fermions, hermitian operators should always be used, whereas for charged spin 1/2 particles, both hermitian and non-hermitian operators are acceptable. This comes from the fact that non-hermitian operators can always be written as a sum of two hermitian operators. For details of discussion, we refer to Appendix A and references listed there. Here, we just present the results.

When one uses hermitian fermion operators, the following equal-time anticommutation relation is obtained

$$\{\psi_a(x), \psi_b(x')\}_{x^0 = x'^0} = \delta_{ab} \delta(\vec{x} - \vec{x}').$$ (200)

Here, $\psi^\dagger(x) = \psi(x)$. When non-hermitian field operators are used, we obtain the equal-time anticommutation relation,

$$\{\psi_a(x), \psi^\dagger_b(x')\}_{x^0 = x'^0} = \delta_{ab} \delta(\vec{x} - \vec{x}'),$$

$$\{\psi_a(x), \psi_b(x')\}_{x^0 = x'^0} = 0 = \{\psi^\dagger_a(x), \psi^\dagger_b(x')\}_{x^0 = x'^0}$$ (201) (202)

where $\psi^\dagger(x) \neq \psi(x)$.

As mentioned above, since non-hermitian field operator can be obtained through a linear combination of hermitian operators, it is convenient to start with hermitian operators. Since, in this case, the anticommutation relation, Eq.(200), indicates that the field operator itself corresponds to the conjugate momentum (with some constant factor),
it is not possible to obtain a simple prescription as in the bosonic case. However, they can be represented by a linear combination of their eigenvalues and the functional differential operators;

\[ \psi_a(\vec{x}) = \alpha \theta_a(\vec{x}) + \beta \frac{\delta}{\delta \theta_a(\vec{x})} \]  

(203)

where \( \theta_a(\vec{x})^* = \theta_a(\vec{x}) \) and \( \{ \theta_a(\vec{x}), \theta_b(\vec{x}) \} = 0 \). It must satisfy the equal-time anticommutation relations, Eq.(200) and this imposes a condition for the constants \( \alpha \) and \( \beta \), \( \alpha \beta = \frac{1}{2} \).

**Problem** Show that \( \alpha \beta = \frac{1}{2} \).

Thus, a simple choice for the hermitian fermion field operators is to take \( |\alpha| = |\beta| = 1/\sqrt{2} \), which gives two equivalent representations

\[ \psi_1(\vec{x}) = \frac{1}{\sqrt{2}} \left[ \theta_1(\vec{x}) + \frac{\delta}{\delta \theta_1(\vec{x})} \right] \]  

(204)

and

\[ \psi_2(\vec{x}) = \frac{1}{\sqrt{2}} \left[ \theta_2(\vec{x}) - \frac{\delta}{\delta \theta_2(\vec{x})} \right] . \]  

(205)

The representation for the non-hermitian spinor field operators, which are charge eigenvalues, can be constructed combining two hermitian field \( \psi_1 \) and \( \psi_2 \),

\[ \psi = \psi_1 + i \psi_2. \]  

(206)

We also define a complex Grassmann variable \( \theta(\vec{x}) \);

\[ \theta(\vec{x}) = \theta_1(\vec{x}) + i \theta_2(\vec{x}). \]  

(207)

Using Eq.(204) for both \( \psi_1 \) and \( \psi_2 \),

\[
\begin{align*}
\psi_1 &= \frac{1}{\sqrt{2}} \left( \theta_1 + \frac{\delta}{\delta \theta_1} \right), \\
\psi_2 &= \frac{1}{\sqrt{2}} \left( \theta_2 + \frac{\delta}{\delta \theta_2} \right),
\end{align*}
\]

(208)

we have

\[
\begin{align*}
\psi &= \frac{1}{\sqrt{2}} \left[ \theta(\vec{x}) + \frac{\delta}{\delta \theta^*(\vec{x})} \right], \\
\psi^\dagger &= \frac{1}{\sqrt{2}} \left[ \theta^*(\vec{x}) + \frac{\delta}{\delta \theta(\vec{x})} \right].
\end{align*}
\]

(209)

This prescription was first proposed by Floreanini and Jackiw [1].

Another way to obtain a representation for the non-hermitian field is to use Eq.(204) and (205) together with a real Grassmann variable \( \theta \) (\( \theta^*(\vec{x}) = \theta(\vec{x}) \)).

\[
\begin{align*}
\psi_1 &= \frac{1}{\sqrt{2}} \left( \theta + \frac{\delta}{\delta \theta} \right), \\
\psi_2 &= \frac{1}{\sqrt{2i}} \left( \theta - \frac{\delta}{\delta \theta} \right),
\end{align*}
\]

(210)

From these expressions, we obtain

\[
\begin{align*}
\psi &= \theta(\vec{x}), \\
\psi^\dagger &= \frac{\delta}{\delta \theta(\vec{x})},
\end{align*}
\]

(211)
which was first proposed by Duncan, Meyer-Ortmans and Roskies (DMR) [2]. It should be noted that, in this prescription, the hermitian conjugate of \( \theta(\vec{x}) \) is not given by the transpose of \( \theta(\vec{x}) \) but

\[
[\theta(\vec{x})]^\dagger = \frac{\delta}{\delta \theta(\vec{x})}.
\]  

(212)

It can be shown easily that the above two representations Eq.(209) and (211) both satisfy the anticommutation relations Eq.(201) and (202). For charged particles including electrons, any of the above two representations can be used. We show, in the next chapter, examples of applications for both representations to physical problems. However, for neutral spin-\( \frac{1}{2} \) particles, Eq.(204) or (203) with \( \alpha\beta = \frac{1}{2} \) should be used.

Using the above prescription, we can readily write down the functional Schrödinger equation for fermionic particles. Especially when the Hamiltonian is time-independent,

\[
H[\psi^\dagger, \psi]|\Psi\rangle = H \left[ \frac{1}{\sqrt{2}} \left( \theta^* + \frac{\delta}{\delta \theta} \right), \frac{1}{\sqrt{2}} \left( \theta + \frac{\delta}{\delta \theta^*} \right) \right] |\Psi\rangle
\]  

(213)

with the Floreanini-Jackiw prescription. When the DMR prescription is used, we have

\[
H[\psi^\dagger, \psi]|\Psi\rangle = H \left[ \frac{\delta}{\delta \theta}, \theta \right] |\Psi\rangle.
\]  

(214)

In the functional Schrödinger picture representation of fermionic many-particles, the physical information is given by the state functional \( \langle \theta, t | \Psi \rangle \) and also by the scalar product between states,

\[
\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_2 | \Psi_1 \rangle^*.
\]  

(215)

Unlike the bosonic case, the dual to the state ket, here, is not a simple hermitian conjugate. In order to investigate this problem, we first consider a system of one degree of freedom described by annihilation and creation operators, \( a^\dagger \) and \( a \), which satisfy

\[
\{a, a^\dagger\} = 1, \\
\{a, a\} = 0 = \{a^\dagger, a^\dagger\}.
\]  

(216)

The Hilbert space of the system consists of vacuum and 1-particle states, \( |0\rangle \) and \( |1\rangle \);

\[
a|0\rangle = 0, a|1\rangle = |0\rangle \\
a^\dagger |0\rangle = |1\rangle, \quad a^\dagger |1\rangle = 0
\]  

(217)

We now want to represent the Hilbert space by functional \( \Psi[\theta] \) of real Grassmann number \( \theta \), which satisfies \( \theta \theta = 0 \). The most general functional of \( \theta \) may be written as

\[
\Psi[\theta] = \alpha + \beta \theta \quad (\alpha, \beta = \text{constants}),
\]  

(218)

which implies that the Hilbert space is described by the two component basis \((1, \theta)\). Thus, a natural choice for the \( \theta \)-representation is to take

\[
|0\rangle \rightarrow 1, \quad |1\rangle \rightarrow \theta,
\]  

(219)

which imply

\[
\langle \theta | 0 \rangle = 1 \quad \text{and} \quad \langle \theta | 1 \rangle = \theta.
\]  

(220)

From the above relation, we obtain the transformation function

\[
\langle \theta' | \theta \rangle = \langle \theta' | 0 \rangle \langle 0 | \theta \rangle + \langle \theta' | 1 \rangle \langle 1 | \theta \rangle \\
= 1 + \theta' \theta = e^{\theta' \theta}.
\]  

(221)

This relation shows that the \( \theta \)-basis is not orthonormal. With the above relation, we now define the \( \theta \)-representation of the dual state,
\[\langle \Psi_1 | \Psi_2 \rangle = \int D\theta D\theta' \langle \Psi_1 | \theta' \rangle \langle \theta' | \theta \rangle \langle \theta | \Psi_2 \rangle \]
\[\equiv \int D\theta \bar{\Psi}_1 [\theta] \Psi_2 [\theta], \quad (222)\]

where \( \Psi_2 [\theta] = \langle \theta | \Psi_2 \rangle \). Thus, the dual state \( \bar{\Psi}[\theta] \) of \( \Psi[\theta] \) is defined by
\[\bar{\Psi}[\theta] = \int D\theta' \langle \Psi | \theta' \rangle \langle \theta' | \theta \rangle \]
\[\equiv \int D\theta \Psi^\dagger [\theta'] e^{\theta' \theta}, \quad (223)\]

where \( \Psi^\dagger \) is the Hermitian conjugate of \( \Psi \). This can be easily generalized to the case of infinite degree of freedom as follows
\[\bar{\Psi}[\theta(\vec{x})] = \int D\theta' (\Psi | \theta'(\vec{x})) e^{\theta'(\vec{x})\theta(\vec{x})}, \quad (224)\]

where the variable \( \theta \) can have components in the internal space and the integral convention is used for the repeated variables \( \vec{x} \).

As an example, we consider the dual state of a Gaussian functional
\[\Psi[\theta] = e^{\frac{1}{2} \theta_\alpha (\vec{x}) G_{\alpha \beta}(\vec{x},\vec{y}) \theta_\beta (\vec{y})}, \quad (225)\]

It can be shown easily that the dual is given by another Gaussian functional (See Appendix B.)
\[\bar{\Psi}[\theta] = C e^{\frac{1}{2} \theta_\alpha (\vec{x}) \bar{G}_{\alpha \beta}(\vec{x},\vec{y}) \theta_\beta (\vec{y})}, \quad (226)\]

where \( C \) is a constant independent of \( \theta \) and \( \bar{G} \) is defined by
\[\bar{G} = [G^\dagger]^{-1}. \quad (227)\]

In the case of the Floreanini-Jakiw representation where complex \( \theta \) is used, the above prescription for the dual becomes slightly modified to become (See Appendix B.)
\[\bar{\Psi}[\theta, \theta^\dagger] = \int D\theta' D\theta'^\dagger \langle \Psi | \theta', \theta'^\dagger \rangle e^{\theta'^\dagger (\vec{x})\theta(\vec{x}) - \theta^\dagger (\vec{x})\theta'(\vec{x})}, \quad (228)\]

where \( \theta^\dagger \) denotes the transpose of the complex conjugate of \( \theta \). However, the dual of a Gaussian functional
\[\Psi[\theta, \theta^\dagger] = e^{\theta^\dagger \theta}, \quad (229)\]

has the same form as in the hermitian case of Eq.(226),
\[\bar{\Psi}[\theta, \theta^\dagger] = C e^{\theta^\dagger \bar{G}\theta}, \quad (230)\]

where \( \bar{G} = G^\dagger^{-1} \). This simple property of the Gaussian functional renders the functional Schrödinger picture useful for computation of physical quantities.

In the next chapter, we show some simple applications of the formalism developed so far.

III. APPLICATIONS TO MANY-BODY PROBLEMS - VARIATIONAL APPROACH

Many-body theoretical schemes, which are essentially non-relativistic field theories have been all based on the Heisenberg (interaction) picture, as we can see easily from the conventional Green’s function method and the functional integral method. Only, very recently the functional Schrödinger picture method has been applied to many-particle systems with some successes.

In this chapter, the functional Schrödinger picture formalism developed in Chapter II will be applied to many-particle systems within variational approximation.
A. Electron Gas and The Hubbard Model

Electron Gas

The Schrödinger picture formalism provides a convenient basis for variational approximation, since, with a trial functional \(\langle u^\dagger, u|\Psi\rangle\), the ground state energy of a many-particle system can be calculated easily.

As an example, we first study an interacting electron gas system [1]. The Hamiltonian is given by

\[
H = \sum_\alpha \int d^3x \psi^\dagger_\alpha(\vec{x}) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \psi_\alpha(\vec{x}) + \frac{1}{2} \sum_{\alpha,\beta} \int d^3xd^3y V(\vec{x}, \vec{y}) \psi^\dagger_\alpha(\vec{x}) \psi^\dagger_\beta(\vec{y}) \psi_\beta(\vec{y}) \psi_\alpha(\vec{x}),
\]

(231)

where \(\alpha\) and \(\beta\) are spin indices. For field operators \(\psi^\dagger\) and \(\psi\), we use the Floreanini-Jackiw formalism,

\[
\psi(\vec{x}) = \frac{1}{\sqrt{2}} \left( u(\vec{x}) + \frac{\delta}{\delta u^\dagger(\vec{x})} \right),
\]

\[
\psi^\dagger(\vec{x}) = \frac{1}{\sqrt{2}} \left( u^\dagger(\vec{x}) + \frac{\delta}{\delta u(\vec{x})} \right).\]

(232)

We note that \(\{\psi_i(\vec{x}, t), \psi^\dagger_j(\vec{x}', t)\} = \delta_{ij} \delta(\vec{x} - \vec{x}')\) and \(u\) and \(u^\dagger\) are anticommuting Grassmann variables. Substitution of field operators into the Hamiltonian turns the many-particle Schrödinger equation into a functional differential equation,

\[
H[\langle 1/\sqrt{2}(u + \delta/\delta u^\dagger), (1/\sqrt{2})(u^\dagger + \delta/\delta u)\rangle|\Psi_0\rangle = E|\Psi_0\rangle.\]

(233)

We now calculate the ground state energy of the above many-particle system using variational approximation. A natural choice for the trial functional is the Gaussian, which becomes an exact solution to non-interacting many-particle systems.

\[
|\Psi_0\rangle = \exp \left( \sum_{\alpha,\beta} \int \int d^3x d^3y u^\dagger_\alpha(\vec{x}) G_{\alpha\beta}(\vec{x}, \vec{y}) u_\beta(\vec{y}) \right)
\]

\[
= \exp(u^\dagger_A G_{AB} u_B),
\]

(234)

\[
\langle \Psi_0 | = \exp \left( \sum_{\alpha,\beta} \int \int d^3x d^3y u^\dagger_\alpha(\vec{x}) \tilde{G}_{\alpha\beta}(\vec{x}, \vec{y}) u_\beta(\vec{y}) \right)
\]

\[
= \exp(u^\dagger_A \tilde{G}_{AB} u_B),
\]

(235)

where \(\tilde{G} = (G^\dagger)^{-1}\). Here, we used Eq.(230).

The expectation value of the Hamiltonian is given by

\[
\langle H \rangle = \frac{\langle \Psi_0 | H |\Psi_0\rangle}{\langle \Psi_0 | \Psi_0 \rangle}
\]

\[
= h_{AB} \frac{\langle \Psi_0 | \psi^\dagger_A \psi_B |\Psi_0\rangle}{\langle \Psi_0 | \Psi_0 \rangle} + \frac{1}{2} V_{AB} \frac{\langle \Psi_0 | \psi^\dagger_A \psi^\dagger_B \psi_B \psi_A |\Psi_0\rangle}{\langle \Psi_0 | \Psi_0 \rangle},
\]

(236)

where

\[
h_{AB} = -\frac{\hbar^2}{2m} \delta_{\alpha\beta} \nabla^2,
\]

(237)

\[
V_{AB} = V(\vec{x}, \vec{y}) = \frac{e^2}{|\vec{x} - \vec{y}|}.
\]

(238)
The normalization constant $\langle \Psi_0 | \Psi_0 \rangle$ is calculated easily

$$
\langle \Psi_0 | \Psi_0 \rangle = \int D\!u D\!u^\dagger e^{u^\dagger (G + \bar{G}) u}
= \int D\!u D\!u^\dagger e^{u^\dagger S u}
= \text{Det} S,
$$

(239)

where $S = G + \bar{G}$ and Eq.(186) was used.

In order to calculate $\langle \Psi_0 | \psi_A^\dagger \psi_B | \Psi_0 \rangle$, we first consider

$$
\psi_A^\dagger \psi_B | \Psi_0 \rangle = \frac{1}{2} \left( u_A^\dagger + \frac{\delta}{\delta u_A} \right) \left( u_B + \frac{\delta}{\delta u_B} \right) e^{u^\dagger G u}
= \frac{1}{2} (u_A^\dagger u_B + \delta_{AB} + u_B u_C^\dagger G_{CA} + u_A^\dagger G_{BC} u_C
+ G_{BA} + G_{BC} u_C u_D^\dagger G_{DA}) | \Psi_0 \rangle.
$$

Thus,

$$
\langle \Psi_0 | \psi_A^\dagger \psi_B | \Psi_0 \rangle
= \frac{1}{2} \left[ (1 + G)_{BA} \langle \Psi_0 | \Psi_0 \rangle + (1 + G)_{BC} (1 - G)_{DA} \langle \Psi_0 | u_D^\dagger u_C | \Psi_0 \rangle \right].
$$

(240)

Also

$$
\langle \Psi_0 | u_D^\dagger u_C | \Psi_0 \rangle
= \int D\!u D\!u^\dagger e^{u^\dagger S u}
= \frac{\partial}{\partial S_{DC}} \langle \Psi_0 | \Psi_0 \rangle = \frac{\partial}{\partial S_{DC}} \text{Det} S
= S_{CD}^{-1} \text{Det} S = S_{CD}^{-1} \langle \Psi_0 | \Psi_0 \rangle.
$$

(241)

Finally, we have

$$
\frac{\langle \Psi_0 | \psi_A^\dagger \psi_B | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{1}{2} \Omega_{BA},
$$

(242)

where

$$
\Omega_{BA} = [(I + G) S^{-1} (I + \bar{G})]_{BA}
= [(I + G) (G + \bar{G})^{-1} (I + \bar{G})]_{BA}.
$$

(243)

Here $I$ is the $2 \times 2$ identity matrix.

Similarly, we obtain

$$
\frac{\langle \Psi_0 | \psi_A^\dagger \psi_L \psi_B \psi_A | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{1}{4} [\Omega_{AA} \Omega_{BB} - \Omega_{BA} \Omega_{AB}],
$$

(244)

<Problem> Derive Eq.(244).

Collecting the above results, we have

$$
\langle H \rangle = \frac{1}{2} \sum_\alpha \int d^3 x d^3 y \left[ -\frac{\hbar^2}{2m} \delta(\vec{x} - \vec{y}) \nabla^2 \Omega_{\alpha\alpha}(\vec{x}, \vec{y}) \right]
+ \frac{1}{8} \sum_{\alpha,\beta} \int d^3 x d^3 y V(\vec{x}, \vec{y}) \Omega_{\alpha\alpha}(\vec{x}, \vec{x}) \Omega_{\beta\beta}(\vec{y}, \vec{y})
- \frac{1}{8} \sum_{\alpha,\beta} \int d^3 x d^3 y V(\vec{x}, \vec{y}) \Omega_{\beta\alpha}(\vec{y}, \vec{x}) \Omega_{\alpha\beta}(\vec{x}, \vec{y}).
$$

(245)
Here, we note that the second term corresponds to the direct term and the third term to the exchange term, respectively.

When the system is homogeneous, it is convenient to use Fourier transformations of $\Omega_{\alpha \beta}(\vec{x}, \vec{y})$ and $V(\vec{x}, \vec{y})$.

$$\Omega_{\alpha \beta}(\vec{x}, \vec{y}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{x} - \vec{y})} \omega_{\alpha \beta}(\vec{k}), \quad \text{(246)}$$

$$V(\vec{x}, \vec{y}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k} \cdot (\vec{x} - \vec{y})} V(\vec{k}). \quad \text{(247)}$$

$V(\vec{k}) = 4\pi e^2/|\vec{k}|^2$ for the Coulomb gas.

These prescriptions allow one to express the expectation value of the Hamiltonian in $\vec{k}$-space.

$$\langle H \rangle = \frac{1}{2} V_g \sum_{\alpha} \int dK \epsilon_0(\vec{k}) \omega_{\alpha \alpha}(\vec{k}) \quad + \frac{1}{8} V_g V(0) \sum_{\alpha,\beta} \int dK dK' \omega_{\alpha \alpha}(\vec{k}) \omega_{\beta \beta}(\vec{k}') \quad - \frac{1}{8} V_g \sum_{\alpha,\beta} \int dK dK' V(\vec{k} - \vec{k}') \omega_{\alpha \alpha}(\vec{k}) \omega_{\alpha \beta}(\vec{k}'), \quad \text{(248)}$$

where $\epsilon_0(k) = \frac{\hbar^2 k^2}{2m}$, $dK = \frac{d^3k}{(2\pi)^3}$ and $V_g$ is the volume of the system.

In order to simplify the above expression, we introduce the particle number $N$,

$$N = \frac{1}{2} V_g \sum_{\alpha} \int dK \omega_{\alpha \alpha}(\vec{k}), \quad \text{(249)}$$

which follows directly from Eq.(242).

Thus,

$$\langle H \rangle = \frac{1}{2} V_g \sum_{\alpha} \int dK \text{Tr}[h \omega] + \frac{1}{2} V(0) N^2 / V_g, \quad \text{(250)}$$

with

$$h_{\alpha \beta}(\vec{k}) = \epsilon_0(\vec{k}) \delta_{\alpha \beta} - \frac{1}{4} \int dK' V(\vec{k} - \vec{k}') \omega_{\alpha \beta}(\vec{k}'). \quad \text{(251)}$$

In order to obtain the ground state energy, it is necessary to take a variation on $\langle H \rangle$ with respect to $g$ or $\bar{g}$, which is the Fourier transformations of $G$ or $\bar{G}$ respectively.

$$\frac{\delta \langle H \rangle}{\delta \bar{g}(\vec{k})} = \frac{1}{2} V_g \frac{\delta \omega_{\beta \alpha}}{\delta \bar{g}} = 0. \quad \text{(252)}$$

Using $\omega = (I + g)(g + \bar{g})^{-1}(I + \bar{g})$, we obtain

$$\frac{1}{(g + \bar{g})^2}(I - g)h(I + g) = 0. \quad \text{(253)}$$

Similarly, we can obtain the condition for $g$. Altogether,

$$(I - g)h(I + g) = 0, \quad (I + \bar{g})h(I - \bar{g}) = 0. \quad \text{(254)}$$

From Eq.(253), we obtain 3 types of solutions, namely, $g = -I$, $g = I$ and the last type $g \neq \pm I$.

$g = -I$ is a trivial solution which gives $\omega = 0$. Next we consider $g = I$. It is known that it gives a trivial solution in the free Dirac theory and the Gross-Neveu model [2, Gen. Ref. 5]. However, it will be shown that $g = I$ gives a Hartree-Fock solution in the electron gas model. We believe that this interesting phenomenon arises due to the difference in the nature of the ground states in the electron gas from that in the Dirac theory. In the Dirac theory,
the vacuum is the Dirac sea with an infinite energy which should be renormalized away, whereas in the electron gas, the vacuum ground state is the fermi sphere which is a very much relevant quantity in condensed matter physics.

When $g = I$, we obtain $\omega = 2I$. Therefore, at $T=0K$, the particle density $\omega_{\alpha\beta}(\vec{k})$ is given by

$$
\omega_{\alpha\beta}(\vec{k}) = 2\delta_{\alpha\beta}\theta(k_F - k),
$$

(254)

where $k_F$ is the fermi wavevector and $\theta(k_F - k) = 1$ for $k \leq k_F$ and 0 for $k > k_F$.

When this result is substituted in Eq.(250), we obtain the variational ground state energy in the Gaussian functional as follows,

$$
\langle H \rangle = (2S + 1)V_g \int dK[\epsilon_0(\vec{k}) + \Sigma(\vec{k})]\theta(k_F - k),
$$

(255)

where $S$ represents the spin. The self-energy $\Sigma(\vec{k})$ is defined as

$$
\Sigma(\vec{k}) = \frac{1}{2}nV(0) - \frac{1}{2} \int dK'V(\vec{k} - \vec{k}')\theta(k_F - k).
$$

(256)

Here $n = N/V_g$ is the electron density. We note the above result is the standard Hartree-Fock result (Eq.(10.22) in Gen. Ref. 3).

**Hubbard Model**

Most of the theories of strongly correlated electron systems begin with the Hubbard model [3]. Therefore, it is a natural choice to be studied by the new many-body theory via the functional Schrödinger picture.

The Hubbard model Hamiltonian is given by

$$
H = -\sum_{ij\alpha} \epsilon_{ij}\epsilon_{\alpha} c_{\alpha}^i c_{\alpha}^j + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} \\
= -\sum_{A,B} t_{AB} c_A^\dagger c_B + h.c. + \frac{1}{2}U \sum_{AB} T_{AB} n_A n_B.
$$

(257)

Here, the first term represents the hopping term, the second the hermitian conjugate of the first term, and the third the on-site Coulomb repulsion. We used the notation $A = (i, \alpha)$, $B = (j, \beta)$, $t_{AB} = \epsilon_{ij}\delta_{\alpha\beta}$, and $T_{AB} = \delta_{ij}(1 - \delta_{\alpha\beta})$. $i$ and $j$ represent the lattice site and $\alpha$ and $\beta$ the spin indices.

Since, now, we are dealing with discrete lattice sites, we should generalize the Floreanini-Jackiw formalism to the discrete case by writing

$$
c_A = \frac{1}{\sqrt{2}} \left( u_A + \frac{\delta}{\delta u_A} \right), \quad c_A^\dagger = \frac{1}{\sqrt{2}} \left( u_A^\dagger + \frac{\delta}{\delta u_A} \right).
$$

(258)

Here, $u_A$ and $u_A^\dagger$ are Grassmann variables which satisfy $\{u_A, u_B^\dagger\} = \delta_{AB}$. The Gaussian trial wavefunction assumes the same form as Eqs.(234) and (235),

$$
|\Psi_0\rangle = e^{u_A^\dagger G_{AB} u_B}, \\
\langle \Psi_0 | = e^{u_A^\dagger G_{AB} u_B},
$$

(259)

but with the summations on $i$ and $j$ instead of integrals on $\vec{x}$ and $\vec{y}$. Following the same steps, Eqs.(236) ~ (244), we obtain

$$
\langle H \rangle = \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = -\frac{1}{2} \sum_{A,B} t_{AB} \Omega_{BA} + h.c. \\
+ \frac{1}{8} U \sum_{A,B} T_{AB}(\Omega_{AA} \Omega_{BB} - \Omega_{BA} \Omega_{AB}),
$$

(260)

where $\Omega = (I + G)(G + \bar{G})^{-1}(I + \bar{G})$.

In terms of $i, j$ and $\alpha, \beta$, the expectation value becomes
\[
\langle H \rangle = -\frac{1}{2} \sum_{ij\alpha\beta} \epsilon_{ij} \delta_{\alpha\beta} (\Omega_{ij})_{\alpha\beta} + h.c.
+ \frac{1}{8} U \sum_{i,\alpha \neq \beta} [(\Omega_{ii})_{\alpha\alpha} (\Omega_{ii})_{\beta\beta} - (\Omega_{ii})_{\beta\alpha} (\Omega_{ii})_{\alpha\beta}]
= -\frac{1}{2} \sum_{ij\alpha} \epsilon_{ij} (\Omega_{ij})_{\alpha\alpha} + h.c.
+ \frac{1}{8} U \sum_{i,\alpha \neq \beta} [(\Omega_{ii})_{\alpha\alpha} (\Omega_{ii})_{\beta\beta} - (\Omega_{ii})_{\beta\alpha} (\Omega_{ii})_{\alpha\beta}].
\] (261)

Here, we assume the translational symmetry and consider only the nearest neighbor hopping \( t_0 \). Then, the \( k \)-space expression is given by

\[
\langle H \rangle = -t_0 \sum_{k,\alpha} \gamma_k \omega_k |_{\alpha\alpha}
+ \frac{1}{8} U \sum_{kk'\alpha\beta} [\omega_k(\omega_{k'})_{\beta\beta} - (\omega_k)_{\beta\alpha} (\omega_{k'})_{\alpha\beta}],
\] (262)

where, \( N \) is the number of the lattice sites, \( \omega = (I + g)(g + \bar{g})^{-1}(I + g) \) with \( g \) the Fourier transformation of \( G \). \( \gamma_k \) is defined

\[
\gamma_k = \sum_r e^{ik \cdot \vec{r}}
\] (263)

where \( \vec{r} \) is the vector to the nearest neighbor.

In order to study various magnetic ground state, we rewrite \( \langle H \rangle \) using

\[
n = \frac{1}{2} \sum_{k,\alpha} [\omega_k]_{\alpha\alpha}
= \frac{1}{2N} \sum_k \text{Tr}[\omega],
\] (264)

which turns out to be the particle number per site. \( \langle H \rangle \) is now rewritten as,

\[
\langle H \rangle = \frac{1}{2} \sum_k \text{Tr}[h\omega] - \frac{1}{2} U N n^2,
\] (265)

where

\[
h_k = [-2t_0 \gamma_k + Un]I - \frac{1}{4} U \sum_{k'} \omega_{k'}. \] (266)

Taking a variation on \( \langle H \rangle \) with respect to \( \bar{g} \) as done in Eq.(252), we obtain

\[
(I - g)h(I + g) = 0,
\] (267)

which has the identical form for the electron gas model.

As we did for the electron gas model, we first consider \( g = I \). In such a case, as in Eq.(254), we readily find that

\[
\omega = 2\theta(k_F - k)I.
\] (268)

Using this expression and the relation \( \sum_{k\alpha} \theta(k_F - k) = Nn \), we obtain

\[
h_k = [-2t_0 \gamma_k + \frac{3}{4} Un]I,
\]

and
\[ h\omega = 2[-2t_0\gamma_k + \frac{3}{4}Un]\theta(k_F - k)I. \] (269)

Finally, \( \langle H \rangle \) is given by

\[ \langle H \rangle = -2t_0 \sum_{k\sigma} \gamma_k \theta(k_F - k) + \frac{1}{4}n^2NU, \] (270)

which is the well-known paramagnetic mean field result of the Hubbard model [3,4]

In order to study magnetic ground states, we introduce the following order parameter

\[ m = \frac{1}{2N} \sum_k \text{Tr}[\sigma_3\omega], \] (271)

which is the difference between the up-spin and the down-spin electron divided by the number of the sites.

The expectation value of the Hamiltonian can now be rewritten in terms of \( n \) and \( m \),

\[ \langle H \rangle = \frac{1}{2} \sum_k \text{Tr}[h\omega] - \frac{1}{4}UN[n^2 - m^2], \] (272)

where

\[ h = [-2t_0\gamma_k + \frac{1}{2}Un]\sigma_0 - \frac{1}{2}Um\sigma_3. \] (273)

<Problem> Show that Eq.(272) is identical to Eq.(265).

Again taking a variation with respect to \( \bar{g} \), one obtains

\[ (I - g)h(I + g) = 0. \] (274)

The above equation can be solved by expanding \( g \) and \( h \) in terms of the Pauli spin matrices. However, since we seek a solution relevant to ferromagnetic ground state, we assume that \( g \) and \( h \) have \( \sigma_0 \) and \( \sigma_3 \) components only. Thus, \([g, h] = 0\) and \((I - g^2)h = 0\). Therefore we have

\[ g = \pm \sigma_3 \text{ or } \pm I. \] (275)

Since \( g = I \) has been studied already, \( g = \pm \sigma_3 \) will be studied here.

\[ g = \sigma_3, \] (276)

\[ \sigma = \begin{cases} 1 & \text{up-spin} \\ -1 & \text{down-spin} \end{cases} \] (277)

Now, in general \( \omega = \sigma_0 + \sigma_3 \) and can be written

\[ \omega = \theta(k_{F\sigma} - k)(\sigma_0 + \sigma_3) \] (278)

at zero temperature. \( h\omega \) in Eq.(272) is now expressed as a diagonal 2 \( \times \) 2 matrix

\[ h\omega = \begin{pmatrix} (1 + \sigma)(h_0 + h_3)\theta(k_{F\uparrow} - k) & 0 \\ 0 & (1 - \sigma)(h_0 - h_3)\theta(k_{F\downarrow} - k) \end{pmatrix}, \] (279)

where \( h_0 = -t_0\gamma_k + \frac{1}{2}Un \) and \( h_3 = -\frac{1}{2}Um \). This expression allows to write the

\[ \langle H \rangle = \sum_k E_{k\uparrow}\theta(k_{F\uparrow} - k) + \sum_k E_{k\downarrow}\theta(k_{F\downarrow} - k) \\
- \frac{1}{4}UN(n^2 - m^2), \] (280)

where
\[
E_{k\uparrow} = -2t_0\gamma_k + \frac{1}{2}U(n - m), \\
E_{k\downarrow} = -2t_0\gamma_k + \frac{1}{2}U(n + m).
\]  
(281)

The above result clearly shows that the splitting due to the mean-field magnetization.

It can also be written in a more familiar form using \( \sum_{k\sigma} \frac{1}{2}Un = \frac{1}{2}Nn^2 \).

\[
\langle H \rangle = \sum_{k\sigma} E_{k\sigma} + \frac{1}{4}UN(n^2 + m^2),
\]
(282)

where

\[
E_{k\sigma} = -2t_0\gamma_k - \frac{1}{2}\sigma U m,
\]
(283)

which is the ferromagnetic Hartree-Fock result [4].

A more interesting case is provided by the antiferromagnetic ordering. For simplicity, only one dimensional case will be considered. The order parameter in this case is the staggered magnetization,

\[
m_l = (-1)^l m = me^{iQr},
\]
(284)

where \( Q = \pi/a \) and \( r = la \). This is readily reduced to the paramagnetic state by setting \( m = 0 \), and to the ferromagnetic state by setting \( Q = 0 \). The Hamiltonian can be expressed in terms of this order parameter as follows,

\[
\langle H \rangle = -\frac{1}{2}N \int dK Tr(h_k\omega_k) + \frac{1}{4}U m^2 + \frac{1}{4}Un^2,
\]
(285)

where

\[
h_k = \epsilon_k\sigma_0 + MQ\sigma_3.
\]
(286)

Here, \( dK = dk/2\pi \) and \( MQ = \frac{1}{2}U me^{iQr} \).

For the antiferromagnetic ordering, the Brillouin zone should be folded in half. This zone folding can be carried out by separating the \( k \)-contributions into two parts

\[
\langle H \rangle = -\frac{1}{2}N \int dK' \left( \begin{array}{cc}
\epsilon_k\sigma_0 & MQ\sigma_3 \\
MQ\sigma_3 & \epsilon_{k+Q}\sigma_0
\end{array} \right) \left( \begin{array}{c}
\omega_k \\
\omega_{k+Q}
\end{array} \right) + \frac{1}{4}Um^2 + \frac{1}{4}Un^2,
\]
(287)

where the prime on the integral signifies the zone-folding. This Hamiltonian is diagonalized under the nesting condition \( \epsilon_{k+Q} = -\epsilon_k \). Now, we take a variation in \( \tilde{g} \) and obtain \( (\sigma_0 - \tilde{g})h(\sigma_0 + \tilde{g}) = 0 \). Among the solutions, we choose \( g = \sigma_0 \), because the antiferromagnetic gap occurs due to the nesting and the zone-folding and, thus, requires no further symmetry breaking in terms of spin variables. Finally, we obtain

\[
\langle H \rangle = \pm N \sum_{\sigma} \int dK' \sqrt{\epsilon_k^2 + \left( \frac{1}{2}Um \right)^2} + \frac{1}{4}UN(m^2 + n^2),
\]
(288)

which gives two antiferromagnetic bands degenerate with spin indices [4]. The paramagnetic ground state is readily obtained by requiring \( m = 0 \), and the ferromagnetic state is obtained by setting \( Q = 0 \) in Eq.(286).

When the on-site Coulomb interaction \( U \) is large (\( U \gg t \)), doubly occupied sites are energetically very expensive. Thus, the restricted Hilbert space now consists of configurations made of empty sites (holes), and up and down spins. The effective Hamiltonian which describes this situation is called t-J model and has been studied intensively in possible connection with high \( T_c \) superconductivity and 2-dimensional antiferromagnetism [5]. Functional Schrödinger picture approaches coupled with the slave-boson and the slave-fermion techniques have been shown to produce correct mean-field results on the 2-dimensional t-J systems [6].

The above results shows versatility of the functional Schrödinger picture in obtaining various ground state energies within the Gaussian approximation. However, at the same time, one may notice that the variational method coupled with a Gaussian trial functional invariably leads into mean-field or Hartree-Fock results. This has been early noted that in the field theory and the mean-field results are often called Gaussian. In the later sections and chapters, efforts going beyond the Gaussian approximation will be described.
B. BCS Superconductivity

The phenomenon of superconductivity is a rare example of a simple field theoretic many-body theory being able to explain most of the essential features. Since Bardeen, Cooper, and Schrieffer (BCS) introduced their variational theory in 1957, several alternative methods including the canonical transformation technique and the Green’s function method have been successfully applied to superconductivity [Gen. Ref. 3]. Therefore, it appears imperative that any new many-body theoretical technique should stand the test of the BCS superconductivity.

In this section, the functional Schrödinger picture formalism is applied to the BCS superconductivity [1]. Here, instead of the Floreanini-Jackiw formalism, we employ the DMR formalism, Eq.(211) to solve the BCS equation. It was shown that the DMR formalism require a non-conventional definition of the hermitian conjugate. However, it will be shown that in order to obtain the gap equation, we do not require the dual of the ground state. Therefore, no complications due to non-standard hermitian conjugate arise. The same problem can also be solved using the Floreanini-Jackiw formalism [2]. But it will be left as a problem.

The model grand canonical Hamiltonian for the BCS superconductivity is given by [Gen. Ref. 3]

\[
H = \sum_\alpha \int d^3x \psi_\alpha^\dagger(\vec{x}) \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \psi_\alpha(\vec{x}) + \frac{1}{2} g \sum_{\alpha \beta} \int d^3x \psi_\alpha^\dagger(\vec{x}) i \sigma^{(2)}_{\alpha \beta} \psi_\beta(\vec{x}) i \sigma^{(2)}_{\beta \alpha} \psi_\alpha(\vec{x}),
\]

where \(\mu\) is the chemical potential and

\[
\sigma^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]

is introduced to insure the s-type pairing. In the process of factorizing the quadratic interaction, the usual Hartee-Fock terms are neglected. Eq.(289) is, then, reduced to

\[
H = \sum_\alpha \int d^3x \: \xi(\vec{x}) \psi_\alpha^\dagger(\vec{x}) \psi_\alpha(\vec{x})
+ \frac{1}{2} \Delta^* \sum_{\alpha \beta} \int d^3x \: \psi_\beta(\vec{x}) i \sigma^{(2)}_{\alpha \beta} \psi_\alpha(\vec{x})
- \frac{1}{2} \Delta \sum_{\alpha \beta} \int d^3x \: \psi_\alpha^\dagger(\vec{x}) i \sigma^{(2)}_{\alpha \beta} \psi_\beta(\vec{x})
+ V |\Delta|^2 \frac{g}{g},
\]

when \(\xi(\vec{x}) = -(\hbar^2/2m) \nabla^2 \delta(\vec{x}^\prime - \vec{x}) - \mu\). \(\vec{x}^\prime\) denotes a coordinate infinitesimally larger then \(\vec{x}\), which ensures the proper operation of \(\xi(\vec{x})\) on \(\psi_\alpha(\vec{x})\). The gap function is defined by

\[
\Delta = -g \langle \psi_\alpha(\vec{x}) i \sigma^{(2)}_{\alpha \beta} \psi_\beta(\vec{x}) \rangle
= -g \langle \psi_\uparrow(\vec{x}) \psi_\downarrow(\vec{x}) \rangle
= g \langle \psi_\downarrow(\vec{x}) \psi_\uparrow(\vec{x}) \rangle.
\]

In the DMR formalism, the fermion field operators are expressed as

\[
\psi_\alpha(\vec{x}) = \varphi_\alpha(\vec{x}),
\psi_\alpha^\dagger(\vec{x}) = \frac{\delta}{\delta \varphi_\alpha(\vec{x})},
\]

where \(\varphi(\vec{x})\) is a real Grassmann function. With the above prescription, the time-independent Schrödinger equation is given by
However, the DMR formalism employed in this section requires the s-wave pairing. Substituting Eq.(294) into Eq.(293) and equating terms with same order, we obtain two equations, therefore, we write

\[
\Phi[\varphi] = E\Phi[\varphi],
\]

where \(\Phi[\varphi]\) is the wavefunctional which satisfies the functional differential equation.

Here, it should be noted that we do not need the troublesome dual of \(\Phi[\varphi]\), since it is not necessary to evaluate \(\langle H \rangle\). Power counting indicates that \(G[\varphi]\) should minimally be quadratic in \(\varphi\) so that the second functional derivative of \(G\) yields a number while the square of the first derivative is still quadratic in \(\varphi\).

Therefore, we write \(G[\varphi]\) as a quadratic form in \(\varphi\) (For the power counting technique, see Chapter. 10, Gen. Ref. 1.).

In the mean field theory of the electron gas and the Hubbard model in the previous section, \(G\) has a form, \(\psi^\dagger g\psi\). However, the DMR formalism employed in this section requires \(G\) to be written in the form \(\psi F\psi\), which reflects the pairing. With this prescription, \(G[\varphi]\) is written

\[
G[\varphi] = \sum_{\alpha\beta} \int d^3x d^3y \varphi_\alpha(\vec{x}) F_{\alpha\beta}(\vec{x}, \vec{y}) \varphi_\beta(\vec{y}).
\]

We note that \(F_{\alpha\beta}(\vec{x}, \vec{y})\) must be symmetric in coordinate space and antisymmetric in spin space so that \(\Phi[\varphi]\) represents the s-wave pairing. Substituting Eq.(294) into Eq.(293) and equating terms with same order, we obtain two equations,

\[
E = \sum_{\alpha\beta} \int d^3x \left[ \xi(x) \delta_{\alpha\beta} + i\Delta^{(2)}_{\alpha\beta} F_{\alpha\beta}(\vec{x}, \vec{x}) \right] + \frac{|\Delta|^2}{g} V,
\]

\[
\sum_{\alpha\beta} \int d^3x d^3y \left( 2\xi(\vec{x}) F_{\alpha\beta}(\vec{x}, \vec{y}) + i\Delta^{*}\sigma_{\alpha\beta}(\vec{x} - \vec{y}) \right) + 2\sum_{\gamma\delta} \int d^3z \frac{\alpha\beta}{2} \Delta^{(2)}_{\alpha\beta} F_{\delta\gamma}(\vec{x}, \vec{z}) = 0.
\]

Eq.(296) can be written in a simple matrix form

\[
2\xi K + \frac{1}{2} i\Delta^{*}\sigma^{(0)} + 2i\Delta K^2 = 0,
\]

where \(K = F_{\sigma^{(2)}}\). It is convenient to solve Eq.(297) in momentum space. For this purpose, we define \(K(\vec{k})\), the Fourier transformation of \(K(\vec{x}, \vec{y})\),

\[
K(\vec{x}, \vec{y}) = \int dK \exp[-i\vec{k} \cdot (\vec{x} - \vec{y})] \sum_{i=0}^{3} K_i(\vec{k}) \sigma^{(i)},
\]

where \(dK = d^3k/(2\pi)^3\). This Fourier transformation reduces Eq.(297) to a set of coupled equations,

\[
2\xi K_0 + \frac{i}{2} \Delta^{*} + 2i\Delta K_0^2 + 2i\Delta \sum_{i=1}^{3} K_i^2 = 0,
\]

\[
2\xi K_1 + 4i\Delta K_0 K_l = 0,
\]

where \(\xi = E_k - \mu = \hbar^2 k^2/2m - \mu\).

The above equations are readily solved to yield

\[
K_1 = K_2 = K_3 = 0, \quad K_0 = i(\xi_k + \sqrt{\xi_k^2 + |\Delta|^2})/2\Delta.
\]

Now \(F(\vec{x}, \vec{y})\) is given as

\[
F(\vec{x}, \vec{y}) = i\sigma^{(2)} \int dK \exp[-i\vec{k} \cdot (\vec{x} - \vec{y})] \frac{\xi_k + E_k}{2\Delta},
\]

\[
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\]
where $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$ represents the excitation energy. The wavefunctional which satisfies Eq.(293) is given by

$$\Phi[\varphi] = \exp \left( \frac{1}{2} \int dK \ \frac{\xi_k + E_k}{\Delta} \left[ \varphi_\uparrow(\vec{k})\varphi_\downarrow(-\vec{k}) - \varphi_\downarrow(\vec{k})\varphi_\uparrow(-\vec{k}) \right] \right).$$

(302)

It is obvious that the above wavefunctional has the correct BCS state features. Also the ground state energy is obtained from Eq.(295) and given by

$$E = V \int dK \ (\xi_k - E_k) + V \frac{\Delta^2}{g}$$

(303)

Here, $\Delta$ is assumed real. Since the characteristic energy range in forming the Cooper pairs is $\hbar w_c$, the ground state energy per volume is

$$\epsilon_s = E_s/V = N(0) \int_{k_{wc}} d\xi \ (\xi - \sqrt{\xi^2 + \Delta^2}) + \frac{\Delta^2}{g},$$

(304)

where $\hbar w_c$ is the phonon energy and $N(0)$ the density of states at the Fermi energy. The gap equation can be obtained by minimizing Eq.(303) with respect to $\Delta$,

$$\Delta = \frac{g}{2} \int d^3k \ \frac{\Delta}{(2\pi)^3} \sqrt{\xi^2 + \Delta^2},$$

(305)

which can be reduced to the standard BCS result [3]

$$\Delta = \frac{\hbar w_c}{\sinh\left[1/N(0)g\right]}$$

(306)

It is shown that the functional Schrödinger picture method via the DMR formalism can be used to construct a consistent theory of the BCS superconductivity. It should be noted that we could avoid the problem of the nonconventional hermitian conjugate in the DMR representation since one does not have to calculate the expectation value of the Hamiltonian. It is because that the factorized form of the BCS Hamiltonian is only quadratic and, thus, can be solved exactly without resorting to the variational process.

Since, the Floreanini-Jackiw formalism is also a valid representation for fermions, it should be possible to solve the BCS superconductivity problem using this formalism. This is done in the literature and will be left as a problem.

<Problem> Obtain the gap equation using the Floreanini-Jackiw formalism (Reference.2).

C. Dilute Bose Gas and Bose-Einstein Condensation

It has been shown that, in Section II.B, the functional Schrödinger picture formalism assumes an easy and straightforward form in the bosonic scalar field theory. However, when this formalism is applied to boson particles, occurrence of the Bose-Einstein condensation makes the calculation less straightforward.

In this section, the bosonic functional Schrödinger picture is generalized to include the Bose-Einstein condensation. Also, we try a shifted Gaussian trial functional in order to reach beyond the Gaussian approximation [1].

The standard model Hamiltonian for an interacting Bose gas is given by [Chap. 10, Gen. Ref. 3]

$$H = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{U}{2V} \sum_{k_1k_2k_3k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \delta_{k_1+k_2,k_3+k_4}.$$  

(307)

The constant matrix element $U$ can be determined by requiring that $H$ correctly reproduce the two-body scattering properties in vacuum. We assume that the scattering length is much less than the inter-particle spacing $n^{1/3}$, where $n = N/V$. Therefore, the validity of the present calculation is restricted by the condition $na^3 \ll 1$. Under this assumption, the zero momentum operators $a_0$ and $a_0^\dagger$ become nearly classical due to occurrence of condensate. The interacting part of the Hamiltonian is rewritten explicitly in terms of $a_0$ and $a_0^\dagger$ as
\[
H_{\text{int}} = \frac{U}{2V} a_0^\dagger a_0 a_0 + \frac{U}{2V} \sum_{k \neq 0} \left[ 2(a_k^\dagger a_0 a_k a_0 + a_{-k}^\dagger a_0^\dagger a_{-k} a_0) \\
+ a_k^\dagger a_{-k} a_0 a_0 + a_0^\dagger a_k a_{-k} \right] \\
+ \frac{U}{V} \sum_{\vec{k}, \vec{q} \neq \vec{0}} \left[ a_{\vec{k}+\vec{q}}^\dagger a_0^\dagger a_{\vec{q}} a_k + a_{\vec{k}+\vec{q}} a_{\vec{k}-\vec{q}}^\dagger a_0 a_0 \right],
\]

(308)

where only terms of order of \( N_0^2 \), \( N_0 \) and \( \sqrt{N_0} \) have been retained. The three-zero-momentum operator terms do not exist, because momentum conservation makes the fourth term also have zero momentum. It should be noted that the last term, which is generally neglected in text book calculations originates from the interaction of particles with condensate, thus representing the condensation fluctuation.

In order to handle the contribution from the last term, we introduce a new variable \( \gamma_k \),

\[
\gamma_k = \sum_{q \neq 0} a_{k+q}^\dagger a_q.
\]

(309)

We approximate \( \gamma_k \) as a c-number. Replacing the operators \( a_0 \) and \( a_0^\dagger \) by \( \sqrt{N_0} \), \( H_{\text{int}} \) becomes

\[
H_{\text{int}} = \frac{U}{2V} N_0^2 + \frac{U}{2V} N_0 \sum_{k \neq 0} \left[ 2(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) \\
+ a_k^\dagger a_{-k} + a_k a_{-k} \right] + \frac{U}{V} \sqrt{N_0} \sum_{k \neq 0} \gamma_k (a_k + a_{-k}).
\]

(310)

The number operator satisfies the relation

\[
N_0 = N - \frac{1}{2} \sum_{k \neq 0} (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}).
\]

(311)

Using this relation and keeping up to the \( \sqrt{N} \) terms, the model Hamiltonain becomes

\[
H = \frac{1}{2} n^2 V U + \frac{1}{2} \sum_{k \neq 0} \left[ \epsilon_k^0 + nU \right] \left( a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right) \\
+ nU (a_k^\dagger a_{-k} + a_k a_{-k}) + \frac{nU}{\sqrt{N}} \sum_{k \neq 0} \gamma_k (a_k + a_{-k}),
\]

(312)

where \( \epsilon_k^0 = \hbar^2 k^2 / 2m \).

When there is no Bose-Einstein condensation, the bosonic operators can be simply written \( a_k = \phi(\vec{k}) \) and \( a_k^\dagger = -\delta / \delta \phi(\vec{k}) \). However, due to Bose-Einstein condensation, such simple prescription does not work. With reasons which will become transparent below, we introduce Bose-Einstein weighting factor, \( \alpha_k (k \neq 0) \) and express the operators,

\[
a_k = \alpha_k \phi(\vec{k}), \quad a_k^\dagger = -\alpha_k \frac{\delta}{\delta \phi(\vec{k})}.
\]

(313)

When these expressions are introduced to the commutation relation \([a_k, a_{k'}^\dagger] = \delta_{kk'}\), we obtain a constraint relation for \( \alpha_k \), namely

\[
\alpha_k \alpha_{k'} \delta(k - k') = \delta_{kk'}.
\]

(314)

Note that \( \alpha_k^2 \delta(0) = 1 \) except \( k = 0 \). The Hamiltonian is now given by

\[
H \left( \phi(\vec{k}), \frac{\delta}{\delta \phi(\vec{k})} \right) = \frac{1}{2} n^2 V U \\
+ \frac{1}{2} \sum_{k \neq 0} \alpha_k^2 \left( \epsilon_k^0 + nU \right) \left[ \frac{\delta}{\delta \phi(\vec{k})} \phi(\vec{k}) + \frac{\delta}{\delta \phi(-\vec{k})} \phi(-\vec{k}) \right]
\]

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The Schrödinger equation becomes

\[
\Phi_k + nU \left[ \frac{\delta}{\delta \phi(k)} \frac{\delta}{\delta \phi(-k)} \phi(k) \phi(-k) \right] + \frac{nU}{\sqrt{N}} \sum_{k \neq 0} \alpha_k \gamma_k \left[ \phi(\bar{k}) - \frac{\delta}{\delta \phi(-k)} \right].
\]

Here, we assume that the ground state functional is real and positive and has no nodes. Thus we write

\[
\Phi_k = Ce^{G[\phi]},
\]

where \(C\) is the normalization constant.

The Schrödinger equation becomes

\[
\frac{1}{2} n^2 V U - \frac{1}{2} \sum_{k \neq 0} \alpha_k^2 \left( \epsilon_k^0 + nU \right) \times \left[ 2 \delta(0) + \phi(k) \frac{\delta G}{\delta \phi(0)} + \phi(-k) \frac{\delta G}{\delta \phi(-k)} \right] + \frac{nU}{2} \sum_{k \neq 0} \alpha_k^2 \left[ \frac{\delta^2 G}{\delta \phi(k) \delta \phi(-k)} + \frac{\delta G}{\delta \phi(k)} \frac{\delta G}{\delta \phi(-k)} + \phi(k) \phi(-k) \right] + \frac{nU}{\sqrt{N}} \sum_{k \neq 0} \alpha_k \gamma_k \left[ \phi(k) - \frac{\delta G}{\delta \phi(-k)} \right] = E_g.
\]

The power counting technique indicates that \(G[\phi]\) should be at least quadratic in \(\phi(k)\). Therefore, a simple form of \(G[\phi]\) can be expressed as a shifted Gaussian in \(\phi\),

\[
G[\phi] = \int d^3k [g(k) \phi(k) \phi(-k) + f(k) \phi(k)],
\]

where \(\phi(k) = -\phi(-k)\) to ensure convergence and \(g(k)\) and \(f(k)\) are function parameters that will be determined below. It should be noted that the linear term in the above expression has no contribution if the fluctuation contribution is not included in the calculation. Substituting Eq.(318) into Eq.(317), we obtain the following relation,

\[
E_g = \frac{1}{2} n^2 V U + \sum_{k \neq 0} \alpha_k^2 \delta(0) \left[ nU g(k) - (\epsilon_k^0 + nU) \right] + \frac{nU}{2} \sum_{k \neq 0} \alpha_k^2 f(k) \left[ f(-k) - \frac{2 \alpha_k \gamma_k \sqrt{N}}{\alpha_k \sqrt{N}} f(k) \right] + \sum_{k \neq 0} \alpha_k^2 \left[ - (\epsilon_k^0 + nU) f(k) + 2 nU g(k) f(k) + \frac{nU \gamma_k}{\alpha_k \sqrt{N}} (1 - 2 g(k)) \right] f(k) + \frac{1}{2} \sum_{k \neq 0} \alpha_k^2 \left[ - 4 (\epsilon_k^0 + nU) g(k) + 4 nU g(k)^2 + nU \right] \phi(k) \phi(-k)
\]

Power counting of the above equation readily yields,

\[
4 nU g(k)^2 - 4 (\epsilon_k^0 + nU) g(k) + nU = 0, \tag{320}
\]

\[
-(\epsilon_k^0 + nU) f(k) + 2 nU g(k) f(k) + \frac{nU \gamma_k}{\alpha_k \sqrt{N}} (1 - 2 g(k)) = 0, \tag{321}
\]

\[
E_g = \frac{1}{2} n^2 V U + \sum_{k \neq 0} \left[ nU g(k) - (\epsilon_k^0 + nU) \right] + \frac{nU}{2} \sum_{k \neq 0} \alpha_k^2 \left[ f(k) f(-k) - \frac{2 \alpha_k \gamma_k \sqrt{N}}{\alpha_k \sqrt{N}} f(k) \right]. \tag{322}
\]

In deriving the above relations, we used Eq.(314). Function parameters are now determined to be
\[ g(k) = \frac{\epsilon_k^0 + nU + E(k)}{2nU}, \quad (323) \]
\[ f(k) = \frac{\gamma_k}{\alpha_k \sqrt{N}} \frac{\epsilon_k^0 + E(k)}{E(k)}, \quad (324) \]

where
\[ E(k) = \sqrt{\left(\epsilon_k^0 + nU\right)^2 - (nU)^2}. \quad (325) \]

Finally, the ground state energy is given by
\[ E_g = E_0 + E_1 + E_2 = \frac{1}{2} n^2 VU - \frac{1}{2} \sum_{k \neq 0} \left( (\epsilon_k^0 + nU) - E(k) \right) - \frac{nU^2}{V} \sum_{k \neq 0} \frac{\gamma_k \gamma_{-k}}{\epsilon_k^0 + 2nU}. \quad (326) \]

The first two terms, \(E_0\) and \(E_1\), are the standard results which can be obtained by a canonical transformation [p.317, Gen. Ref. 3]. The last term, \(E_2\), is the fluctuation contribution from the condensation. Following the standard step relating the scattering length to the interaction [p.314, Gen. Ref. 3]
\[ \frac{4\pi \hbar^2 a}{m} = U - \frac{U^2}{2V} \sum_{k \neq 0} \frac{1}{\epsilon_k} + \cdots, \quad (327) \]

we obtain the ground state energy density
\[ \frac{E}{V} = \frac{2\pi \hbar^2 a n^2}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right], \quad (328) \]
which is the standard textbook result. Note that we have not yet evaluated the fluctuation contribution from the condensation.

Before we evaluate the new correction term to the ground state energy, it is interesting to check whether the present formalism predicts the particle depletion from the zero momentum correctly. The depletion is defined by
\[ \frac{N - N_0}{N} = \frac{1}{N} \sum_{k \neq 0} \langle a_k^\dagger a_k \rangle \quad (329) \]

This value is equal to \(\gamma_0/N\) and can be calculated using Eq.(313), (314) and (316). We obtain for \(n_k = \langle a_k^\dagger a_k \rangle \)
\[ n_k = \left\langle -\alpha_k^2 \left[ \delta(0) + \phi(k) \frac{\delta G}{\delta \phi(k)} \right] \right\rangle \\
= \left\langle -1 + 2\alpha_k^2 g(k) \phi(k)^2 - \alpha_k^2 f(k) \phi(k) \right\rangle, \quad (330) \]

where we used \(\phi(k) = -\phi(-k)\).

The expectation value of \(\phi(k)^2\) and \(\phi(k)\) can be evaluated by carrying out the Gaussian integrals
\[ \frac{\langle \Phi_0 | \phi(k)^2 | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \frac{1}{4g(k)} + \frac{f(k)^2}{4g(k)^2}, \quad (331) \]
and
\[ \frac{\langle \Phi_0 | \phi(k) | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \frac{f(k)}{2g(k)}. \quad (332) \]

\textbf{Problem} Prove Eqs.(331) and (332).
Using these expressions, we obtain
\[ n_k = -1 + \frac{\alpha_k^2}{2}, \] (333)
where \( k \neq 0 \).

In order to obtain \( \alpha_k \), which is introduced as a measure in the k-space to conserve the particle numbers, we use a simple physical argument. We note that \( n_k \) should satisfy the following conditions
\[ \lim_{k \to 0} n_k = \infty \quad \text{and} \quad \lim_{k \to \infty} n_k = 0. \] (334)

Also, we obtain from Eq.(323) the following properties
\[ g(0) \simeq \frac{1}{2} \quad \text{and} \quad E(0) \simeq 0 \quad \text{for} \quad k \to 0 \] (335)
and
\[ nUg(k) \sim E(k) \quad \text{for} \quad k \to \infty. \] (336)

The simplest function to satisfy the above properties for \( n_k \) is given by
\[ \frac{\alpha_k^2}{2} = \frac{nUg(k)}{E(k)}. \] (337)

Indeed, we note that \( n_k \) has the desired properties of a very sharp peak at \( k = 0 \) and almost zero elsewhere.

The particle depletion is now calculated using Eqs.(333) and (337) to yield
\[ \frac{N - N_0}{N} = \frac{1}{N} \sum_{k \neq 0} \left[ \frac{nUg(k)}{E(k)} - 1 \right] \]
\[ = \frac{1}{2N} \sum_{k \neq 0} \left[ \frac{\epsilon_k^0 + nU}{E(k)} - 1 \right], \] (338)
which gives the standard textbook result, \( \frac{8}{3} \left( \frac{na^3}{\pi} \right)^{1/2} \) after carrying out the \( k \) summation [p.317, Gen. Ref. 3]. So far, we have shown that the functional Schrödinger picture can handle dilute bose gas successfully even when the Bose-Einstein condensation occurs. Next, it will be shown that the functional Schrödinger picture scheme coupled with a shifted Gaussian function enables us to calculate the fluctuation contribution from the condensation.

The ground state energy of dilute bose gas is generally given (See for example Eq.(22.21), Gen. Ref. 3.)
\[ E_V = \frac{2\pi n^2 a \hbar^2}{m} \left[ 1 + \frac{128}{15} \left( \frac{na^3}{\pi} \right)^{1/2} \right. \]
\[ \left. + 8 \left( \frac{4}{3} \pi - \sqrt{3} \right) (na)^3 \ln(na^3) + \mathcal{O}(na^3) + \cdots \right]. \] (339)

We note that the first two terms are the Gaussian results discussed above. The next order correction term originates from the second term of \( H_{int} \), Eq.(308). However, the coefficient of the last term has never been determined.

Below, we show that the fluctuation contribution, the last term in Eq.(326) produces a term in \( na^3 \). Indeed, a rough estimate of this contribution showed that this contribution would be of the order \( na^3 \) [p.318, Gen. Ref. 3]. The fluctuation contribution, \( E_2 \), carries the same ultraviolet divergence as in \( E_1 \). The divergence in \( E_1 \) was handled through the expression of the scattering length \( a \) to order of \( U^2 \) as given in Eq.(327). However, for the calculation of \( E_2 \), such a simple cancellation scheme does not exist, because it is now necessary to expand \( a \) up to \( U^3 \). Therefore, we resort to an alternative cutoff procedure called minimal subtraction [2]. In minimal subtraction, ultraviolet divergences are removed as part of the regularization power of \( k \) from the momentum space integrated. Following this prescription, we obtain \( E_2 \) in a dimensionless form
\[ \frac{E_2}{E_c} = -\frac{2U}{NV} \sum_{k \neq 0} \gamma_k \gamma_{-k} \left[ \frac{1}{\epsilon_k^0 + 2nU} - \frac{1}{\epsilon_k^0} \right], \] (340)
where \( E_c = 2\pi \hbar^2 a n^2 V/m \). Now, it is necessary to evaluate \( \gamma_k \gamma_{-k} \). It is known that a dominant contribution arises when a particle interacts with itself, which happens when \( \vec{q}' = \vec{k} + \vec{q} \). Therefore,

\[
\gamma_k \gamma_{-k} = \sum_{qq'} a_{k+q} \dagger a_{q-k} \dagger a_q a_{q'}
\]

\[
\simeq \sum_q a_{k+q} \dagger a_{k+q} a_q a_{q-k} \dagger
\]

\[
\simeq \sum_{q \neq 0} n_q^2
\]

\[
= \sum_{q \neq 0} \left[ \frac{e_q^0 + nU - E(q)}{2E(q)} \right]^2.
\]

(341)

This approximation gives a simple result for the condensation fluctuation correction \( E \),

\[
E_2/E_c = 16 \left( \pi - \frac{8}{3} \right) na^3.
\]

(342)

Here, we note that the above result is obtained through a rather drastic approximation of Eq.(341). Also, there are indications that there might be \( na^3 \) order terms from other sources [p.319, Gen. Ref. 3]. A calculation which produces a \( na^3 \) order term from the particle-particle interaction has been reported [3].

In this section, we generalized the bosonic functional Schrödinger picture to the case when Bose-Einstein condensation exists. Also, a shifted Gaussian functional is employed to calculate the fluctuation contribution from the condensation.

D. Finite Temperature Formalism of The Electron Gas

So far, we have presented only zero-temperature formalism. In order that the functional Schrödinger picture many-body theory be truly useful, it requires extension to finite temperature. In this section, a finite temperature formulation of many-body theory based on the functional Schrödinger picture is presented [1]. It is shown that a Gaussian approximation of the theory produces the finite temperature Hartree-Fock results both for the para- and ferromagnetic phases in a simple and convenient fashion. It is also shown that the self-consistent equation for the ferromagnetic splitting yields the Stoner condition for the ferromagnetism.

A finite temperature quantum field theory using the functional Schrödinger picture has been recently formulated by generalizing the Gaussian approximation of the variational calculation in quantum mechanics [2]. The method is based on density matrix formalism in statistical mechanics [3].

Here, we briefly introduce the concept of the density matrix. When \(|\phi_i\rangle\) is an eigenket, \( E_i \) the corresponding eigenvalue of the Hamiltonian \( H \) of the system and \( Q \) the partition function, the probability that the system is in the state \(|\phi_i\rangle\) is \((1/Q) e^{-\beta E_i}\). Thus, the density matrix is defined to be

\[
\rho = \sum_n \omega_n |\phi_n\rangle \langle \phi_n|,
\]

(343)

where \( \omega_n = (1/Q) e^{-\beta E_n} \) and \( \beta = 1/k_B T \).

We can readily show that \( \langle A \rangle = \text{Tr} \rho A \) and \( \text{Tr} \rho = 1 \). Because \( H|\phi_n\rangle = E_n|\phi_n\rangle \), we can write

\[
\rho = \frac{1}{Q} \sum_n e^{-\beta E_n} |\phi_n\rangle \langle \phi_n| = e^{-\beta H}/Q,
\]

(344)

where

\[
e^{-\beta F} = Q = \sum_n e^{-\beta E_n} = \text{Tr} e^{-\beta H},
\]

(345)

and, thus,
\[
\rho = \frac{e^{-\beta H}}{\text{Tr}e^{-\beta H}}. \tag{346}
\]

Now we regard the density matrix as a function of \(\beta\). The unnormalized \(\rho\) is defined by
\[
\rho_U(\beta) = e^{-\beta H}. \tag{347}
\]
In place of \(\rho_U\), we will hereafter write \(\rho\). \(\rho(\beta)\) obeys the differential equation
\[
-\frac{\partial \rho}{\partial \beta} = H\rho. \tag{348}
\]

\textbf{Problem} Using the energy representation, \(H|i\rangle = E_i|i\rangle\), prove Eq.(348).

Solving this differential equation, one can obtain \(\rho(\beta)\), \(F\) and other physical properties of the model system represented by \(H\) [3]. In order to develop a finite temperature many-body theory, we first study non-interacting fermion system which has a grand Hamiltonian given by
\[
K = H - \mu N = \sum_{A} \int d^3x \psi_\alpha^\dagger(\vec{x}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + \right] \psi_\alpha(\vec{x}) - \mu N, \tag{349}
\]
where \(N\) represents the number operator and \(\mu\) the chemical potential. Using the Floreanini-Jackiw prescription, the grand Hamiltonian is expressed as
\[
K = \frac{1}{2} \sum_{AB} \xi_{AB} \left( u_A^\dagger + \frac{\delta}{\delta u_A} \right) \left( u_B + \frac{\delta}{\delta u_B} \right), \tag{350}
\]
where \(\xi_{AB} = -\left(\frac{\hbar^2}{2m}\right)\delta(\vec{x} - \vec{y})\nabla^2\delta_{\alpha\beta} - \mu\delta_{AB}\) and \(A = (\vec{x}, \alpha), B = (\vec{y}, \beta)\).

We choose a Gaussian trial density matrix
\[
\rho = \exp(u_A^\dagger F_{AB}u_B + J_Au_A + u_A^\dagger L_A + C). \tag{351}
\]
Substituting Eq.(351) into Eq.(348), we obtain the following relation.
\[
-u^\dagger \frac{\partial F}{\partial \beta} u - u^\dagger \frac{\partial J}{\partial \beta} u - u^\dagger \frac{\partial L}{\partial \beta} - \frac{\partial C}{\partial \beta} = \frac{1}{2} \left( u^\dagger (\xi + F\xi)u + (-J\xi - J\xi F)u + u^\dagger (\xi L - F\xi L) + (\xi + F\xi - J\xi L) \right). \tag{352}
\]
Since the above equation is valid for any Grassmann variables \(u\) and \(u^\dagger\), we obtain four differential equations,
\[
-\frac{\partial F}{\partial \beta} = \frac{1}{2}(I - F^2)\xi, \tag{353}
\]
\[
-\frac{\partial J}{\partial \beta} = -\frac{1}{2} J(I + F)\xi, \tag{354}
\]
\[
-\frac{\partial L}{\partial \beta} = \frac{1}{2}(I - F)\xi L, \tag{355}
\]
\[
-\frac{\partial C}{\partial \beta} = \text{Tr}[(I + F - JL)\xi]. \tag{356}
\]
These equations are readily solved to yield
\[ F = - \coth \left( \frac{1}{2} \beta \xi \right) \]  
(357)

\[ J = - v^\dagger e^{\beta \xi} \left[ \sinh \left( \frac{1}{2} \beta \xi \right) \right]^{-1} \]  
(358)

\[ L = - ve^{-\frac{1}{2} \beta \xi} \left[ \sinh \left( \frac{1}{2} \beta \xi \right) \right]^{-1} \]  
(359)

\[ C = \text{Tr} \left[ - \frac{1}{2} \beta \xi + \ln \left[ \sinh \left( \frac{1}{2} \beta \xi \right) \right] - v^\dagger v \coth \left( \frac{1}{2} \beta \xi \right) \right]. \]  
(360)

In the above Grassmann variables \( v \) and \( v^\dagger \) are introduced as constants of integrations in order to make \( \rho \) as a Gaussian type density matrix.

Collecting these expressions, we obtain

\[ (\rho_{\text{nor}})_{uv} = \frac{1}{N} e^{\text{Tr} \left[ - \frac{1}{2} \beta \xi \right]} \text{Det} \left[ \sinh \left( \frac{1}{2} \beta \xi \right) \right] e^{u^\dagger v - v^\dagger u} e^{-\left( u^\dagger + v^\dagger \right) \left[ \coth \left( \frac{1}{2} \beta \xi \right) \right]} \]  
(361)

where the normalization constant \( N \) is to be obtained by the relation, \( \text{Tr}[\rho_{\text{nor}}] = 1 \).

**Problem**

Prove Eqs.(357) \( \sim \) (361).

We note that \( N = \text{Tr}[\rho] \). Carrying out the integral, we obtain

\[ N = \int D u^\dagger D u \rho_{uu} \]  
\[ = e^{\text{Tr} \left[ - \frac{1}{2} \beta \xi \right]} \text{Det} \left[ \sinh \left( \frac{1}{2} \beta \xi \right) \right] \int D u^\dagger D u e^{-u^\dagger \left[ 4 \coth \left( \frac{1}{2} \beta \xi \right) \right] u} \]  
(362)

where we used Eq.(185). The normalized density corresponding to the above density matrix is given by

\[ \hat{\rho}_{\text{nor}} = \frac{e^{\text{Tr} \left[ \frac{1}{2} \beta \xi \right]} \text{Det} \left[ 4 \cosh \left( \frac{1}{2} \beta \xi \right) \right]}{e^{-\beta K}} \]  
(363)

The Helmholtz free energy is defined by

\[ \beta F \equiv \langle \ln \hat{\rho}_{\text{nor}} \rangle + \beta \langle H \rangle. \]  
(364)

Substituting Eqs.(349) and (363) into Eq.(364), we obtain

\[ F = N \mu - k_B T \text{Tr} \left[ \ln \left( 1 + e^{-\beta \xi} \right) \right] - \text{Tr} \left[ \ln 2 \right] \]  
\[ = N \mu - k_B T \sum_{k,\sigma} \left[ \ln \left( 1 + e^{-\beta \xi} \right) \right] - N \ln 2, \]  
(365)

where \( \xi_k = \epsilon_k^0 - \mu \) and \( \sigma \) is the spin index. For the second expression, we carried out the Fourier transform.

The total energy is calculated through

\[ E = \langle H \rangle \]  
\[ = \sum_{AB} \int D u^\dagger D u h_{AB} \psi_A^\dagger \psi_B \rho_{uv} \big|_{u=v} \]  
\[ = \sum_{AB} \int D u^\dagger D u h_{AB} \left( u_A^\dagger + \frac{\delta}{\delta u_A} \right) \left( u_B^\dagger + \frac{\delta}{\delta u_B} \right) \rho_{uv} \big|_{u=v} \]  
\[ = \frac{1}{2} \text{Tr} \left\{ h \left[ 1 - \tanh \left( \frac{1}{2} \beta \xi \right) \right] \right\} \]  
\[ = \sum_{k,\sigma} \epsilon_k^{0} n_k, \]  
(366)
where \( h_{AB} = \xi_{AB} + \mu \) and \( n_k = 1/(1 + e^{\beta(\epsilon_k^0 - \mu)}) \).

**Problem** Prove Eqs.(365) and (366).

We observe the well-known results of non-interacting fermionic particles, Eqs.(365) and (366) clearly confirm that a finite temperature many-particle theory can be successfully formulated using the density matrix method based on the functional Schrödinger picture approach.

Next, we investigate the interacting electron gas system of which the grand Hamiltonian is given by

\[
K = \sum_{AB} \xi_{AB} \psi_A \psi_B + \frac{1}{2} \sum_{AB} V_{AB} \psi_A \psi_B \psi_A \psi_B, \tag{367}
\]

where \( V_{AB} \) is any appropriate particle-particle interaction potential. The density matrix for an interacting system is not a Gaussian and generally quite complicated. As a first approximation, we choose a trial Gaussian density with a variable function, which will be chosen from minimization of the thermodynamic potential. Thus, the normalized trial density matrix is given by

\[
[\rho_{nor}]_{uv} = \frac{1}{\text{Det}[4 \coth(\beta Q/2)]} e^{u^\dagger v - v^\dagger u} \times e^{-(u^\dagger + v^\dagger)\text{coth}(\beta Q/2)(u + v)}, \tag{368}
\]

where \( Q \) is the adjustable parameter matrix. The corresponding normalized density operator is written in the form

\[
\hat{\rho}_{nor} = \frac{e^{\text{Tr}[\beta Q/2]}}{\text{Det}[4 \cosh(\beta Q/2)]} e^{-\beta \psi^\dagger Q \psi}, \tag{369}
\]

in analogy to the free particle case.

The thermodynamic potential is given by

\[
\beta \Omega = \beta (F - \mu N) = \langle \ln \hat{\rho}_{nor} \rangle + \beta \langle H \rangle - \beta \mu \beta \langle N \rangle = \langle \ln \hat{\rho}_{nor} \rangle + \beta \langle K \rangle. \tag{370}
\]

Substituting Eq.(369) into Eq.(370), one can obtain the following expression

\[
\beta \Omega = \text{Tr}[\beta Q/2] - \langle \ln \text{Det}[4 \cosh(\beta Q/2)] \rangle - \beta \langle \psi^\dagger Q \psi \rangle + \beta \langle K \rangle. \tag{371}
\]

The third term is calculated using the same steps used in Eq.(366).

\[
\langle \psi^\dagger Q \psi \rangle = \sum_{AB} \langle \psi_A^\dagger Q_{AB} \psi_B \rangle = \sum_{AB} Q_{AB} \int D u^\dagger D u \frac{1}{2} \left( u_A^\dagger + \frac{\delta}{\delta u_A} \right) \left( u_B + \frac{\delta}{\delta u_B} \right) \rho_{uv} \bigg|_{u=v} = \frac{1}{2} \sum_{AB} Q_{AB} G_{BA}, \tag{372}
\]

where \( G = \sigma_0 - \tanh(\beta Q/2) \).

Similarly, we obtain

\[
\langle \psi^\dagger \xi \psi \rangle = \frac{1}{2} \sum_{AB} \xi_{AB} G_{BA}, \tag{373}
\]

\[
\langle \psi_A^\dagger \psi_B^\dagger V_{AB} \psi_B \psi_A \rangle = \frac{1}{4} \sum_{AB} V_{AB} [G_{AA} G_{BB} - G_{BA} G_{AB}]. \tag{374}
\]

Collecting terms, the thermodynamic potential is expressed as
\[
\beta \Omega = \frac{1}{2} \beta \sum_A Q_{AA} - \sum_A \left[ \ln \left[ 4 \cosh \left( \frac{1}{2} \beta Q \right) \right] \right]_{AA} \\
- \frac{1}{2} \beta \sum_{AB} Q_{AB} G_{BA} + \frac{1}{2} \beta \sum_{AB} \xi_{AB} G_{BA} \\
+ \frac{1}{8} \beta \sum_{AB} V_{AB} [G_{AA} G_{BB} - G_{BA} G_{AB}].
\] (375)

For a homogenous system, it is more convenient to carry out the calculation in \( \vec{k} \)-space. Thus,
\[
\beta \Omega = -V \int dK \text{tr} [\ln [4 \cosh A(\vec{k})]] \\
+ V \int dK \text{tr} [A(\vec{k}) \tanh A(\vec{k})] \\
+ \frac{1}{2} V \int dK \text{tr} [\xi(\vec{k}) G(\vec{k})] \\
+ \frac{1}{8} V \int dK \text{tr} [G(\vec{k})] \int dK' \text{tr} [G(\vec{k}')] \\
- \frac{1}{8} V \beta \int dK dK' V(\vec{k} - \vec{k}') \text{tr} [G(\vec{k}) G(\vec{k}')],
\] (376)

where \( A(\vec{k}) = \beta Q(\vec{k})/2, G(\vec{k}) = \sigma_0 - \tanh(\beta Q(\vec{k})/2) \) and \( \text{tr} \) is the trace for the spin indices only.

Introducing a constraint parameter \( N \),
\[
N \equiv \frac{1}{2} V \int dK \text{tr} [G(\vec{k})],
\] (377)

we rewrite the thermodynamic potential as follows
\[
\beta \Omega = \alpha \left[ N - \frac{1}{2} V \int dK \text{tr} [G(\vec{k})] \right] \\
- V \int dK \text{tr} [\ln [4 \cosh A(\vec{k})]] \\
+ V \int dK \text{tr} [A(\vec{k}) \tanh A(\vec{k})] \\
+ \frac{1}{2} V \beta \int dK \text{tr} [\xi(\vec{k}) G(\vec{k})] \\
+ \frac{1}{2} V(0) \beta N^2 \\
- \frac{1}{8} V \beta \int dK dK' V(\vec{k} - \vec{k}') \text{tr} [G(\vec{k}) G(\vec{k}')],
\] (378)

where \( \alpha \) is the Lagrange’s undetermined multiplier. Taking variations on \( \beta \Omega \) with respect to \( N \) and \( A(\vec{k}) \), we obtain
\[
\alpha = -V(0) \beta N / V, \quad (379)
\]
\[
\beta Q(\vec{k}) = (\beta \xi(\vec{k}) - \alpha) \sigma_0 - \frac{1}{2} \beta \int dK' V(\vec{k} - \vec{k}') G(\vec{k}').
\] (380)

**<Problem>** Prove Eq.(380).

Eq.(380) is a self-consistent equation which determines \( Q(\vec{k}) \). Since all functions in the above equation are \( 2 \times 2 \) matrices, \( Q(\vec{k}) \) and \( G(\vec{k}) \) are also expressed as linear combinations of Pauli matrices. First, we consider the symmetry conserving paramagnetic case. In this case, the eigenvalues of \( G(\vec{k}) \) are same for both spins, and, thus, \( Q(\vec{k}) \) and \( G(\vec{k}) \) must be multiples of the \( 2 \times 2 \) identity matrix same as in the zero-temperature case,
\[ Q(\vec{k}) = q(\vec{k})\sigma_0. \]
\[ G(\vec{k}) = g(\vec{k})\sigma_0. \]  
(381)

By defining \( q(\vec{k}) \equiv \epsilon_k - \mu \), \( g(\vec{k}) \) can be written as
\[
g(\vec{k}) = 1 - \tanh\left[ \frac{1}{2}\beta(\epsilon_k - \mu) \right]
= \frac{2}{1 + e^{\beta(\epsilon_k - \mu)}} = 2n_k. \]  
(382)

Here, \( n_k \) is the Fermi distribution function of the interacting system. The energy spectrum of the interacting system is obtained from Eq.(380)
\[
\epsilon_k = \epsilon_k^0 + (2S + 1)V(0)n - \int dK'V(\vec{k} - \vec{k}')n_{k'}. \]  
(383)

where \( n = N/V \) is the number density. The above equation is the familiar self-consistent Hartree-Fock equation, which determines the energy spectrum of the interacting electron gas system. The total energy is obtained using Eqs.(373), (374), (381) and (382).
\[
E = \langle H \rangle
= \frac{1}{2}V \int dK \text{tr}[h(\vec{k})G(\vec{k})]
\frac{1}{8}VV(0) \int dK \text{tr}[G(\vec{k})] \int dK' \text{tr}[G(\vec{k}')]
- \frac{1}{8}V \int dK dK'V(\vec{k} - \vec{k}')\text{tr}[G(\vec{k})G(\vec{k}')]
= (2S + 1)V \int dK \epsilon_k^0 n_k
\frac{1}{8}VV(0)(2S + 1)^2 \int dK 2n_k \int dK' 2n_{k'}
- \frac{1}{8}V(2S + 1) \int dK dK'V(\vec{k} - \vec{k}')4n_k n_{k'}
= (2S + 1)V \int dK (\epsilon_k^0 + \frac{1}{2}\Sigma_k)n_k, \]  
(384)

where the self-energy \( \Sigma_k \) is given by
\[
\Sigma_k = (2S + 1)V(0)n - \int dK'V(\vec{k} - \vec{k}')n_{k'}. \]  
(385)

The thermodynamic potential is obtained using Eqs.(376), and (381) \sim (384),
\[
\Omega = -Nk_B T \ln 2
- k_B T(2S + 1)V \int dK \ln \left[ 1 + e^{-(\epsilon_k - \mu)/k_BT} \right]. \]  
(386)

<Problem> Prove Eq.(386).

As we discussed in Section III.A, there exist solutions other than the simple paramagnetic solution. In order to consider a magnetic symmetry breaking solution, we express \( Q(\vec{k}) \),
\[
Q(\vec{k}) = (\epsilon_k - \mu)\sigma_0 + \gamma_k \sigma_3. \]  
(387)

Assuming that \( \gamma_k \) is much smaller than \( \epsilon_k \) and expanding to the first order of \( \gamma_k \), we obtain
tanh \left[ \frac{1}{2} \beta (\epsilon_k - \mu) \right]
\approx \sigma_0 \tanh \left[ \frac{1}{2} \beta (\epsilon_k - \mu) \right] + \sigma_0 \frac{1}{2} \beta \gamma_k \sech^2 \left[ \frac{1}{2} \beta (\epsilon_k - \mu) \right].
\tag{388}

Substituting this result into Eqs. (380) and (382), we obtain for the ferromagnetic state
\begin{align*}
\beta \left[ (\epsilon_k - \mu) \sigma_0 + \gamma_k \sigma_3 \right] &= (\beta \xi_k - \alpha) \sigma_0 \\
- \frac{1}{2} \beta \int dK' V(\vec{k} - \vec{k}') \left[ \sigma_0 \left( 1 - \tanh \left( \frac{1}{2} \beta (\epsilon_{k'} - \mu) \right) \right) \right. \\
&\left. - \sigma_3 \frac{1}{2} \beta \gamma_{k'} \sech^2 \left( \frac{1}{2} \beta (\epsilon_{k'} - \mu) \right) \right].
\tag{389}
\end{align*}

From this identity equation, we obtain two self-consistent equations as follows
\begin{align*}
\epsilon_{k\sigma} &= e_{k\sigma}^0 + (2S + 1)V(0)n - \int dK' V(\vec{k} - \vec{k}') n_{k'\sigma}, \\
\gamma_k &= \frac{1}{4} \beta \int dK' V(\vec{k} - \vec{k}') \gamma_{k'} \sech^2 \left( \frac{1}{2} \beta (\epsilon_{k'} - \mu) \right).
\tag{390}
\end{align*}

Solving Eq. (391) self-consistently, one can obtain the magnitude of the splitting between the up- and down-spin energy spectrum. The zeroth order approximation of Eq. (391) yields the celebrated Stoner condition for ferromagnetism,
\begin{align*}
1 &= \tilde{V}(0) \int dK \left[ - \frac{\partial n(\epsilon_k)}{\partial \epsilon_k} \right] \\
&= \tilde{V}N(0) \approx \tilde{V}N(0).
\tag{392}
\end{align*}

Here, \( F(0), N(0), \) and \( \tilde{V}(0) \) represent the static Lindhard function, the density of states at the Fermi surface and the average exchange interaction respectively. The total energy and the thermodynamic potential are obtained in the same fashion as for the paramagnetic case,
\begin{align*}
E &= V \sum_\sigma \int dK \left[ e_{k\sigma}^0 + \frac{1}{2} \Sigma_{k\sigma} \right] n_{k\sigma}, \\
\Omega &= - \frac{1}{\beta} \ln 2 - \frac{1}{\beta} V \sum_\sigma \int dK \ln \left[ 1 + e^{-\beta (\epsilon_{k\sigma} - \mu)} \right],
\tag{393}
\end{align*}
where
\begin{align*}
\Sigma_{k\sigma} &= \frac{1}{2} V(0)n - \frac{1}{2} \int dK' V(\vec{k} - \vec{k}') n_{k'\sigma}, \\
n_{k\sigma} &= \frac{1}{1 + e^{\beta (\epsilon_{k\sigma} - \mu)}}.
\tag{394}
\end{align*}

\( \epsilon_{k\sigma} \) and \( n_{k\sigma} \) can be determined self-consistently once \( \gamma_k \) is obtained.

In this chapter, we have shown that the functional Schrödinger picture formalism can produce the well-known Hartree-Fock or mean field results through variational process with Gaussian trial functionals.

We also have shown that, in certain special cases, a shifted Gaussian can be employed to obtain higher terms which do not appear in the Gaussian approximation. Although the present method is quite versatile and can be applied to any models, including the electron gas, the Hubbard, and the nonlinear sigma model \cite{4}, it is quite clear that the variational method lacks means for systematic improvement. Therefore, it is not possible to go beyond the Hartree-Fock result within the theoretical schemes presented in this chapter.

In order to overcome this problem, a time-dependent functional Schrödinger picture theory is constructed \cite{5}. It is known that infinitesimal time-dependent Hartree-Fock fluctuations around the Hartree-Fock ground state yield the random-phase-approximation (RPA) results (p. 292, Gen. Ref. 2). Indeed, it was shown that, in the small oscillation regime around the Hartree-Fock solutions, the RPA results can be obtained. The theory was applied to the electron gas to yield the electron-hole excitation spectrum, the collective plasma oscillation, and the spin wave energy. However, again it should be noted that this line of approach is limited to the RPA results. Often, for systems with strong correlations, the RPA results are not satisfactory. Therefore, it is necessary to provide a theoretical scheme which can go beyond the Gaussian and the RPA results.

In the next chapter, we discuss such efforts using the functional Schrödinger picture.
IV. FURTHER DEVELOPMENT OF THE FUNCTIONAL SCHröDINGER PICTURE METHOD

A basic problem inherent to any variational calculation is that it lacks means for systematic improvement. Therefore, in order to devise a many-body theoretical scheme applicable to wide range of problems, it is necessary to overcome this problem.

In undergraduate quantum mechanics courses, students are taught generally two types of approximation schemes, perturbation and variational methods. Each method is known to have its own advantages and limitations. Perturbation theory is applicable only when the perturbing term is small, whereas the variational method lacks systematic means for improvement as mentioned above. Efforts to combine these two approximations and provide a new scheme which retains the advantages of both methods have been existed in various field of physics. In this chapter, we review these efforts and introduce the variational perturbation theory and the optimized perturbation theory in plain quantum mechanics languages. Then, we construct the variational perturbation scheme based on the functional Schrödinger picture. The theory is applied to the $\lambda\phi^4$ field theory in order to compare the scheme with other existing methods. In the remaining section, the theory will be extended to the optimized perturbation with the $\lambda\phi^4$ as a model system.

A. Variational and Optimized Perturbation Theories in Quantum Mechanics

Perturbation Theory

In order to explain the salient features of perturbation theory, we reproduce the discussion on perturbation theory from Negele and Orland (Chapt. 2, Gen. Ref. 2). In the process, we will show that how the new concepts of variational perturbation and optimized perturbation are related to plain perturbation theory.

Perturbation theory is based on the belief that the behavior of a physical system is continuous in some 'small' parameter describing the difference between a solvable problem and the actual system. It is crucial to note, however, that in general perturbation theory yields an asymptotic rather than a convergent series. Only under appropriate circumstances, it may yield a useful physical approximation, but it cannot be applied systematically to arbitrary precision.

The salient feature of asymptotic expansions may be illustrated by the following simple integral

$$Z(g) = \int \frac{dx}{\sqrt{2\pi}} e^{-x^2/2 - gx^4/4}$$

(397)

corresponding to the classical partition function $Z = \int dx e^{-V(x)}$ for a particle in a potential, $V(x) = x^2/2 + gx^4/4$. Physically, the classical or quantum behavior in this potential changes completely when $g$ changes sign, since a particle is localized when $g > 0$ and not when $g < 0$. Thus, we expect that the theory is nonanalytic at $g = 0$ and that an expansion in powers of $g$ has zero radius of convergence.

The perturbation series for $Z(g)$ is easily obtained by expanding $e^{-gx^4/4}$, with the result

$$Z(g) = \sum_n g^n Z_n$$

(398)

with

$$g^n Z_n = \frac{(-g)^n}{n!} \frac{1}{4^n} \int dx \sqrt{2\pi} e^{-x^2/2} x^{4n}$$

$$= \frac{(-g)^n (4n-1)!!}{n! 4^n}$$

$$= \frac{(-g)^n (4n)!}{n! 16^n (2n)!}$$

$$\sim \frac{1}{\sqrt{n\pi}} \left( \frac{4gn}{e} \right)^n, \quad n \to \infty$$

(399)

where the asymptotic behavior in the last line is obtained using Stirling’s formula $n! = \sqrt{2\pi n^{n+1/2}} e^{-n}$. Since $Z_n$ grows like $n!$, the series diverges as expected from the non-analyticity at $g = 0$. 

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The crucial point for the present discussion is the fact that, under appropriate circumstances, a finite number of terms of an asymptotic series may give an excellent approximation. The residual error after \( n \) terms is bounded by the \((n+1)\)st term

\[
R_n \equiv |Z(g) - \sum_{m=0}^{n} g^m Z_m| = \int \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} |e^{-g x^4/4} - \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{-g x^4}{4} \right)^m | \leq \int \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{(n+1)!} \left( \frac{g x^4}{4} \right)^{n+1} = g^{n+1} |Z_{n+1}|, \tag{400}
\]

so the approximation continues improve as long as \( g^n Z_n \) decreases. Fig. IV.1 shows \( R_n \) and \( g^n|Z_n| \) as a function of \( n \) for several values of the coupling constant \( g \). From the asymptotic expression for \( g^n Z_n \), Eq.(399), we note that the minimum occurs for \( n \sim \frac{1}{g^2} \), so that the minimum error is \( g^n Z_n|_{min} \sim \sqrt{4g/\pi e^{-1/4g}} \). This exponential dependence on the inverse coupling constant is characteristics of perturbation theory for weak coupling.

The real problem comes at large coupling constant where the series begins to diverge in very low order. At \( g = 0.1 \), for example, one must stop at the third term after only attaining an accuracy of \( R_3/R_0 = 25\% \).

---

**Fig. IV.1** Asymptotic expansion of \( Z(g) \). For five values of the coupling constant, \( \frac{1}{2} g^n |Z_n| \) is plotted at each integer \( n \) and the residual error \( R_n \) is plotted at each half integer \( n + \frac{1}{2} \). The arrow symbolizes the variation process carried out for the variational perturbation theory, whereas the solid line connecting the minima corresponds to the optimized perturbation approximation. (from Gen. Ref. 2).
In order to overcome this problem, many prescriptions including the Borel summation (Section 7.5, Gen. Ref. 2) have been proposed. In this lecture, we discuss two systematic approaches to overcome this problem, namely the variational perturbation theory and the optimized perturbation theory. Fig. IV.1, which is Fig. II.2 in General Reference 2, is reproduced here to explain the relationship between the plain perturbation and the two methods mentioned above.

Variational Perturbation Theory

Here, we explain the concept of variational perturbation theory using a simple quantum mechanical language [1]. Although this concept has been studied intensively in connection with path integrals [2], field theories and other physics subfields [3], we believe that it had never been discussed in a plain quantum mechanical language before Ref. 1.

In a variational calculation, one first chooses a trial function $\Psi(\lambda)$ as a function of a variational parameter $\lambda$ for a given Hamiltonian $H$. Then, the ground state energy is estimated by minimizing the expectation value, $\langle \Psi(\lambda) | H | \Psi(\lambda) \rangle$ against $\lambda$.

In the present formalism, we also first choose a trial function $\Psi_n(\lambda)$, but we require $H_\Lambda | \Psi_n(\lambda) \rangle = E_n(\lambda) | \Psi_n(\lambda) \rangle$, where $H_\Lambda$ is called a parent Hamiltonian. We will discuss implications of this requirement below. The original Hamiltonian is now rewritten

$$H = H_\Lambda + H - H_\Lambda = H_{\Lambda} + H', \quad (401)$$

where $H' = H - H_\Lambda$ is the new renormalized perturbing Hamiltonian. Clearly, success of the following perturbation calculation depends how small $H'$ can be made. In order to obtain an optimum $H_\Lambda$, we first determine $\lambda$ through the condition,

$$\delta \langle \Psi_n(\lambda) | H | \Psi_n(\lambda) \rangle = 0. \quad (402)$$

Here, we note that this condition is not limited to the ground state only, but is valid for all excited states. Therefore, $\lambda$ will be generally dependent on the state number $n$, of which energy we want to estimate.

The standard Rayleigh-Schrödinger perturbation expansion is given by [4]

$$|n\rangle = \sum_{l=0}^{\infty} Q_n \frac{1}{H_0 - E_n^{(0)}} (E_n - E_n^{(0)} - H_I) \left| n^{(0)} \right\rangle, \quad (403)$$

$$E_n = E_n^{(0)} + \sum_{l=0}^{\infty} \langle n | H_I | n \rangle \left[ Q_n \frac{1}{H_0 - E_n^{(0)}} (E_n - E_n^{(0)} - H_I) \right] \left| n^{(0)} \right\rangle \quad (404)$$

where $Q_n = 1 - P_n = 1 - |n\rangle^{(0)} (n\rangle^{(0)}$ is the number operator.

In the present theoretical scheme, we use $H_0 = H_\Lambda$ and $H' = H - H_\Lambda$. The energy expression up to the second order is given by

$$E_n = \langle \Psi_n(\lambda_n) | H_{\Lambda n} | \Psi_n(\lambda_n) \rangle + \langle \Psi_n(\lambda_n) | H' | \Psi_n(\lambda_n) \rangle + \sum_{k \neq n} \frac{|\langle \Psi_k(\lambda_n) | H' | \Psi_n(\lambda_n) \rangle|^2}{E_n^{(0)}(\lambda_n) - E_k^{(0)}(\lambda_n)} + \cdots. \quad (405)$$

where $H_{\Lambda n} | \Psi_n(\lambda_n) \rangle = E_n^{(0)}(\lambda_n) | \Psi_n(\lambda_n) \rangle$. We note that the first two terms correspond to the variational calculation result $\langle \Psi_n(\lambda) | H | \Psi_n(\lambda) \rangle_{\lambda = \lambda_n}$ with $\lambda_n$ determined through minimization. The third term is the second order perturbation term with a renormalized perturbation which provides a systematic improvement over the simple variational ground state energy. The perturbation expansion, Eq.(405) differs from that obtained through conventional perturbation theory. The basis function used in the perturbation are those obtained through a variational process.

As a simple example of the variational perturbation scheme, we consider the anharmonic oscillator problem. We will see that seemingly simple example exhibits all the salient features of the variational perturbation theory.

The Hamiltonian is given by
\[
H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 + bx^4 ,
\]
where \( b \) is positive. An obvious choice for the trial function is given by
\[
\Psi_\Omega(x) = \left(\frac{m\Omega}{\pi \hbar}\right)^\frac{1}{4} e^{-\frac{m\Omega}{2\hbar} x^2} ,
\]
for the ground state, where \( \Omega \) is the variational parameter. The corresponding parent Hamiltonian is given by
\[
H_\Omega = \frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 .
\]
Using this parent Hamiltonian, the original Hamiltonian is rewritten as
\[
H = H_\Omega + H' = \frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 + \frac{m}{2} (\omega^2 - \Omega^2) x^2 + bx^4 .
\]
We denote the \( n \)th eigenstate of \( H_\Omega \) by \( |n\Omega\rangle \). Then, the expectation value of \( \langle n\Omega|H|n\Omega\rangle \) is given by
\[
\langle n\Omega|H|n\Omega\rangle = \langle n\Omega|H_\Omega|n\Omega\rangle + \langle n|H'|n\rangle = \langle n\Omega|H_\Omega|n\Omega\rangle - \frac{m(\Omega^2 - \omega^2)}{2} \langle n\Omega|x^2|n\Omega\rangle + b\langle n\Omega|x^4|n\Omega\rangle
= \hbar \Omega \left( n + \frac{1}{2} \right) - \frac{\hbar(\Omega^2 - \omega^2)}{4\Omega} (2n + 1) + \frac{3\hbar^2}{4m^2\Omega^2} (2n^2 + 2n + 1) .
\]
Here, we used the standard quantum mechanical results [5]
\[
\langle n\Omega|x^2|n\Omega\rangle = \frac{\hbar}{2m\Omega} (2n + 1) ,
\langle n\Omega|x^4|n\Omega\rangle = \left( \frac{\hbar}{2m\Omega} \right)^2 (6n^2 + 6n + 3) .
\]
Taking a variation on \( \langle n\Omega|H|n\Omega\rangle \), we obtain a relation which determines \( \Omega_n \),
\[
\Omega_n^3 - \omega^2 \Omega_n - \frac{6\hbar^2}{m^2} \frac{2n^2 + 2n + 1}{2n + 1} = 0 .
\]

| TABLE I. Comparison of the ground state energies(in eV) obtained using different approximation schemes. The values in the parentheses are the ratios to the exact values. The values of \( \frac{1}{2} m\Omega_0^2 \) are also shown as references. |
|---|---|---|---|
| b(eVÅ⁻¹) | 0.01 | 0.05 | 0.25 |
| Perturbation | 1.4318427 | 1.5279252 | does not converge. |
| Theory | (99.935%) | (95.962%) | |
| Variational | 1.4333279 | 1.5968858 | 2.0664772 |
| Calculation | (100.038%) | (100.293%) | (100.929%) |
| Present | 1.4327726 | 1.5912088 | 2.0412648 |
| Method | (99.997%) | (99.937%) | (99.679%) |
| Exact | 1.4327725 | 1.5922195 | 2.0474629 |
| Energy Value | \( \frac{1}{2} m\Omega_0^2(eVÅ⁻¹) \) | 0.5770839 | 0.8227827 | 1.6423320 |
Substituting these results into Eq.(405), we obtain
\[
E_n = \frac{\hbar \Omega}{2}(2n + 1) - \frac{3\hbar^2}{4m^2\Omega^2_n}(2n^2 + 2n + 1)
+ \frac{1}{4\hbar \Omega_n} \left( \frac{\hbar^2}{4m^2\Omega^2_n} \right)^2 \frac{64n^5 + 160n^4 - 336n^3 - 664n^2 - 280n - 24}{(2n + 1)^2}.
\]

(413)

**Problem** Show that \( E_n \) to the second order is given by Eq.(413).

In order to show the systematic improvement achieved by the variational perturbation theory over the variational or the plain perturbation theory, we have carried out numerical calculations. For this purpose, we choose \( \frac{\omega}{\Omega} = 0.5eV\AA^{-2} \) and carry out calculations for various values of \( b \). The results for the ground state energy are given in Table 4.1 [Table I, Ref.1]. The result shows that the present method is clearly superior to the conventional perturbation theory and provides a systematic mean for improvement over the variational calculation. First of all, the present method gives highly accurate values in the regime where the conventional perturbation theory is not applicable. This is because the perturbing Hamiltonian has been renormalized through the variational process.

Before we discuss the convergence problem of the variational perturbation theory, we briefly mention that the method can be applied problems other than anharmonic potentials such as helium atom and also to excited states [1]. Also, any well-behaving potential can be expanded around local minima

\[
V(x) = V(x_0) + \sum_{n=2}^{\infty} \frac{1}{n!} V^{(n)}(x)_{x=x_0} (x - x_0)^n.
\]

(414)

Therefore, we observe that above discussion on anharmonic oscillator is generally applicable to any well-behaving potentials. In the next section, we will show that this approximation corresponds to the variational perturbation process based on the Gaussian basis.

Next, we discuss the convergence problem of the variational perturbation process. Recently, this problem has been studied in detail and has been shown that the expansion does not converge at higher orders for strong coupling constants [6]. In fact, this behavior is not totally unexpected.

In the early part of this section, we have shown that perturbation theory is only asymptotically convergent and eventually divergent. The variational perturbation is also basically a perturbation expansion only with a renormalized perturbation. This process is explained on Fig.IV.1. As indicated by the arrow, the variational process renormalizes the the coupling constant first. Then, perturbation calculation is carried out with the renormalized coupling constant. As shown by the anharmonic example, this renormalized perturbation generally allows one to obtain much higher accuracy than allowed in the original perturbation expansion, although the variational perturbation theory will also eventually diverges at higher orders.

**Optimized Perturbation Theory**

Optimized perturbation theory was proposed to overcome the convergence problem in the perturbation theory[7,8]. It may look formidable in the field theory, but, in quantum mechanics, it is a rather simple and straightforward idea. In the optimized perturbation expansion, the variational process is not made in the beginning, but at the last stage of the perturbation calculation. In the process, the Hamiltonian is divided as in the variational perturbation method. And the perturbation calculation is carried out using Eqs.(403) and (404). Variation is made on \( E^{(l)}(\lambda) \), the \( l \)th order perturbation result, and, then the obtained \( \lambda_n \) is substituted into \( E_n^{(l)}(\lambda) \). Therefore, the value of \( \lambda_n^{(l)} \) is different on different \( l \).

We believe the method is best understood through a simple example of anharmonic oscillator[9]. We use the same Hamiltonian, Eq.(409)

\[
H = H\Omega + H' = \frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 + \frac{m}{2}(\omega^2 - \Omega^2)x^2 + bx^4,
\]

and the same trial function, Eq.(407)

\[
\psi_{\Omega}(x) = \left( \frac{m\Omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\Omega}{\hbar} x^2}.
\]

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We carry out the perturbation calculation on $E_n$ using Eq.(404) but without the variational condition, Eq(412). Then, to the second order, we obtain

$$E_n = \langle n\Omega | H \Omega | n\Omega \rangle + \langle n\Omega | H' | n\Omega \rangle + \sum_{k \neq n} \frac{|\langle k\Omega | H' | n\Omega \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$= \frac{\hbar \Omega}{2} (2n + 1) - \frac{\hbar (\Omega^2 - \omega^2)}{4\Omega} (2n + 1)$$

$$+ \frac{3\hbar^2}{4m^2 \Omega^2 (2n^2 + 2n + 1)}$$

$$+ \frac{3\hbar^2}{4m^2 \Omega^2 (2n^2 + 2n + 1)} - \frac{\hbar (\Omega^2 - \omega^2)^2}{16\Omega^3} (2n + 1)$$

$$- \frac{b^2 \hbar^3}{8m^4 \Omega^5} (34n^3 + 51n^2 + 59n + 21).$$

(415)

We find that, by taking a variation on $E_n$ with respect to $\Omega$, $\partial E_n / \partial \Omega = 0$, $\Omega$ does not any real roots. In order to cope with this problem, we examine the Hamiltonian, Eq.(409) and the perturbation expansion, Eq.(404). We note that, if the perturbation calculation is to be carried out to infinite or der, then, the final result will be independent of $\Omega$, since the original Hamiltonian does not have $\Omega$. The $\Omega$ dependence in the energy values comes from 'incomplete' perturbation calculation.

Therefore, unlike in the variational perturbation where one looks for minimum, here, we search for a point where the energy value is least sensitive to the variational parameter $\Omega$. This is called the principle of minimal sensitivity’ [8,9]. In the principle of minimal sensitivity, one takes the point which satisfies $\partial^2 E_n / \partial \Omega^2 = 0$, as the point of the least sensitivity, when there is no real value to satisfy $\partial E_n / \partial \Omega = 0$. It will be shown that in the odd order approximation, there exists at least one real value of $\Omega$, whereas in the even order, one should choose an $\Omega$ value which satisfies $\partial^2 E_n / \partial \Omega^2 = 0$. This comes from the fact that, at the odd order, the highest order of $\Omega$ is even and odd for the even order.

Therefore we take $\partial^2 E_n / \partial \Omega^2 = 0$ for Eq.(415) and, by numerically solving the equation, obtain $\Omega_{ls}$. The value of $\Omega_{ls}$ is substituted into Eq.(415) to obtain the energy value $E_n$. Here, we note that, in the optimized perturbation theory, it is not possible to obtain an analytic expression for the energy unlike in the variational perturbation theory, Eq.(413).

In order to study the convergence problem of the three perturbation theories, we have carried out the optimized perturbation calculation up to the third order,

$$E_n = \langle n\Omega | H \Omega | n\Omega \rangle + \langle n | H' | n \rangle$$

$$+ \sum_{k \neq n} \frac{|\langle k\Omega | H' | n\Omega \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$+ \sum_{k \neq n} \frac{\langle n\Omega | H' | k\Omega \rangle \langle k\Omega | H' | n\Omega \rangle}{(E_n^{(0)} - E_k^{(0)})}$$

$$- \frac{\hbar \Omega}{2} (2n + 1) - \frac{\hbar (\Omega^2 - \omega^2)}{4\Omega} (2n + 1)$$

$$+ \frac{3\hbar^2}{4m^2 \Omega^2 (2n^2 + 2n + 1)}$$

$$+ \frac{3\hbar^2 (\Omega^2 - \omega^2)}{4m^2 \Omega^4 (2n^2 + 2n + 1)} - \frac{\hbar (\Omega^2 - \omega^2)^2}{16\Omega^3} (2n + 1)$$

$$- \frac{b^2 \hbar^3}{8m^4 \Omega^5} (34n^3 + 51n^2 + 59n + 21)$$

$$- \frac{\hbar (\Omega^2 - \omega^2)^3}{32\Omega^6} (2n + 1) + \frac{b^2 \hbar^3 (\Omega^2 - \omega^2)^2}{4m^2 \Omega^6} (6n^2 + 6n + 3)$$

$$- \frac{b^2 \hbar^3 (\Omega^2 - \omega^2)^3}{16m^4 \Omega^7} (170n^3 + 255n^2 + 292n + 105)$$

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Problem 1  

Prove Eq. (415) and (416).

This equation has a real solution for \( \partial E_n/\partial \Omega = 0 \), which can be substituted into the equation to obtain the energy value. In Fig. IV.2, we compare the three perturbation methods for the ground state \( (n = 0) \) with parameters \( m\omega^2/2 = 0.5 \text{eV} \text{Å}^{-2} \) and \( b = 0.01 \text{eV} \text{Å}^{-4} \). The figure shows clearly that the optimized perturbation has the best convergence. Now, we consider the relation between the optimized perturbation theory and the conventional perturbation.

\[
\frac{b^3 \hbar^4}{16m^6\Omega^8}(375n^4 + 750n^3 + 1416n^2 + 1041n + 333).
\]

\[ (416) \]

<Problem> Prove Eq. (415) and (416).

The optimized perturbation theory renormalizes the perturbation (coupling constant) at each order and choose the minimum (or near minimum) point for \( E_n \). Therefore, the optimized perturbation theory can be pictorially represented by solid line in Fig. IV.1.

Here, it should be mentioned that although the optimized perturbation theory may solve the problem of convergence, its practical use is rather limited due to the complicated nature of the detailed calculation. Quite often, the one-time renormalization scheme of the variational perturbation theory allows enough accuracy required.

The variational and the optimized perturbation theories in quantum mechanics via path integral have been intensively studied by Kleinert and his colleagues and any higher terms can be readily generated through computer[2]. In the remaining sections, the variation and the optimized perturbation theories will be applied to bosonic field theories using the \( \lambda\phi^4 \) model as a model system.

B. Variational Perturbation Theory in The Functional Schrödinger Picture

It has been shown that in Chapter III, Gaussian approximations invariably lead into mean-field results. In order to go beyond Gaussian results, various approximations schemes including functional integrals and background field methods have been proposed[1~3]. Among these methods, except several variational calculations with correlated or non-Gaussian trial functions, majority of the schemes are basically based on the concepts of the variational or the optimized perturbation theory. Therefore, here again the approaches going beyond the Gaussian approximations can be classified by the methodologies employed, namely, the operator (Green’s function method), the functional integrals,
and the functional Schrödinger picture methods. It has been observed that the first two methods naturally lead into
Feynman diagrams again albeit renormalized and somewhat simplified. Therefore, in order to go beyond the second
order, careful enumerations on inequivalent diagrams are still required. However, functional Schrödinger picture does
not require such counting processes. Being a basic perturbation theory but with a Gaussian basis, it is enough to carry
out the standard Rayleigh-Schrödinger perturbation calculation given by Eqs.(403) and (404). The only modification
is that the basis are now functionals instead of functions.

Here, we present a bosonic Rayleigh-Schrödinger perturbation theory based on Gaussian wavefunctional. We
consider a model with the Lagrangian density

$$L = \frac{1}{2} \partial_\mu \phi x \partial^\mu \phi x - V(\phi x),$$

(417)

where $x = (x^1, x^2, \cdots, x^D)$ represents a position in $D$-dimensional space and $\phi x = \phi(\vec{x})$ is the field at $\vec{x}$. We note
that this model can be readily reduced to non-relativistic many-body theory by changing the kinetic part. Also, the
$\phi$ classical constant $\varphi$ is equal to the Gaussian vacuum expectation value of $\phi x$:

$$\varphi = \langle 0 | \phi x | 0 \rangle.$$

(419)

The Hamiltonian density corresponding to Eq.(417) is given by

$$\mathcal{H} = \pi_x \partial_t \phi x - L$$

$$= \frac{1}{2} \pi_x^2 + \frac{1}{2} (\partial_x \phi x)^2 + V(\phi x),$$

(420)

where $\pi_x = \frac{1}{i} \frac{\partial}{\partial \phi x}$ as shown in Eq.(190). Here, we set $c = \hbar = 1$ following the field theoretical notation. In order to
calculate the ground energy state density $\epsilon = \langle H \rangle$, it is necessary to evaluate the following matrix elements$[4]$, \(0\langle \phi x | (\partial_x \phi x)^2 | 0 \rangle = (\partial_x \varphi)^2 - ((\phi x - \varphi) \partial_x^2 (\phi x - \varphi))

= (\partial_x \varphi)^2 - \frac{1}{2} \int \delta(x - y) \partial_x^2 f_{xy}^{-1}

= (\partial_x \varphi)^2 + \frac{1}{2} \int \frac{d^D p}{(2\pi)^D} \frac{p^2}{f(p)},

(421)

where we utilized the Gaussian functional integrals, Eq.(154). We also have

$$0\langle \phi x | (\frac{\delta}{\delta \phi x})^2 | 0 \rangle = \left\langle \left( \frac{\delta}{\delta \phi x} \right)^2 \right\rangle$$

$$= \pi_x^2 + \frac{1}{2} \int \frac{d^D p}{(2\pi)^D} \frac{p^2}{f(p)},$$

(422)

$$0\langle \phi x | V(\phi x) | 0 \rangle = \int_{-\infty}^{\infty} \frac{d\beta}{\sqrt{2\pi}} \tilde{V}(\beta)(e^{i\beta \varphi})$$

$$= \int_{-\infty}^{\infty} \frac{d\beta}{\sqrt{2\pi}} \tilde{V}(\beta) e^{-\frac{1}{2} \beta^2 f_{xx}^1} e^{i\beta \varphi}$$

$$= \int_{-\infty}^{\infty} \frac{d\beta}{\sqrt{2\pi}} \tilde{V}(\beta) \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{2\pi}} e^{-\alpha^2/2} e^{\sqrt{2}(\beta f_{xx}^1 + i\varphi)} \left\langle 0 \left| \alpha \sqrt{f_{xx}^1} + \varphi \right\rangleight.$$
Collecting the results, we obtain for the ground state energy density, which is also called effective potential in the field theory, for the Gaussian trial functional.

\[
\epsilon [\varphi, P_x, f] = \langle 0 | \hat{H}_x | 0 \rangle^{(0)} = \frac{1}{2} (\partial_x \varphi)^2 + \frac{1}{2} P_x^2 + \frac{1}{4} \int \frac{d^D p}{(2\pi)^D} f(p) \frac{p^2}{2} + \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2} V(\alpha \sqrt{f_{xx}^{-1}} + \varphi)
\]

As the first process of the variational perturbation theory, we take variations on \( \epsilon \) with respect to \( P_x \) and \( f(p) \).

\[
\frac{\delta \epsilon}{\delta f(p)} = 0 = \frac{1}{4(2\pi)^D} \left( \partial \varphi \right)^2 + \frac{1}{4(2\pi)^D} \left( -\frac{1}{f^2(p)} \right)
\]

where we used the second relation in Eq.(423). This equation can be arranged as

\[
f^2(p) = p^2 + \int_{-\infty}^{\infty} \frac{d\beta}{\sqrt{2\pi}} \tilde{V}(\beta) e^{i\beta \phi} e^{-\frac{1}{4} \beta^2 f_{xx}^{-1}} (-\beta^2)
\]

\[
= p^2 + \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2} V^{(2)}(\alpha \sqrt{f_{xx}^{-1}} + \varphi) + \mu^2,
\]

where \( V^{(n)}(z) = d^n V(z)/dz^n = \int_{-\infty}^{\infty} (dq/\sqrt{2\pi}) (iq)^n \hat{V}(q) e^{iqz} \).

The renormalized mass or coupling constant \( \mu^2 \) is given by

\[
\mu^2(\varphi) = \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2} V^{(2)}(\alpha \sqrt{f_{xx}^{-1}} + \varphi).
\]

Here, it is convenient to introduce the following notation

\[
I_n(Q^2) = \int \frac{d^D p}{(2\pi)^D} \left[ \sqrt{p^2 + Q^2}/(p^2 + Q^2)^n \right].
\]

Note that \( f_{xx}^{-1} = I_1(\mu^2) \).

Substituting the above relations, Eq(426)~(428), into Eq(424) and noting that \( \partial \varphi / \partial x = 0 \), the Gaussian effective potential becomes

\[
\mathcal{V}_G(\varphi) = \frac{1}{2} I_0(\mu^2) - \frac{\mu^2}{4} I_1(\mu^2)
\]

\[
+ \int_{-\infty}^{\infty} \frac{d\alpha}{2\sqrt{\pi}} e^{-\alpha^2} \sqrt{\frac{\alpha}{2}} \sqrt{I_1(\mu^2) + \varphi}. \]

We note that when \( \mathcal{V}_G(\varphi) \) has the absolute minimum at \( \varphi_0 \), \( \mu(\varphi_0) \) becomes the physical mass(or the renormalized mass) and \( \mathcal{V}_G(\varphi) \) represents the vacuum(ground) state energy. The symmetry of the ground state can be discussed using Eq.(429).

For the second stage of the variational perturbation theory, it is necessary to partition the Hamiltonian in two parts as we did in Eq.(401) and (409). This can be best achieved constructing annihilation and creation operators for
Gaussian particles (Gaussians), of which the Gaussian functions are exact solutions. Following Ref. [4], we define

\[
A_f(p) = \left( \frac{1}{2(2\pi)^3 f(p)} \right)^{1/2} \int_x e^{-ipx} [f(p)(\phi_x - \varphi) + i\pi_x],
\]

\[
A_f^\dagger(p) = \left( \frac{1}{2(2\pi)^3 f(p)} \right)^{1/2} \int_x e^{ipx} [f(p)(\phi_x - \varphi) - i\pi_x].
\]

(430)

We can readily show that these operators satisfy \([A_f(p), A_f^\dagger(p')] = \delta(p' - p)\). Based on these operators, one can construct the parent Hamiltonian

\[
H_0 = \int dp f(p) A_f^\dagger(p) A_f(p)
\]

\[
= \int_x \left[ \frac{1}{2\pi^2} + \frac{1}{2}(\partial_x \phi_x)^2 + \frac{1}{2} \mu^2 (\phi_x - \varphi)^2 - \frac{1}{2} f_0(\mu^2) \right]
\]

(431)

<Problem> Show that \([A_f(p), A_f^\dagger(p')] = \delta(p' - p)\) and prove Eq.(431).

The Gaussian ground state (vacuum), Eq.(418) is the ground state of \(H_0\) with the zero energy eigenvalue \(E_0^{(0)}\). The exited states of \(H_0\) are

\[
|n\rangle^{(0)} = \frac{1}{\sqrt{n!}} \prod_{i=1}^n A_f^\dagger(p_i)|0\rangle^{(0)} , \quad n = 1, 2, \cdots,
\]

(432)

with the corresponding energy eigenvalues

\[
E_n^{(0)} = \sum_{i=1}^n f(p_i).
\]

(433)

\(|n\rangle^{(0)}\) are normalized,

\[
(0)\langle n|n\rangle^{(0)} = \frac{1}{n!} \sum_{P_i(n)} \prod_{k=1}^n \delta(p_k' - p_k),
\]

(434)

where the \(P_i(n)\) represents a permutation of the set \(\{i_k\} = \{1, 2, \cdots, n\}\) and the summation is over all \(P_i(n)\)s. \(|n\rangle^{(0)}\) describes a \(n\)-particle state with the continuous momenta \(p_1, p_2, \cdots, p_n\). \(|0\rangle^{(0)}\) and \(|n\rangle^{(0)}\) with \(n = 1, 2, \cdots, \infty\) constitute the complete set for \(H_0\).

We note that the above Gaussian formalism is quite general and convenient for any system with a well behaving potential \(V(\phi_x)\). Now, the Hamiltonian is rewritten \(H = H_0 + H_I = H_0 + (H - H_0)\) with

\[
H_I = \int_x \left[ -\frac{1}{2} \mu^2 (\phi_x - \varphi)^2 + \frac{1}{2} f_0(\mu^2) + V(\phi_x) \right].
\]

(435)

Following the Rayleigh-Schrödinger perturbation procedures, Eq.(403) and (404), we write

\[
|n\rangle = \sum_{l=0}^\infty \left[ Q_n \frac{1}{H_0 - E_n^{(0)}} (E_n - E_n^{(0)} - H_I) \right]^l |n\rangle^{(0)},
\]

(436)

and

\[
E_n(\varphi) = E_n^{(0)} + \sum_{l=0}^\infty \langle 0|H_I \left[ Q_n \frac{1}{H_0 - E_n^{(0)}} (E_n - E_n^{(0)} - H_I) \right]^l |n\rangle^{(0)},
\]

(437)

where \(Q_n = \sum_{j\neq n} \int d^Dp_1 d^Dp_2 \cdots d^Dp_j (j)^{(0)}(0)\langle j|\).

For the case, \(n = 0\) and \(l = 0\), Eq.(437) gives the vacuum (ground state) energy up the first order \(E_n^1 = E_n^{(0)} + E_n^{(1)} = \).
\[ \int_x \mathcal{V}_G(\varphi), \] which is just the product of the Gaussian effective potential and the space volume.

**Application to the \( \lambda \phi^4 \) Field Theory.**

As an example, we consider the potential, \( V(\varphi) = \frac{1}{2} m^2 \varphi^2 + (\lambda/4!) \varphi^4 \), which was widely studied in connection with the Gaussian approximation[5]. Thus, this model allows direct comparisons with existing results and can be readily reduced to non-relativistic many-body theory and quantum mechanics.

With the above potential, Eq.(427) becomes

\[
\mu^2(\varphi) = \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2} V^{(2)}(\alpha \sqrt{I_1} + \varphi) \\
= m^2 + \frac{1}{2} \lambda \varphi^2 + \frac{1}{4} \lambda I_1(\mu^2),
\]

(438)

where we used \( \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} \alpha^{2n+1} e^{-\alpha^2} = 0 \) and \( \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} \alpha^{2n} e^{-\alpha^2} = 2^{-n} \cdot 1 \cdot 3 \cdot 5 \cdots (2n-1) \). Also, Eq.(429) becomes

\[
\mathcal{V}_G(\varphi) = \frac{1}{2} m^2 \varphi^2 + \frac{1}{4} \lambda \varphi^4 + \frac{1}{2} I_0(\mu) - \frac{1}{32} \lambda I_1^2(\mu^2),
\]

(439)

which is the standard Gaussian effective potential for the \( \lambda \phi^4 \) model.

**Problem** Prove Eqs.(438) and (439).

To obtain the effective potential of the \( \lambda \phi^4 \) model up to a given order using Eqs.(436) and (437), we need the following matrix elements:

\[
\langle n| H_f | n \rangle^{(0)} = \frac{1}{n! (n-1)!} \left\{ \frac{\lambda \varphi}{2 \sqrt{2(2\pi)^D}} \sum_{P_{ij}(n-2)} \prod_{k=1}^{n-2} \Delta(p_{ik} - p'_{jk}) \right. \\
\times \delta(p'_{j(n-1)} - p_{j(n-1)} - p_{in}) \times [f(p'_{j(n-1)}) f(p_{j(n-1)}) f(p_{in})]^{-\frac{1}{2}},
\]

(440)

\[
\langle n| H_f | n - 1 \rangle^{(0)} = \frac{1}{n! (n-1)!} \left\{ \frac{\lambda \varphi}{2 \sqrt{2(2\pi)^D}} \sum_{P_{ij}(n-2)} \prod_{k=1}^{n-2} \Delta(p_{ik} - p'_{jk}) \right. \\
\times \delta(p'_{j(n-1)} - p_{j(n-1)} - p_{in}) \times [f(p'_{j(n-1)}) f(p_{j(n-1)}) f(p_{in})]^{-\frac{1}{2}} + \sqrt{\frac{(2\pi)^D}{2}} (\mu^2 - \frac{\lambda}{3} \varphi^2) \varphi \right. \\
\left. \times \prod_{P_{ij}(n-1)} \Delta(p_{ik} - p'_{jk}) \delta(p_{in}) [f(p_{in})]^{-\frac{1}{2}} \right\},
\]

(441)

\[
\langle n| H_f | n - 2 \rangle^{(0)} = \frac{1}{n! (n-2)!} \left\{ \frac{\lambda \varphi}{2 \sqrt{2(2\pi)^D}} \sum_{P_{ij}(n-3)} \prod_{k=1}^{n-3} \Delta(p_{ik} - p'_{jk}) \right. \\
\times \delta(p'_{j(n-2)} - p_{j(n-2)} - p_{in}) \times [f(p'_{j(n-2)}) f(p_{j(n-2)}) f(p_{in})]^{-\frac{1}{2}},
\]

(442)

\[
\langle n| H_f | n - 3 \rangle^{(0)} = \frac{1}{n! (n-3)!} \left\{ \frac{\lambda \varphi}{2 \sqrt{2(2\pi)^D}} \sum_{P_{ij}(n-3)} \prod_{k=1}^{n-3} \Delta(p_{ik} - p'_{jk}) \right. \\
\times \delta(p_{2(n-2)} + p_{i(n-1)} + p_{in}) \times [f(p_{2(n-2)}) f(p_{i(n-1)}) f(p_{in})]^{-\frac{1}{2}}
\]

(443)

\[
\langle n| H_f | n - 4 \rangle^{(0)} = \frac{1}{n! (n-4)!} \left\{ \frac{\lambda \varphi}{2 \sqrt{2(2\pi)^D}} \sum_{P_{ij}(n-4)} \prod_{k=1}^{n-4} \Delta(p_{ik} - p'_{jk}) \right. \\
\times \delta(p_{3(n-2)} + p_{i(n-1)} + p_{in}) \times [f(p_{3(n-2)}) f(p_{i(n-1)}) f(p_{in})]^{-\frac{1}{2}}.
\]

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ordering process beforehand [See Appendix C.].

Here, the index \( i_k \in \{1, 2, \cdots, n\} \) with \( k = 1, 2, \cdots, n \) corresponds to \( \{n\}^{0)} \) and \( j_k \in \{1, 2, \cdots, n'\} \) with \( k = 1, 2, \cdots, n' \) to \( (0)\{n'\} \). \( P_{ij}(l) \) represents a given permutation of \( l \) momenta \( p_i, p_2, \cdots, p_l \) paired respectively with \( p'_j, p'_j, \cdots, p'_j \), and \( \sum_{i,j(l)} \) is over all different \( P_{ij}(l) \).s. For any \( P_{ij}(l), i_1, i_2, \cdots, i_l \) are different from one another, and so are \( j_1, j_2, \cdots, j_l \).

**Problem** Prove Eqs.(440)∼(444). For the calculation, it is much more convenient to carry out the normal ordering process beforehand [See Appendix C.].

Employing the above matrix elements, a straightforward, yet lengthy calculation according to Eq.(437) gives the effective potential of the \( \lambda \phi^4 \) field theory up to the third order as

\[
V^{iii}(\varphi) = \frac{E_0^{iii}}{(2\pi)^D\delta(0)} = V_G(\varphi) - \frac{1}{2}\lambda \varphi^2(\mu^2 - \frac{\lambda}{3})^2 - \frac{A \lambda^2}{48 \mu^4 - 2D \varphi^2} - \frac{B \lambda^2}{384 \mu^6 - 3D} + \frac{A + A_1 + A_2 \lambda^2}{48 \mu^6 - 2D \varphi^2(\mu^2 - \frac{\lambda}{3})^2} + \frac{2B_1 + B_2 \lambda^3}{128 \mu^6 - 3D \varphi^2} + \frac{C \lambda^3}{512 \mu^8 - 4D}
\]

with

\[
A = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}[f_1(x)f_1(y)f_1(x + y) - 1]f_1(x) + f_1(y) + f_1(x + y) - 1,
\]

\[
A_1 = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}[f_1(x)f_1(y)f_1(x + y) - 1][1 + f_1(x) + f_1(y) + f_1(x + y)] - 1,
\]

\[
A_2 = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}[f_1(x)f_1(y)f_1(x + y) - 1][f_1(x) + f_1(y) + f_1(x + y)] - 1
\times [1 + f_1(x) + f_1(y) + f_1(x + y)] - 1,
\]

\[
B = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}\frac{dz}{(2\pi)^D}[f_1(x)f_1(y)f_1(z)f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(z) + f_1(x + y + z)] - 1,
\]

\[
B_1 = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}\frac{dz}{(2\pi)^D}[f_1(x)f_1(y)f_1(z)f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(z) + f_1(x + y + z)] - 1,
\]

\[
B_2 = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}\frac{dz}{(2\pi)^D}[f_1(x)f_1(y)f_1(z)f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(z) + f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(z)] - 1,
\]

\[
C = \int \frac{dx}{(2\pi)^D}\frac{dy}{(2\pi)^D}\frac{dz}{(2\pi)^D}[f_1(x)f_1(y)f_1(z)f_1(x + y + z)f_1(x + y + \omega)] - 1
\times [f_1(x) + f_1(y) + f_1(z) + f_1(x + y + z)] - 1
\times [f_1(x) + f_1(y) + f_1(z) + f_1(x + y + z) + f_1(x + y + \omega)] - 1,
\]

and \( f_1(w) = \sqrt{1 + w^2} \). In Eq.(445), the second, third, and fourth terms are the second order corrections and the last three terms represent the third order corrections to the Gaussian effective potential.

**Problem.** Prove Eq.(445).

Quite surprisingly, we note that the second order result of Eq.(445) has an additional term, \(-\frac{1}{2}(1/\mu^2)\varphi^2[\mu^2 - (\lambda/3)\varphi^2]^2 \) which does not appear in other references[6]. In order to see the origin of this term, we note that the normal ordered form of \( H_I \) is given by [See Eq.(513).]

\[
H_I = \int_x \left\{ V_G(\varphi) + \varphi \left( \mu^2 - \frac{\lambda}{3} \varphi^2 \right) : (\varphi_x - \varphi) + \frac{\lambda}{3!} \varphi : (\varphi_x - \varphi)^3 + \frac{\lambda}{4!} : (\varphi^2 - \varphi)^4 : \right\},
\]

(446)
where : : denotes normal ordering. The additional term arises from the second term, which disappears if we choose $< \phi_x > = \varphi$. However, we note that this result is from the simple Gaussian calculation and does not include higher order contribution. Therefore, when higher order contribution is included self-consistently, it is expected that this term produces nonvanishing contribution.

It should be noted that in obtaining the above results, no diagrammatic considerations are made. Although the calculation maybe lengthy, it is rather straightforward and conceptually simple. We believe that the complexity in selecting relevant diagrams and corresponding symmetry factors have, so far, prevented obtaining the third order results using the operator and the function integral method based on the Heisenberg picture.

Before concluding this section, we compare the present results with the ones in the quantum mechanics, Eqs. (413) and (416). Quantum mechanics requires $D = 0$; $\varphi(x, y) \rightarrow x(t)$, $d^D p = 1$ and $(2\pi)^D = 1$. Also, we observe $\varphi = 0$ for anharmonic oscillator. Then, Eq. (445) is reduced to become

$$V_G(0) = \frac{1}{2} I_0(\mu^2) - \frac{1}{32} \lambda I_1^2(\mu^2) - \frac{B}{384 \mu^6} + \frac{C}{512 \mu^8}$$

$$= \frac{1}{2} \mu - \frac{3 b}{4 \mu^2} - \frac{3 b^2}{8 \mu^3} + \frac{27 b^3}{16 \mu^5} \quad (447)$$

Here, we used $I_0 = \mu$, $I_1 = \frac{1}{\mu}$, $B = \frac{1}{4}$, $C = \frac{1}{16}$ and $b = \lambda/46$. Eq. (447) can be directly compared with Eq. (413) and (416) and confirms the correctness of the present calculation.

The discussion in this section has been confined to the bosonic case. In order that the variational perturbation theory can be applied to condensed matter systems, it is necessary to develop Rayleigh-Schrödinger perturbation theory for fermionic functionals, which is a future subject.

### C. Optimized Perturbation Theory in The Functional Schrödinger Picture

In this section, we present an optimized perturbation theory in the functional Schrödinger picture with an external source $J_x \equiv J(\vec{x})$, is given by

$$H^I_0 = \int \frac{1}{2} \phi_x^2 + \frac{1}{2} (\partial_x \phi_x)^2 + \frac{1}{2} \mu^2 \phi_x^2$$

$$- J_x \phi_x - \frac{1}{2} f_{xx} + \frac{1}{2} \int y J_y h_{xy}^{-1} J_y \rangle, \quad (448)$$

where $f_{xy} \equiv (\sqrt{-\partial_x^2 + \mu^2}) \delta(x - y)$ with $\int \phi x f_{xy} \rightarrow \phi(x) \phi(y)$ and $h_{xy} \equiv (-\partial_x^2 + \mu^2) \delta(x - y)$ with $\int h_x h_y \rightarrow \delta(x - y)$. The last term is introduced to make $E_0^I[J] = 0$ in the presence of the external source term $-J_x \phi_x$ (Compare with Eq. (429)). The functional Schrödinger equation is readily solved using the power-counting method. The ground state wavefunctional is a Gaussian-type functional

$$|0; J^{(0)} \rangle = N \exp \left\{-\frac{1}{2} \int x y \left[ \phi_x - \int y h_{xz}^{-1} J_z \right] f_{xy} \left[ \phi_y - \int h_{yz}^{-1} J_z \right] \right\}, \quad (449)$$

where $N$ is the normalization constant. It should be noted that, here, $|0; J^{(0)} \rangle = \int z h_{xz}^{-1} J_z$ which, unlike in Section IV.B, is dependent on $x$. Then, accordingly, annihilation and creation operators can be constructed as

$$A_f(p; J) = \left( \frac{1}{2(2\pi)^D f(p)} \right)^{1/2} \int x e^{-ipx} [f(p)(\phi_x - \int h_{xz}^{-1} J_z) + i\pi_x], \quad (450)$$

and

$$A_f^*(p; J) = \left( \frac{1}{2(2\pi)^D f(p)} \right)^{1/2} \int x e^{ipx} [f(p)(\phi_x - \int h_{xz}^{-1} J_z) - i\pi_x], \quad (451)$$
with \([A_f(p; J), A_f^\dagger(p'; J)] = \delta(p' - p)\) and \(A_f(p; J)|0\rangle^{(0)} = 0\).

**Problem.** Show that \(H_0^J, \mu = \int d^Dp \int f(p)A_f^\dagger(p; J)A_f(p; J)\), where \(f(p) = \sqrt{p^2 + \mu^2}\).

The eigenwavefunctionals for exited states can be written as

\[
|n; J\rangle^{(0)} = \frac{1}{\sqrt{n!}} \prod_{i=1}^n A_f^\dagger(p_i; J)|0; J\rangle^{(0)}, \quad n = 1, 2, \ldots, \infty
\]

and the corresponding eingenergies are

\[
E_n^{(0)}[J] = \sum_{i=1}^n f(p_i).
\]

The eigenwavefunctionals \(|n; J\rangle^{(0)}\) and \(|0; J\rangle^{(0)}\) are orthogonal and normalized, \((0)\langle J; m|n; J\rangle^{(0)} = \delta_{mn} \prod_{k=1}^n \delta(p_k' - p_{ik})\). Here \(P_i(n)\) represents a permutation of the set \(\{i_k\} = \{1, 2, \ldots, n\}\) and the summation is over all \(P_i(n)\)'s. \(|n; J\rangle^{(0)}\) describe a n-particle state with the continuous momenta \(p_1, p_2, \ldots, p_n\). \(|0; J\rangle^{(0)}\) and \(|n; J\rangle^{(0)}\) with \(n = 1, 2, \ldots, \infty\) constitute the complete set for \(H_0^J, \mu\) and satisfy the closure \(|0; J\rangle^{(0)}\langle J; 0| + \sum_{n=1}^\infty \int d^Dp_1 d^Dp_2 \cdots d^Dp_n|n; J\rangle^{(0)}\langle J; n| = 1\).

We now introduce the model potential through the following scalar Lagrangian density

\[
\mathcal{L} = \frac{1}{2} \partial_\mu \phi_x \partial^\mu \phi_x - V(\phi_x).
\]

We assume that \(V(\phi_x) = \int \frac{d\Omega}{\sqrt{2\pi}} V(\Omega)e^{i\Omega x}\phi_x\), at least, in a sense of tempered distributions[3]. In fact, this assumption also applies to the previous section. For the system, Eq.(454), the time-independent functional Schrödinger equation in the presence of an external source of \(J_x\) is

\[
\left( H - \int_x J_x \phi_x \right) |\Psi_n\rangle = E_n^{(0)}[J]|\Psi_n\rangle
\]

with the Hamiltonian \(H = \int_x \left[ \frac{1}{2} \partial_x^2 + \frac{1}{4} (\partial_x \phi_x)^2 + V(\phi_x) \right]\).

Here, the eigenvalue \(E_n[J]\) is a functional of \(J_x\). For convenience in the calculation, we shift \(\phi_x \rightarrow \phi_x + \Phi\) (\(\Phi\) is a constant). Thus, the above equation is modified

\[
H(\phi_x + \Phi) - \int_x J_x(\phi_x + \Phi) \Psi_n[\phi_x + \Phi, J] = E_n[J; \Phi]\Psi_n[\phi_x + \Phi, J].
\]

This shift is made in the spirit of the background field method[4]. However, we will not go into the background field method.

Therefore, the above shift can be regarded as a just mathematical convenience. Normal ordering the Hamiltonian with respect to a normal-ordering mass \(M\)(See Appendix C.) and inserting a vanishing term \(\int_x \left[ \frac{1}{2} \mu^2 \phi_x^2 - \frac{1}{2} \mu^2 \phi_x^2 \right]\) with \(\mu\) an arbitrary mass parameter into the Hamiltonian, we have

\[
N_M \left[ H(\phi_x + \Phi) - \int_x J_x(\phi_x + \Phi) \right] = H_0^{J, \mu} + H_I^{J, \Phi} - C
\]

with

\[
H_0^{J, \mu} = \int_x \left\{ -\frac{1}{2} \mu^2 \phi_x^2 + N_M [V(\phi_x + \Phi)] \right\}
\]

and

\[
C = \int_x \left[ -\frac{1}{2} f_{xx} + \frac{1}{2} \int_y J_y h_{xy}^{-1} J_y + \frac{1}{2} I_0(M^2) - \frac{M^2}{4} I_1(M^2) + J_x \Phi \right].
\]
Here, the normal ordering of the shifted potential is given by[5]

\[
N_M[V(\phi_x + \Phi)] = \int \frac{d\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega)e^{\Omega(\phi_x + \Phi) + \frac{i}{\sqrt{\Omega}} I_1(M^2)}. \tag{460}
\]

For \( I_n(M^2) \), see Eq.(426). Since \( C \) is a constant, we can now carry out the Rayleigh-Schrödinger perturbation calculation only for \( H^\mu_1^\phi \). To check the order of the perturbation calculation, an index factor \( \delta \) will be attached to \( H^\mu_1^\phi \), so that Eq.(456) is modified to become

\[
[H^\mu_0^J + \delta H^\mu_1^J,\Phi_n][\phi_x + \Phi, J; \delta] = (E_n[J; \Phi, \delta] + C)\Psi_n[\phi_x + \Phi, J; \delta]. \tag{461}
\]

Now, we carry out the optimized perturbation expansion as explained in Section IV.A. Obviously, the zeroth-order approximation to \( E_0[J; \Phi, \delta], E_0^{(0)}[J; \Phi] \) satisfies

\[
E_0^{(0)}[J; \Phi] + C = E_0^{(0)} = 0. \tag{462}
\]

To the \( n \)th order of \( \delta \),

\[
E_0^{(0)}[J; \Phi] = \langle 0; J|0|H^\mu_1^\phi \left[ Q_n \frac{1}{H_0^{J,\mu} - E_0^{(0)}[J]} \left( E_0^{(1)}[J; \Phi] - H^\mu_1^\phi \right) \right]^{n-1}|0; J \rangle^{(0)}, \tag{463}
\]

with \( Q_n = \sum_{j \neq n}^{\infty} \int d^Dp_1 d^Dp_2 \cdots d^Dp_j |j; J \rangle^{(0)}(0)|J; j \rangle \).

Thus \( E_0[J; \Phi, \delta] = E_0^{(0)}[J; \Phi] + \sum_{n=1}^{\infty} \delta^n E_0^{(n)}[J; \Phi] \).

Before carrying out the perturbation calculation, we note that a Legendre transformation of \( E_0[J; \Phi, \delta] \) yields the static effective action[6]

\[
\Gamma_s[\varphi; \Phi, \delta] = -E_0[J; \Phi, \delta] - \int_x J_x \varphi_x. \tag{464}
\]

To calculate the effective potential, one can conveniently take \( \phi_x = \Phi \) to fix the arbitrary shifted parameter \( \Phi[n] \).

Then, the effective potential is given by

\[
\varphi(\Phi) \equiv -\frac{\Gamma_s[\varphi; \Phi, \delta]}{\int_x} \bigg|_{\varphi = \Phi, \delta = 1} \tag{465}
\]

When truncated at a given order of \( \delta \), \( \varphi(\Phi) \) will depend on \( \mu \). To obtain an approximated effective potential, one determines \( \mu \) according to the principle of minimal sensitivity explained in Section IV.A.

The matrix elements, which appear in Eq.(463), involve only Gaussian integrals except commutators of creation and annihilation operators and, thus, can be readily calculated as follows,

\[
(0|m|N_M[V(\phi_x + \Phi)][m]^{(0)}) = \frac{1}{\sqrt{n!m!}} \sum_{i=0}^{n} C_i^n C_{m-n+i}^{n-i}(n-i)! \left(2(2\pi)^D \right)^{-\frac{m-n+2i}{2}}
\times \left( \prod_{j=n-i+1}^{m} f(p_j) \prod_{k=n-i+1}^{m} f(p_k) \right) e^{i(\sum_{k=n-i+1}^{m} \sum_{j=n-i+1}^{m} p_{k} \cdot p_{l})} \prod_{l=1}^{n-i} (p_l^i - p_l)
\times \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2} V(m-n+2i) \left( \alpha \sqrt{\int_{-1}^{1} J^2} + \Phi + \int \frac{h_{xx}^{-1} J_x}{x} \right). \tag{466}
\]

with \( n \leq m \). In Eq.(466), \( V^k(z) \equiv \frac{d^k V(z)}{dz^k} \). For simplicity, in getting the above results, we have employed the permutation symmetry of momenta in Eq.(463) for various products of \( \delta \) functions. Note that matrix elements of \( \phi^2_x \) are special cases of Eq.(466). Substituting the above matrix elements into Eq.(463), one can obtain the first- and the second-order corrections to \( E_0[J; \delta] \) as

66
\begin{align}
E_0^{(1)}[J; \phi] &= \int_{x} \left\{ \frac{\mu^4}{2} \left[ \int_{z} h_{xx}^{-1} J_z^2 + \frac{1}{2} f_{xx}^{-1} \right] \right. \\
& \quad + \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi \right) \\
& \quad \left. + \int_{z} h_{xx}^{-1} J_z \right\} \\
(467)
\end{align}

and
\begin{align}
E_0^{(2)}[J; \phi] &= -\frac{\mu^4}{2} \int \frac{d^D p}{(2\pi)^D} \frac{1}{f^2(p)} \left[ \int_{xx} e^{ipx} h_{xx}^{-1} J_z \right] ^2 - \frac{\mu^4}{16} \int \frac{d^D p}{(2\pi)^D} \frac{1}{f^3(p)} \int_{x}
+ \mu^2 \int \frac{d^D p}{(2\pi)^D} \frac{1}{f^2(p)} \int_{xx} e^{-ipx} h_{xx}^{-1} J_z \int_{xx} e^{ipx} \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V}
\times V^{(1)} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi + \int_{z} h_{xx}^{-1} J_z \right)
+ \frac{\mu^2}{8} \int \frac{d^D p}{(2\pi)^D} \frac{1}{f^3(p)} \int_{xx} \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V^{(2)}} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi + \int_{z} h_{xx}^{-1} J_z \right)
- \sum_{j \neq 0} \frac{1}{|j|^2} \int \int \frac{d^D p_k}{(2\pi)^D} \frac{1}{f(p_k)(\sum_{k=1}^{j} f(p_k))}
\times \left[ \int_{x} e^{ip} \sum_{k=1}^{j} p_j \right] \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V^{(j)}} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi + \int_{z} h_{xx}^{-1} J_z \right)^2,
(468)
\end{align}

respectively. Here, "|⋯|" represents the absolute value.

Next, we extract the approximated effective potential for the system order by order.

At the zeroth order, \( E_0^{(0)}[J; \phi] = -C \) from Eq.(462), and so, taking \( \frac{\delta E_0^{(0)}[J; \phi]}{\delta J_x} = \int_{y} h_{xy}^{-1} J_y + \Phi = \varphi^{(0)}_x \) as \( \Phi \), one has \( J^{(0)} = 0 \). Consequently, the effective potential at the zeroth-order of \( \delta \) is
\begin{align}
\mathcal{V}^{(0)}(\Phi) = -\frac{\Gamma^{(0)}[\varphi; \Phi, \delta]}{\int_{x}} = \frac{1}{2} f_{xx} - \frac{1}{2} I_0(M^2) + \frac{M^2}{4} I_1(M^2).
(469)
\end{align}

Up to the first order (Hereafter, any Greek-number superscript, such as "I", "II", means “up to the order whose number is consistent with the Greek number”),
\begin{align}
E_0^{(1)}[\Phi, \delta; J] = E_0^{(0)}[J; \phi] + \delta E_0^{(1)}[J; \phi]
(470)
\end{align}

and \( \frac{\delta E_0^{(\Phi, \delta; J)}}{\delta J_x} = \varphi^{(0)}_x = \Phi \) yields
\begin{align}
\int_{y} h_{xy}^{-1} J_y + \delta \int_{y} h_{xy}^{-1} \left\{ \mu^2 \int_{z} h_{xx}^{-1} J_z \right. \\
- \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V^{(1)}} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi + \int_{z} h_{xx}^{-1} J_z \right) \right\} = 0.
(471)
\end{align}

When extracting the effective potential up to first order, Eqs.(464), (465) and (470) imply that only the \( J_x \) up to the first order, \( J^I \), is necessary. Owing to \( J^{(0)} = 0 \), it is enough to take \( J_x = 0 \) for the last term in the left-hand of Eq.(471). Thus, \( J^I \) can be solved from Eq.(471) as
\begin{align}
J^I = \delta \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V^{(1)}} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2)} + \Phi \right).
(472)
\end{align}

Even \( J^I \) will not be needed to get the effective potential up to the first order of \( \delta \), because there exists no linear, but the quadratic term of \( J_x \) in the zeroth-order term of \( (E_0^{(1)}[J; \Phi, \delta] - \int_{x} J_x \Phi) \) as shown in Eq.(459). In fact, to obtain
the effective potential up to the $n$th order, one need the approximated $J$ only up to the $(n - 1)$th order. Now, one can write down the effective potential up to the first order
\[
V_I(\Phi, \delta) = \frac{1}{2}[f_{xx} - I_0(M^2)] + \frac{1}{4}M^2 I_1(M^2) - \frac{1}{4}\mu^2 f_{xx}^{-1}
+ \delta \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2) + \Phi} \right).
\] (473)

Obviously, this result will yield nothing but the Gaussian effective potential[5].

Finally, we consider the second order. $\varphi_x = \varphi^I_x = \frac{\delta E^I_x[J, \Phi, \delta]}{\delta J}$ can be solved for $J^{II}$. In the present case, however, it is enough to use only $J^I$ for the effective potential. Substituting $J^I$ into Eq.(465), we obtain the effective potential for the system, Eq.(454), up to the second order as
\[
V^{II}(\Phi, \delta) = \frac{1}{2}[f_{xx} - I_0(M^2)] + \frac{1}{4}M^2 I_1(M^2) - \frac{1}{4}\mu^2 f_{xx}^{-1}
+ \delta \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2) + \Phi} \right)
+ \delta^2 \frac{\mu^2}{16} \int \frac{d^Dp}{(2\pi)^D} \frac{1}{f^{3}(p)} \left[ \mu^2 - 2 \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V(2)} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2) + \Phi} \right) \right]
- \delta^2 \sum_{j=2}^{\infty} \frac{1}{f(\sum_{k=1}^{j-1} p_k) \prod_{k=1}^{j-1} f(p_k)} \left[ \int_{-\infty}^{\infty} \frac{d\alpha}{\sqrt{\pi}} e^{-\alpha^2 V(2)} \left( \alpha \sqrt{f_{xx}^{-1} - I_1(M^2) + \Phi} \right) \right]^2,
\] (474)

where, one should take $\delta = 1$ after renormalizing $V^{II}(\Phi, \delta)$, and $\mu$ is determined from the stationary condition
\[
\frac{\partial V^{II}(\Phi)}{\partial \mu} = 0.
\] (475)

Here, $V^{II}(\Phi)$ is the effective potential after $V^{II}(\Phi, \delta)$ is renormalized. If Eq.(475) has no real solutions, $\mu$ can be fixed by $\frac{\partial^2 V^{II}(\Phi)}{\partial \mu^2} = 0$ as explained in Section IV.A. Note that in (1+1) dimensions, $\{ \frac{1}{2}[f_{xx} - I_0(M^2)] + \frac{1}{4}M^2 I_1(M^2) - \frac{1}{4}\mu^2 f_{xx}^{-1} \}$ and $[f_{xx}^{-1} - I_1(M^2)]$ in Eq.(474) with $\delta = 1$ is finite and, thus, for any (1+1)-dimensional theories which make the series in Eq.(474) finite, no renormalization procedure is needed. Similarly, employing Eq.(466), one can obtain higher order corrections from the Gaussian effective potential from Eq.(463).

As an example of the above optimized perturbation theory, we consider the potential,
\[
V(\phi_x) = \frac{1}{2}m^2 \phi_x^2 + \lambda \phi_x^4,
\] (476)

which was also studied with the variational perturbation technique.

Substituting Eq.(476) into Eq.(474), and noting that $\int_{-\infty}^{\infty} \alpha^{2n+2} e^{-\alpha^2} d\alpha = 0$ for $n = 1, 2, \cdots$ and $\int_{-\infty}^{\infty} \alpha^n e^{-\alpha^2} d\alpha = 2^{-n} \cdot 1 \cdot 3 \cdots (2n - 1)$ for $n = 0, 1, 2, \cdots$, one can easily obtain the effective potential for the system up to the second order
\[
V^{II}(\Phi, \delta) = \frac{1}{2}(f_{xx} - I_0(M^2)) + \frac{1}{4}M^2 I_1(M^2) + \delta(\frac{1}{2}m^2 \Phi^2 + \lambda \Phi^4 - \frac{1}{4}\mu^2 f_{xx}^{-1})
+ \delta^2 \frac{1}{16} \int \frac{d^Dp}{(2\pi)^D} \frac{1}{f^{3}(p)} \left[ m^2 - \mu^2 + 12\lambda \Phi^2 + 6\lambda(f_{xx}^{-1} - I_1(M^2)) \right]^2
- \delta^2 \frac{3}{2} \lambda \int \frac{d^Dp_1 d^Dp_2 d^Dp_3}{(2\pi)^{3D}} \frac{1}{f(p_1) f(p_2) f(p_1 + p_2)} \frac{1}{f(p_1) f(p_2) f(p_1 + p_2)} \times \int \frac{d^Dp_1 d^Dp_2 d^Dp_3}{(2\pi)^{3D}} \frac{1}{f(\sum_{k=1}^{3} p_k) \prod_{k=1}^{3} f(p_k)}.
\] (477)
Discarding terms with \( I_n(M^2)(n = 0, 1) \), the above result becomes identical to Eq.(2.36) in Ref.7(1990) in Section IV.A. This can be verified by carrying out integrations of \( I_n(\Omega)(n = 0, 1) \) and \( I^{(n)}(\Omega)(n = 2, 3, 4) \) in the above reference over one component of each Euclidean momentum. Using \( \mu \) fixed at the Gaussian approximation result for each order will simultaneously imply that up to each order, the vacuum expectation value of the field operator \( \phi_x \) is identical to that in the Gaussian approximation. If one chooses to do so, Eq.(477) will yield the second order result of the variational perturbation theory in Eq.(443).

Finally, we point out that taking \( \mu = m \) will lead to the conventional perturbation result on the effective potential.

V. SUMMARY AND FUTURE WORKS

In this lecture note, we have presented a theoretical schemes for study of many-particle systems based on the functional Schrödinger picture. In Chapter I, the basic conventional tools for many-body theory including the second quantization and the Green’s function method are briefly reviewed. In Chapter II, basic ingredients for functional Schrödinger picture are treated. They include functional calculus, Grassmann algebra, and the basic functional Schrödinger picture formalism. In Chapter III, functional Schrödinger picture formalism is applied to various condensed matter problems including electron gas, the Hubbard model, the BCS super conductivity, and dilute bose gas with the Bose-Einstein condensation. However, the formalism in the Chapter III is limited to the variational approximation and shown that it only leads to mean-field(Gaussian) results.

In Chapter IV, recent efforts to go beyond the Gaussian approximation are presented. Two methods, the variational and the optimized perturbation methods are first introduced with quantum mechanical languages. Then, they are discussed in depth using scalar field theory. As results of the study, the effective potential(the ground state energy) are given, up to the third order in the variational perturbation method and up to the second order in the optimized perturbation theory.

However, it should be noted that no concrete condensed matter models are discussed using above two methods. This is because the theory presented in Chapter IV is limited to bosonic case and, thus, cannot be applied to electronic systems such as electron gas and the Hubbard model. The work extending the variational and the optimized perturbation theories to fermionic system is currently under study. Only when this extension is successful, the functional Schrödinger picture approach to many-particle systems can be claimed truly useful.

VI. APPENDICES

A. Anticommutation Relations for Fermionic Field Theory

In order to obtain anticommutation relation for fermion field, it is necessary to start from the spinor field theory [1-3]. In general, the fermionic field theory can be studied through either non-hermitian or hermitian field operators. Here, we start with a non-hermitian field operators. It is an easy matter to see that the Dirac equation

\[
(i\gamma^\mu \partial_\mu - m)\psi = 0
\]  

(478)

follows from the Euler-Lagrange equation

\[
\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi)} \right) = 0,
\]  

(479)

if we choose

\[
\mathcal{L} = i\bar{\psi}\gamma^\mu \partial_\mu \psi - m\bar{\psi}\psi
\]

\[
= i\frac{1}{2} [\bar{\psi}\gamma^\mu (\partial_\mu \psi) - (\partial_\mu \bar{\psi})\gamma^\mu \psi] - m\bar{\psi}\psi,
\]  

(480)

where

\[
\bar{\psi} = \psi^\dagger \gamma^0
\]  

(481)

and

\[
A\partial^\mu B = \frac{1}{2} [A\partial^\mu B - (\partial^\mu A)B].
\]  

(482)
The $4 \times 4$ Dirac matrices are defined by the relation
\[
\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu},
\]
where the metric tensor $g^{\mu\nu}$ is given by
\[
g^{\mu\nu} = g_{\mu\nu} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix},
\]
in Minkowski space.

From $\mathcal{L}$, we find the canonical momentum field $\pi(x)$
\[
\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\psi^\dagger(x).
\]
This relation naturally leads into the anticommutation relations [1],
\[
\{ \psi_i(\vec{x}, t), \psi^\dagger_j(\vec{x}', t) \} = \delta^3(\vec{x} - \vec{x}')\delta_{ij},
\]
\[
\{ \psi_i(\vec{x}, t), \psi_j(\vec{x}', t) \} = 0 = \{ \psi^\dagger_i(\vec{x}, t), \psi^\dagger_j(\vec{x}', t) \}.
\]
Note that the above non-hermitian field operators $\psi$ and $\psi^\dagger$ are eigenstates of the charge operator.

Fermionic field theory can also be studied using hermitian field operators [2,3], $\psi^\dagger(\vec{x}) = \psi(\vec{x})$. Non-hermitian field operator can be constructed from the hermitian operators as follows
\[
\psi_{\text{charge eigenstate}} = \psi^\dagger_{\text{hermitian}} + i\psi^2_{\text{hermitian}},
\]
In such a case, the Lagrangian density is expressed as
\[
\mathcal{L} = \frac{i}{2} \psi^\alpha \partial_\mu \psi - \frac{1}{2} m\psi^2 \psi,
\]
where $\{ \alpha^i, \alpha^j \} = 2\delta^{ij}$, $\{ \alpha, \beta \} = 0, \beta^2 = 1, \alpha^0 = 1$.

In this case, we can readily show that
\[
\{ \psi_a(x), \psi_b(x') \}_{x^\mu = x'^\mu} = \delta_{ab}\delta(\vec{x} - \vec{x}').
\]
However, we note that the second half of Eq.(486) is not satisfied in this case.

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B. Dual for Gaussian Functionals

Here, we prove that the dual to a Gaussian functional is given by another Gaussian functional. Specifically we prove Eqs.(226)~(230).

For a real $\theta(\vec{x})$ basis, Eq.(223) show that the dual $\Psi[\theta]$ of $\Psi[\theta]$ is given by
\[ \Psi[\theta] = \int D\theta' \Psi'[\theta'] e^{\theta' \theta}, \] (490)

where \( \Psi[\theta] = e^{\frac{1}{2} \theta M \theta} \). First, the kernel \( M \) should have the antisymmetric property to have nonvanishing contribution,

\[ M^i = -M. \] (491)

This property can be proved easily as follows,

\[ \theta_i M_{ij} \theta_j = \theta_i (M_{ij})^t \theta_j = -\theta_j (M_{ij})^t \theta_i \\
= -\theta_j (M^j)^t \theta_i = -\theta_i (M_i)^j \theta_j. \]

Thus, we have \( M^i = -M \).

Upon substituting \( \Psi[\theta] = e^{\frac{1}{2} \theta M \theta} \) into Eq.(490), we have

\[ \int D\theta' e^{\frac{1}{2} \theta' M^i \theta' \theta}. \] (492)

Let \( \theta_i' = u_i + K_{ij} \theta_j \), then

\[ \theta' \theta = (u_i + K_{ij} \theta_j) \theta_i = u \theta - \theta K \theta \] (493)

\[ \int \frac{1}{2} \theta' M^i \theta' + \theta' \theta \\
= \frac{1}{2} u M^i u + \frac{1}{2} (u M^i K - \theta K M^i u) + \frac{1}{2} \theta \tilde{K} M^i K \theta. \] (494)

Here, we require \( M^i K - \tilde{M}^i K + 2 = 0 \).

Using \( \tilde{M} = -M \), we have

\[ 2M^i K = -2, \]

which gives

\[ K = -(M^i)^{-1}, \] (495)

or

\[ \tilde{K} = (M^i)^{-1}. \] (496)

Here, we used \( \tilde{K} = -K \), which is required for \( K \) as a new kernel.

Using \( K = -(M^i)^{-1} \), we have

\[ \int D\theta' e^{\frac{1}{2} \theta' M^i \theta' \theta} = \int D\theta e^{\frac{1}{2} u M^i u + \frac{1}{2} \theta \tilde{K} \theta} \\
= \det(M)^{1/2} e^{\frac{1}{2} \theta (M^i)^{-1} \theta}. \] (498)
which is Eq.(226). Here, we used Eq.(179).

Now, we continue to prove Eq.(228), where complex Grassmann variables are used.

For complex variables,

\[ u = \frac{1}{\sqrt{2}}(u_1 + iu_2), \quad u^\dagger = \frac{1}{\sqrt{2}}(u_1 - iu_2), \]  

(499)

and

\[ u_1 = \frac{1}{\sqrt{2}}(u + u^\dagger), \quad u_2 = \frac{1}{\sqrt{2i}}(u - u^\dagger). \]  

(500)

The dual vector for \( \Psi(u_1, u_2) = \langle u_1, u_2 | \Psi \rangle \) is given by

\[ \bar{\Psi}[u_1, u_2] = \int D\bar{u}D\bar{u}^\dagger e^{u_1 \bar{u}} e^{u_2 \bar{u}} \Psi^\dagger[\bar{u}_1, \bar{u}_2]. \]  

(501)

Now,

\[ \bar{u}_1 u_1 + \bar{u}_2 u_2 \]

\[ = \frac{1}{2}[(\bar{u} + \bar{u}^\dagger)(u + u^\dagger) - (\bar{u} - \bar{u}^\dagger)(u - u^\dagger)] \]

\[ = \bar{u}u^\dagger + \bar{u}^\dagger u = \bar{u}u - u^\dagger \bar{u}. \]  

(502)

Thus,

\[ \bar{\Psi}[u, u^\dagger] = \int D\bar{u}D\bar{u}^\dagger (\Psi|\bar{u}, \bar{u}^\dagger) e^{\bar{u}u - u^\dagger \bar{u}} \]  

(503)

which is Eq.(228).

When \( \Psi[u, u^\dagger] = e^{u^\dagger G_u} \), \( \Psi^\dagger[u, u^\dagger] = e^{u^\dagger G^\dagger u} \).

Thus, we have

\[ \bar{\Psi}[u, u^\dagger] = \int D\bar{u}D\bar{u}^\dagger e^{u^\dagger G_u \bar{u} + \bar{u}u - u^\dagger \bar{u}} \]

\[ = e^{u^\dagger (G^\dagger)^{-1} u} \int D\bar{u}D\bar{u}^\dagger e^{\bar{u}^\dagger - u^\dagger (G^\dagger)^{-1} G^\dagger (\bar{u} + (G^\dagger)^{-1} u)} \]

\[ = Ce^{u^\dagger G_u}, \]  

(504)

which is Eq.(230).

C. Normal-Ordering of \( H_I \)

A normal-ordered product of field operators is very convenient for calculation of the ground state energy (effective potential), because its expectation value vanishes identically. Therefore before carrying out calculations on matrix elements, Eqs.(438)\textasciitilde(442), it is necessary to normal order \( H_I \). \( \phi_x \) can be rewritten using Eq.(428),

\[ \phi_x = \varphi + \int \frac{d^D p}{(2\pi)^{D/2}} \frac{1}{(2f(p))^{1/2}} [A_f(p)e^{ipx} + A_f^\dagger(p)e^{-ipx}] \]

\[ = \varphi + \varphi^- + \varphi^+, \]  

(505)

where

\[ \varphi^- = \int \frac{d^D p}{(2\pi)^{D/2}} \frac{1}{(2f(p))^{1/2}} A_f(p)e^{ipx}, \]

\[ \varphi^+ = \int \frac{d^D p}{(2\pi)^{D/2}} \frac{1}{(2f(p))^{1/2}} A_f^\dagger(p)e^{-ipx}. \]  

(506)
Using the above expressions, we readily obtain

\[ [\varphi^-, \varphi^+] = \int \frac{d^Dp}{(2\pi)^D} \frac{1}{2f(p)} = \frac{1}{2} I_1(\mu^2), \]  
\[ \phi_x - \varphi = : (\phi_x - \varphi) :, \]  
\[ (\phi_x - \varphi)^2 = : (\phi_x - \varphi)^2 : + \frac{1}{2} I_1(\mu^2), \]  
\[ (\phi_x - \varphi)^3 = : (\phi_x - \varphi)^3 : + 3[\varphi^-, \varphi^+](\phi_x - \varphi), \]  
\[ (\phi_x - \varphi)^4 = : (\phi_x - \varphi)^4 : + 6[\varphi^-, \varphi^+]: (\phi_x - \varphi) : + 3[\varphi^-, \varphi^+]^2 \]  

\( H_I \) is now rewritten

\[ H_I = \int_x \left\{ \frac{1}{2} m^2 \phi_x^2 - \frac{1}{2} \mu^2 (\phi_x - \varphi)^2 + \frac{\lambda}{4!} \phi_x^4 \right\} 
\quad + \frac{1}{2} \int f_0(\mu^2) \]  
\[ = \int_x \left\{ \frac{1}{2} m^2 \phi_x^2 + \frac{\lambda}{4!} + \frac{1}{2} f_0(\mu^2) 
\quad + (\phi_x - \varphi) \varphi \left[ \frac{\lambda}{6} \phi_x^2 + m^2 \right] 
\quad + (\phi_x - \varphi)^2 \left[ \frac{1}{2} m^2 - \frac{1}{2} \mu^2 + \frac{\lambda}{4} \phi_x^2 \right] 
\quad + \frac{\lambda}{6} \varphi (\phi_x - \varphi)^3 + \frac{\lambda}{4!} (\phi_x - \varphi)^4 \right\} \]  

Substituting Eqs.(507)~(511) into (512), we obtain

\[ H_I = \int_x \left\{ \mathcal{V}_G(\varphi) + (\phi_x - \varphi) \varphi (\mu^2 - \frac{\lambda}{3} \phi_x^2) 
\quad + \frac{\lambda}{6} \varphi : (\phi_x - \varphi)^3 : + \frac{\lambda}{4!} : (\phi_x - \varphi)^4 : \right\}, \]  

which is Eq.(446).

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