A rigorous derivation of the density functional in the Hohenberg-Kohn theory is presented. With no assumption regarding the magnitude of the electric coupling constant $e^2$ (or correlation), this work provides a firm basis for first-principles calculations. Using the auxiliary field method, in which $e^2$ need not be small, we show that the bosonic loop expansion of the exchange-correlation functional can be re-organized so as to be expressed entirely in terms of the Kohn-Sham single-particle orbitals and energies. The excitations of the many-particle system can be obtained within the same formalism. We also explicitly demonstrate at zero-temperature the single-particle limit, the weak-coupling limit of the energy functional, and its application to homogeneous electron gas.

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I. INTRODUCTION

At low energy scale, interactions among electrons largely determine the structure, phases, and stability of matter. Although this fact is well known, pragmatic first-principles/quantum-mechanical calculations to determine various properties of many-electron systems are often hindered by two factors. First, in most condensed matter systems, the typical interaction energy between electrons (the electric coupling constant $e^2$ divided by average electron-electron separation) is often larger than the typical kinetic/Fermi energy of electrons. The result is that a perturbative expansion using $e^2$ as the expansion parameter may not be fruitful. This is particularly true for strongly correlated systems. Second, there is an exponential increase in the number of degrees of freedom as the number of electrons involved increases. When the number of electrons becomes large, according to Kohn,\textsuperscript{1} calculations based on constructing many-electron wave functions soon lose accuracy and will be stopped by an “exponential wall”. It is thus imperative to have a method that goes beyond the conventional perturbative scheme using $e^2$ as the expansion parameter and whose computational complexity does not grow exponentially with the number of electrons involved.

In 1964, Hohenberg and Kohn\textsuperscript{2} proved a theorem stating that there exists a unique description of the ground state of a many-body system in terms of the expectation value of
the particle-density operator. This theorem started the development of the density functional theory (DFT), which offers a possibility of finding the ground state energy $E_g$ by minimizing the energy functional $E_v$ that depends on the charge density $n$ only:

$$E_g = \min_n E_v [n],$$  \hspace{1cm} (1)

with $v$ representing the external one-particle potential of the system. The electronic density $n_g$, which minimizes the energy functional $E_v[n]$, is the ground state electronic density. Hohenberg and Kohn showed that the energy functional $E_v[n]$ can be decomposed into

$$E_v [n] = \int d\mathbf{r} v(\mathbf{r}) n(\mathbf{r}) + F[n],$$  \hspace{1cm} (2)

with $F[n]$ being a universal functional independent of the external potential $v$. Mermin\(^3\) extended this theorem to finite temperature with $E_v$ in (2) replaced by the grand potential, and $F[n]$ replaced by a different universal functional. The electron density $n_T$, minimizing the grand potential functional, corresponds to the electron density at thermal equilibrium.

To make practical use of the DFT, however, a recipe to compute the energy functional is needed. Kohn and Sham\(^4\) proposed a decomposition scheme, aiming to express the energy functional $E_v[n]$ via an auxiliary, noninteracting system that yields a particle density identical to that of the physical ground state. For a typical nonrelativistic many-fermion system, described by the Hamiltonian

$$\hat{H} = \int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x}) \left( -\frac{1}{2m} \nabla^2 + v_{\text{ion}}(\mathbf{x}) - \mu \right) \hat{\psi}(\mathbf{x})$$
$$+\frac{e^2}{2} \int \int \frac{\hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{y}) \hat{\psi}(\mathbf{y}) \hat{\psi}(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y},$$  \hspace{1cm} (3)

the Kohn-Sham decomposition takes the form

$$E_v [n] = T_0 [n] + \int v_{\text{ion}}(\mathbf{x}) n(\mathbf{x}) d\mathbf{x} - \mu N_e$$
$$+\frac{e^2}{2} \int \int \frac{n(\mathbf{x}) n(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} + E_{xc} [n],$$  \hspace{1cm} (4)

where the chemical potential $\mu$ is introduced to ensure $\int n(\mathbf{x}) d\mathbf{x} = N_e$, with $N_e$ being the number of electrons. Here $T_0 [n]$ is the kinetic energy of an auxiliary system of noninteracting fermions that yields the electron density $n(\mathbf{x})$, and the density functional $E_{xc} [n]$ is the so-called exchange-correlation energy functional. Given $E_{xc} [n]$ and provided that it is
differentiable, one may minimize the functional (4) to arrive at the familiar Kohn-Sham
single-particle equations\(^5\)

\[
\left(-\frac{\nabla^2}{2m} + v_{\text{ion}}(x) + \int \frac{n(y)}{|x-y|}dy + \frac{\delta E_{xc}[n]}{\delta n(x)} - \mu\right)\psi_i(x) = \epsilon_i \psi_i(x) \tag{5}
\]

\[
n(x) = \sum_{i=1}^{N_e} \psi_i^*(x) \psi_i(x). \tag{6}
\]

All of the many-particle complexity is now completely hidden in the exchange-correlation
energy functional.

Although \(T_0[n] + E_{xc}[n]\) is universal,\(^2\) there exists no simple means thus far to obtain
it. As a consequence, various \textit{ad hoc} exchange-correlation density functionals have been
suggested/needed to yield acceptable results in different settings\(^6\textsuperscript{–}^9\) when employing the
Kohn-Sham scheme. Limitations of these \textit{approximate} functionals have been discussed.\(^10,11\)

Some of the failures while using \textit{ad hoc} density functionals can be attributed to misuse of the
density-functional theory. For example, it is sometimes neglected that the electron density
\(n(x)\) achievable via introduction of a source potential must obey \(\int n(x)dx = N_e\) and does not
cover the functional space \(\{n(x) \geq 0\}\), a problem also known as the \(\nu\)-representability.\(^12,13\)

As pointed out in reference 15, neglecting these constraints may lead to conclusions\(^16\) that
are not always valid.

The main objective of the DFT is to describe a many-body system in terms of the
expectation value of the particle density operator. In fact, the use of the expectation value
of a suitable operator to describe a many-body system via Legendre transformation, first
introduced into quantum field theory by Jona-Lasinio,\(^17\) is known as the effective action
formalism. As the temperature approaches zero, the effective potential becomes the ground
state energy. This connection suggests that effective action formalism can be used to achieve
the general goal of the DFT: describing a many-particle system in terms of the expectation
value of the density operator. A number of publications\(^18\textsuperscript{–}21\) showed that at zero temperature
the effective action plus \(\mu N_e\) is the ground state energy, linking effective action to the DFT.

Existing methods of expressing DFT via effective action formalism can be classified
roughly into two categories: either (a) by introducing an auxiliary field or (b) by using
a perturbative scheme assuming the electric coupling as a small parameter. The former
category includes a method developed by Fukuda \textit{et al.}\(^18\) and that developed by Polonyi
and Sailer.\(^21\) The latter scheme is used by Valiev and Fernando\(^20\) and by Fukuda \textit{et al.}\(^19\).
The strengths of the auxiliary field approach often come from the simplicity of the effective action expression and from the fact that in principle each term already includes infinitely many Feynman diagrams. However, as pointed out by Fukuda et al., the auxiliary field approach seems to lack a direct connection to the Kohn-Sham scheme. Valiev and Fernando introduced an auxiliary field to compute the exchange-correlation energy. However, the source term they introduced is coupled to the auxiliary field instead of the electron density operator. Furthermore, as pointed out by the authors themselves, an artificial decomposition of the auxiliary field into a sum of the Hartree potential, the exchange correlation potential, and the remaining fluctuations is needed to write down the exchange-correlation energy.

There are two advantages when one uses electric coupling in the perturbative (diagrammatic) expansion without introducing an auxiliary field. First, under the effective action formalism of this type, a direct connection to the Kohn-Sham scheme can be made. Second, there exist other $e^2$ expansion-based developments that can be used to obtain $T_0[n] + E_{xc}[n]$, the universal density functional (UDF). For example, with increasingly complex incorporation of KS orbitals and energies at each order of $e^2$, Görling and Levy wrote $E_g$ as a perturbation series. Employing the Luttinger-Ward method that uses $e^2$ as the perturbative expansion parameter to calculate electron self-energy, Sham and Schlüter expressed $E_{xc}$ as a rather convoluted implicit functional of electron density. As shown by Tokatly and Pankratov, these methods mentioned above can be expressed diagrammatically. However, the problem associated with $e^2$ based expansion remains. As described in reference 29, the expansion using $e^2$ is only good when $e^2$ is very small. Whether one can treat $e^2$ as a small parameter or not depends on the kinetic/Fermi energy of the electrons and the strength as well as the magnitude of variation of the single-particle potential involved. As a matter of fact, the success in employing the GW approximation indicates that not treating $e^2$ as small may lead to results closer to experimental outcomes.

In principle, the problem associated with assuming $e^2$ small can be tamed by summing an infinite subset of Feynman diagrams. However, as pointed out by Hedin, it is nontrivial to devise a systematic resummation scheme where each new term is free from divergence even if $e^2 \gg 1$ and for which the sum of the new terms, each containing an infinitely many Feynman diagrams, accounts completely and non-redundantly for all conventional $e^2$ expansion diagrams. In this paper, without assuming $e^2$ small we develop an auxiliary field
method that makes a direct connection to the Kohn-Sham scheme and at the same time provides equivalently a systematic resummation scheme.

A commonly used approximation for the density functional is the so-called local density approximation (LDA) in which the exchange-correlation energy is approximated by a linear functional $E_{xc}[n] \approx \int d\mathbf{r} \, n(\mathbf{r}) \, e_{xc}(n(\mathbf{r}))$, where $e_{xc}(n)$ is a function of the local density (not a functional of the density profile). See reference 1 for a nontechnical review. This approximation ignores the nonlocal effect of the density profile, i.e., it assumes that $\delta E_{xc}[n]/\delta n(\mathbf{r})$ only depends on the value of $n$ at $\mathbf{r}$ but not on the density $n(\mathbf{r}') \neq \mathbf{r}$ at locations other than $\mathbf{r}$. To complement the LDA by incorporating nonlocal density dependence, Polonyi and Sailer\textsuperscript{21} proposed the $l$-local approximation for the density functional, based on an idea very similar to the cluster expansion in statistical physics. Using this method to obtain explicit expressions for the approximate functional with $l \geq 3$, however, becomes increasingly challenging due to the necessity of going through the coupling constant integration as required by the Hellmann-Feynman theorem\textsuperscript{32,33}

Another route to developing density functionals is via the so-called optimal effective potential (OEP) methods\textsuperscript{34–36}. These methods typically start by introducing \textit{a priori} an approximate, explicitly\textsuperscript{37} orbital-dependent functional. (The approximate functional can be either Hartree-Fock or a more elaborated form.) The procedure then continues with a minimization of the functional via varying single-particle KS orbitals and associated energies. Recently, the definition of OEP methods has been generalized\textsuperscript{38,39} to include functionals dependent on either Green’s function, the self-energy, or the KS potential. Since our effective action based functional is based on self-consistently obtaining the KS potential, it falls exactly in the latter category. The generalized definition of OEP methods is probably becoming the standard definition now. A general characteristic of OEP methods is that the functional arguments –be they KS orbitals/energies, Green’s functions, self energies, or KS potentials– are obtained via self-consistent procedure. Therefore, even with correction terms derived from perturbative expansion, the self-consistency condition for OEP methods distinguishes them from regular perturbative methods. The important matter here is whether an OEP functional can be systematically improved and possibly be asymptotically exact or not.

Based on effective action formalism, the OEP functional proposed here is asymptotically exact and can be shown to give rise to the desired UDF. Containing all the $l$-local interaction
vertices, our method can provide equivalent approximate functionals for \( l \geq 3 \) without going through the Hellmann-Feynman theorem. Since we focus on describing the proposed approach in a manner as self-contained as possible, we have included a non-negligible amount of standard materials available in existing literature/textbooks while keeping only a small portion of the existing literature that we deem closely related to the present manuscript. Readers interested in gaining a broad background are referred to references 10 and 40–43 for reviews on the extensive body of literature in the DFT and related many-body approaches. Expert readers should note that new developments are mainly provided in sections IIIB-D. Although section IV and end of section V also contain some useful developments, they typically rederive/re-express known results within our framework and/or provide contrast with existing methods. Section VI contains some insight of problems shared in post Hartree corrections.

This paper is otherwise organized as follows. We first establish the notation in section II, followed by the development of the general formalism in section III. The purpose of subsection III G is to provide a computational recipe and to give some perspectives on computational complexity: no novelty is claimed here. In section IV, we discuss a number of case studies: the emergence of the universal functional \( F[n] \) in Eq. (2) at arbitrary temperature, the behavior of the effective potential and the single electron limit at zero temperature, the screening effect, as well as the case of homogeneous electron gas. In section V, we then discuss the excitations of the system, and make comparisons with existing studies along this direction. An alternative formalism to obtain the effective action is then discussed in section VI. We conclude with the discussion and future directions section, in which we also provide some more relations/comparisons to other methods as well as some technical remarks.

II. NOTATION

Let us first define useful notation to lighten the exposition of the mathematical formulas. We define a three dimensional integral contraction by a dot

\[
\mathbf{a} \cdot \mathbf{b} \equiv \int d\mathbf{x} \; a(\mathbf{x}) \; b(\mathbf{x})
\]

where \( a \) and \( b \) may be single or composite fields. That is, with \( m \geq 1 \) and \( n \geq 1 \), \( a(\mathbf{x}) \) and
\( b(\mathbf{x}) \) may represent

\[
a(\mathbf{x}) = a_1(\mathbf{x}) \ldots a_m(\mathbf{x}) ,
\]
and

\[
b(\mathbf{x}) = b_1(\mathbf{x}) \ldots b_n(\mathbf{x}) .
\]

Similarly, with a kernel \( M \), we may define

\[
a \cdot b \cdot M = a \cdot M \cdot b = M \cdot a \cdot b = \int \int dx dy \ M(\mathbf{x}, \mathbf{y}) a(\mathbf{x}) b(\mathbf{y}) .
\]

Note that in all expressions \( a \) is in front of \( b \), and that is important when there are Grassmann variables involved. Evidently, one may generalize this notation to include higher order kernels. That is, one may have

\[
a \cdot b \cdot c \cdot M = a \cdot b \cdot M \cdot c = a \cdot M \cdot b \cdot c = M \cdot a \cdot b \cdot c = \int \int \int dx dy dz \ M(\mathbf{x}, \mathbf{y}, \mathbf{z}) a(\mathbf{x}) b(\mathbf{y}) c(\mathbf{z}) .
\]

We define the four dimensional integral contraction by an open circle

\[
a \circ b \equiv \int dx \ a(x) b(x) ,
\]

with

\[
x = (\tau, \mathbf{x}) ,
\]

\[
0 \leq \tau \leq \beta ,
\]

and

\[
\int dx = \int_0^\beta d\tau \int d\mathbf{x} .
\]

Again, \( a \) and \( b \) may be single or composite fields. That is, with \( m \geq 1 \) and \( n \geq 1 \), \( a(x) \) and \( b(x) \) may represent

\[
a(x) = a_1(x) \ldots a_m(x) ,
\]
and

\[
b(x) = b_1(x) \ldots b_n(x) .
\]

Similarly, we may define

\[
a \circ b \circ M = a \circ M \circ b = M \circ a \circ b = \int \int dx dy \ M(x, y) a(x) b(y) ,
\]

and

\[
M \circ a \circ b \circ c = \int \int \int dx dy dz \ M(x, y, z) a(x) b(y) c(z) .
\]
III. RELEVANT FORMULATION

Consider the following generic fermionic Hamiltonian with \( s \) denoting the spins
\[
\hat{H}[\hat{\psi}^\dagger, \hat{\psi}] = \sum_s \int dx \hat{\psi}^\dagger_s(x) \left( -\frac{\nabla^2}{2m} + v_{\text{ion}}(x, s) - \mu_s \right) \hat{\psi}_s(x) \\
+ \frac{1}{2} \sum_{s,s'} \int \int \hat{\psi}^\dagger_s(x) \hat{\psi}^\dagger_{s'}(y) U(x - y) \hat{\psi}_{s'}(y) \hat{\psi}_s(x) dx dy, \tag{7}
\]
\[
= \sum_s \int dx \hat{\psi}^\dagger_s(x) \left( -\frac{\nabla^2}{2m} + v_{\text{ion}}(x, s) - \frac{U(0)}{2} - \mu_s \right) \hat{\psi}_s(x) \\
+ \frac{1}{2} \int \int \left( \sum_s \hat{\psi}^\dagger_s(x) \hat{\psi}_s(x) \right) U(x - y) \left( \sum_s \hat{\psi}^\dagger_s(y) \hat{\psi}_s(y) \right) \\
= \sum_s \int dx \hat{\psi}^\dagger_s(x) \left( -\frac{\nabla^2}{2m} + v_{\text{ion}}(x, s) - \frac{U(0)}{2} - \mu_s \right) \hat{\psi}_s(x) \\
+ \frac{1}{2} \left( \sum_s \hat{\psi}^\dagger_s \hat{\psi}_s \right) U \left( \sum_s \hat{\psi}^\dagger_s \hat{\psi}_s \right). \tag{8}
\]

From this point on, we absorb \(-\frac{U(0)}{2}\) into \(v_{\text{ion}}(x, s)\).

To lighten the notation, we will first ignore the spin degree of freedom but will comment on its effect when clarifications are needed. Let \( \beta \) be the inverse temperature. The partition function \( Z \equiv \text{Tr}[e^{-\beta \hat{H}}] \) contains all the information one needs. To probe the system in terms of the particle density, one often introduces a classical source term \( J(x) \) coupled to \( \hat{\psi}^\dagger(x) \hat{\psi}(x) \). The partition function now becomes a functional of the source \( J \), and we write
\[
Z[J] \Rightarrow e^{-\beta W[J]} = \text{Tr} \left[ e^{-\beta [\hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi})]} \right].
\]

It is easy to show that
\[
\frac{\delta W[J]}{\delta J(x)} = \frac{\text{Tr} \left[ \hat{\psi}^\dagger(x) \hat{\psi}(x) e^{-\beta [\hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi})]} \right]}{Z[J]} = \langle \hat{n}(x) \rangle_J \equiv n_J(x) \tag{9}
\]
Eq. (9) expresses \( n \) in terms of \( J \), or more generally expresses \( n_s \) (charge density of spin \( s \)) in terms of sources \( J_s \) of all spins. Given \( v_{\text{ion}}(x) \) and \( U(x - y) \) (for Coulomb interaction \( U(x - y) = \frac{e^2}{|x - y|} \)), each time-independent configuration of \( \{J(x)\} \) generates a time-independent charge density distribution \( \{n(x)\} \). However, it is not guaranteed that every configuration of \( \{n(x)\} \) is reachable by varying \( J \). The functional variation on \( \{n(x)\} \) is thus limited to the subset of \( \{n(x)\} \) reachable by considering various \( \{J(x)\} \). In this stationary case, the effective action \( \Gamma[n] \) is defined as the Legendre transformation of \( W[J] \),
\[
\Gamma[n,J] = W[J] - J \cdot n_J,
\]
where the subscript \( J \) indicates that the domain of \( \Gamma[n] \) is the set of density profiles reachable by varying \( J \), or the so-called \( \nu \)-representable\(^{12-14} \) densities.

We now show the equivalence between the effective action and the energy functional \( E_\nu[n] \) in (1). Since
\[
e^{-\beta W[J]} = \text{Tr} \left[ e^{-\beta [\hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi})]} \right],
\]
at zero temperature limit \( W[J] \) is simply the ground state energy corresponding to the Hamiltonian \( \hat{H}_J \equiv \hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi}) \),
\[
\hat{H}_J = \int dx \hat{\psi}^\dagger(x) \left[ -\frac{\hbar^2}{2m} \nabla^2 + (v_{\text{ion}}(x) + J(x)) - \mu \right] \hat{\psi}(x) \\
+ \frac{e^2}{2} \int \int \frac{\hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y) \hat{\psi}(y) \hat{\psi}(x)}{|x - y|} dx dy, \tag{10}
\]
while the electron density \( n_J(x) \) is obtained by integrating all but one spatial variable of the ground state wave function corresponding to \( \hat{H}_J \). Evidently, when \( J = 0 \), \( \Gamma[n] |_{n=n_g} = W[J] |_{J=0} = E_g \) where \( E_g \) stands for the ground state energy corresponding to \( \hat{H} \) and \( n_g \) represents the electron density at the physical \( (J = 0) \) ground state. When \( J \neq 0 \) the corresponding electronic density \( n[J \neq 0] \) is different from \( n_g \), and \( \Gamma[n,J] \) represents the expectation value of the original Hamiltonian \( \hat{H} \), calculated using the ground state wave function corresponding to a different Hamiltonian, namely, \( \hat{H} + J \cdot (\hat{\psi}^\dagger \hat{\psi}) \). Since \( n_J \neq n_g \), \( \Gamma[n] |_{n=n[J]} > \Gamma[n] |_{n=n_g} \) by the definition of the ground state. This means that \( \Gamma[n] \) reaches its minimum at \( n_g \), and various other electron density profiles \( n[J] \) producible by introducing different \( J \) form the domain of argument for \( \Gamma[n] \). Thus \( \Gamma[n] \) has all the properties attributed to the energy functional \( E_\nu[n] \) in (1). Since the theorem of Hohenberg and Kohn states that this functional is unique, it must be equal to \( E_\nu[n] \). As we will show in section IV B, \( \Gamma[n] \) can be decomposed exactly in the same manner as in (4).

Within allowable configurations of \( \{n(x)\} \), if one is able to invert the relation (9) to obtain, say, \( J[n] \), then the explicit construction of the effective action becomes possible. In principle, this can be done via an inversion method. Using this scheme, Valiev and Fernando\(^{20} \) proposed a perturbative expansion in terms of \( e^2 \) to express the exchange-correlation functional as a sum of an infinite number of Feynman diagrams and the diagrams’ derivatives with respect to the Kohn-Sham potential.

We approach this problem from two different routes, both involving the introduction of an auxiliary field.\(^{18,21} \) As will be described in section VI A, the second route does not
have an exact correspondence to the Kohn-Sham decomposition, but has the advantage that the correction terms may be obtained without further functional derivatives. The first route, as will be described later in this section, gives a recipe equivalent to the Kohn-Sham decomposition, together with a way to calculate the exchange-correlation functional in a self-consistent manner.

This auxiliary field approach was pursued in an earlier publication, but there it was concluded that it seems infeasible to make a direct connection to the Kohn-Sham scheme. Using the inversion method, we show explicitly how the connection to the Kohn-Sham scheme can be made. One advantage of the auxiliary field method is that each Feynman diagram here corresponds to the sum of infinitely many Feynman diagrams in standard perturbative field theory calculations such as used in reference 20. Subsections III A through III F detail the proposed approach. Subsection III G lays out the computational procedure to give some perspectives on computational complexity.

A. Path Integral

To accommodate a time-dependent probe and to deal with excitations, we express $Z$ as a path integral over Grassmann fields and we have

$$e^{-\beta W[J]} \equiv Z[J] = \int D\psi^\dagger D\psi \exp \left\{ -S[\psi^\dagger, \psi] - J_\circ(\psi^\dagger \psi) \right\},$$  

with

$$S[\psi^\dagger, \psi] = \psi^\dagger \circ G^{-1}_0 \circ \psi + \frac{1}{2} \left( \psi^\dagger \psi \right) \circ U_\circ \left( \psi^\dagger \psi \right),$$

where $\psi^{(t)}$ denote Grassmann fields with $\psi^{(t)}(\beta, \mathbf{x}) = -\psi^{(t)}(0, \mathbf{x})$, and

$$G^{-1}_0(x, x') \equiv \langle x | G^{-1}_0 | x' \rangle = \langle x | x' \rangle = \left( \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(\mathbf{x}) - \mu \right) \delta(x - x'),$$

and

$$U(x, x') = U(x - x') = \delta(\tau - \tau') U(\mathbf{x} - \mathbf{x}'),$$

$$\delta(x - x') = \delta(\tau - \tau') \delta(\mathbf{x} - \mathbf{x'}).$$

For a time-independent source, $J(\tau, \mathbf{x}) = J(\mathbf{x})$ (i.e., $J_\circ(\psi^\dagger \psi) = \int dx J(\mathbf{x}) \psi^\dagger(x) \psi(x)$). For time-dependent probes, $J(x)$ becomes $\tau$-dependent, and $J_\circ(\psi^\dagger \psi) = \int dx J(x) \psi^\dagger(x) \psi(x)$. It
is straightforward to verify that

$$\frac{\delta (\beta W [J])}{\delta J(x)} = \langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle_J = \langle \hat{n}(x) \rangle_J \equiv n_J(x).$$

(13)

This quantity is important for later development.

The quartic fermionic interaction in (12) can be disentangled via introducing an auxiliary real field $\phi$ with $D\phi \equiv \prod_x \frac{d\phi(x)}{\sqrt{2\pi}}$. Note that

$$1 = \sqrt{\det U} \int D\phi \ e^{-\frac{1}{2} \phi \circ U \circ \phi} = \sqrt{\det U} \int D\phi \ e^{-\frac{1}{2} (\phi + Y) \circ U \circ (\phi + Y)},$$

(14)

for an arbitrary field $Y$, provided that $Y(x)$ and $Y(x')$ always commute. Since $U(x,x')$ is diagonal in $\tau$, it suffices that they commute at equal Euclidean times. Let us set $Y(x) = i\hat{\psi}^\dagger(x) \hat{\psi}(x)$, which satisfies the equal time commutation requirement, and then multiply (11) by (14) to obtain

$$Z[J] = \int D\phi D\psi^\dagger D\psi \ \exp \left\{ - S[J,\psi^\dagger,\psi] \right\},$$

(15)

where

$$S[J,\psi^\dagger,\psi] = -\frac{1}{2} \text{Tr} \ln(U) + \frac{1}{2} \phi \circ U \circ \phi + \psi^\dagger \circ G_{\phi^{-1}}^{-1} \circ \psi,$$

(16)

with

$$G_{\phi^{-1}}^{-1}(x,x') = \left( \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + i(U \circ \phi)_x + J(x) \right) \delta(x-x').$$

(17)

If we make a change of variable $\phi' \equiv \phi - iU^{-1} \circ J$ and then rename $\phi'$ by $\phi$, we may rewrite (15-17) as

$$Z[J] = e^{\frac{1}{2} J \circ U^{-1} \circ J} \int D\phi D\psi^\dagger D\psi \ \exp \left\{ - S[J,\psi^\dagger,\psi] \right\},$$

(18)

$$S[J,\psi^\dagger,\psi] = -\frac{1}{2} \text{Tr} \ln(U) + \frac{1}{2} \phi \circ U \circ \phi + i\phi \circ J + \psi^\dagger \circ G_{\phi^{-1}}^{-1} \circ \psi,$$

(19)

$$\langle x | G_{\phi^{-1}}^{-1} | x' \rangle \equiv G_{\phi^{-1}}^{-1}(x,x') = \left( \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + i(U \circ \phi)_x \right) \delta(x-x').$$

(20)

Integrating over the Grassmann fields in (18), we obtain an effective theory in terms of $\phi$

$$e^{-\beta W[J]} = Z[J] = e^{\frac{1}{2} J \circ U^{-1} \circ J} \int D\phi \ \exp \left\{ - I[\phi] - iJ \circ \phi \right\},$$

(21)

where

$$I[\phi] = -\frac{1}{2} \text{Tr} \ln(U) + \frac{1}{2} \phi \circ U \circ \phi - \text{Tr} \ln(G_{\phi}^{-1}).$$

(22)
Let us introduce a new notation $W_\phi[J]$ via

$$e^{-\beta W_\phi[J]} \equiv \int D\phi \ exp \ \{-I[\phi] - iJ \circ \phi\} .$$

(23)

We describe later how to evaluate (23) using well-developed functional integral techniques. Evidently, we have

$$\beta W[J] = \beta W_\phi[J] - \frac{1}{2} J \circ U^{-1} \circ J .$$

(24)

The expectation value, $n_J(x)$, of the density operator in the presence of a source term $J$ is given by

$$n_J(x) = \frac{\delta(\beta W[J])}{\delta J(x)} = \frac{\delta(\beta W_\phi[J])}{\delta J(x)} - (U^{-1} \circ J)_x \equiv i\varphi(x) - (U^{-1} \circ J)_x ,$$

(25)

where

$$(U^{-1} \circ J)_x \equiv \int dy U^{-1}(x,y)J(y) ,$$

and the expectation value of the auxiliary field is defined by

$$i\varphi(x) \equiv \langle i\phi(x) \rangle_J = \frac{\delta(\beta W_\phi)}{\delta J(x)} = \frac{\int D\phi (i\phi(x)) e^{-I[\phi] - iJ \circ \phi} \int D\phi e^{-I[\phi] - iJ \circ \phi}}{\int D\phi e^{-I[\phi] - iJ \circ \phi}} ,$$

(26)

providing a relation between $J$ and $i\varphi$.

Eq. (25) tells us that at the physical limit $J \to 0$, $i\varphi$ is the same as $n$. Since $n$ is a real number, this implies that the expectation value of $\phi(x)$ is an imaginary number, which also implies that when viewed in the complex plane of $\phi(x)$, the saddle point of the integrand is located where the $\phi(x)$s are imaginary numbers.

Now let us write down the effective action. At finite temperature, the effective action is defined as the Legendre transform of $\beta W[J]$:

$$\Gamma[n] \equiv \beta W[J] - \frac{\delta(\beta W[J])}{\delta J} \circ J = \beta W_\phi[J] - \frac{1}{2} J \circ U^{-1} \circ J - n \circ J .$$

(27)

Note that the functional derivative of $\Gamma[n]$ with respect to $n$ reads

$$\frac{\delta \Gamma[n]}{\delta n} = \left[ \frac{\delta(\beta W[J])}{\delta J} - n \right] \frac{\delta J}{\delta n} - J = -J ,$$

(28)

because $\delta(\beta W[J])/\delta J = n$ by Eq. (13). The effective action formalism requires one to express the probe $J$ in terms of an expectation value of some sort, such as the electron density $n$, classical field $i\varphi$, or some equivalent quantity. Below, we will first calculate $\beta W_\phi[J]$, and then use the system’s electron density as the variable and make an explicit connection to the Kohn-Sham decomposition.
B. Evaluation of $e^{-\beta W_\phi[J]}$ via one-particle irreducible diagrams

As shown by Jackiw,\textsuperscript{22} it is possible to express $W_\phi[J]$ as a diagrammatic expansion containing only one-particle irreducible diagrams. The main idea is to shift the field $\phi$ by $\varphi$, $\phi \rightarrow \varphi + \phi$, and note that $J$ is a functional of $\varphi$ via (26). We then rewrite

$$e^{-\beta W_\phi[J]} \equiv e^{-I[\varphi] - iJ \varphi} \int D\phi \; e^{-I[\phi + \varphi] + I[\varphi] - iJ \varphi} \equiv e^{-I[\varphi] - iJ \varphi} Z_\phi[J]$$

where

$$-\ln Z_\phi[J] \equiv \beta W_\phi[J] = -\ln \left[ \int D\phi \; e^{-I[\varphi] + I[\varphi] - iJ \varphi} \right],$$

leading to

$$\beta W_\phi[J] = I[\varphi] + J \varphi + \beta W_\phi[J].$$

(30)

Note that

$$i\varphi(x) = \frac{\delta (\beta W_\phi[J])}{\delta J(x)} = i\varphi(x) + \int dy \left[ \frac{\delta I}{\delta (i\varphi(y))} + \frac{\delta (\beta W_\phi)}{\delta (i\varphi(y))} + J(y) \right] \frac{\delta (i\varphi(y))}{\delta J(x)} ,$$

leading to

$$\frac{\delta I}{\delta (i\varphi(y))} + \frac{\delta (\beta W_\phi)}{\delta (i\varphi(y))} = -J(y).$$

(31)

Using an implicit method and replacing $-J$ in (29) by the left-hand side (LHS) of (31), Jackiw\textsuperscript{22} showed that $\beta W_\phi[J]$ is the sum of all connected one-particle-irreducible (1PI) vacuum graphs governed by the action

$$-I[\phi + \varphi] + I[\varphi] + \phi \frac{\delta I[\varphi]}{\delta \varphi} .$$

To evaluate the expression above, we first rewrite (20) as

$$G_{\phi + \varphi}^{-1}(x, x') = G_{\phi}^{-1}(x, x') + i\delta(x - x')b(x) \equiv G_{\phi}^{-1}(x, x') + V(x, x') ,$$

(32)

with

$$b = U \circ \phi ,$$

and

$$G_{\phi}^{-1}(x, x') = \left[ \partial_t - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + U \circ (i\varphi) \right] \delta(x - x') .$$

(34)

We may then write down

$$G_{\phi + \varphi}^{-1} = G_{\phi}^{-1} [ I + G_{\phi} \circ V ] ,$$

$$G_{\phi + \varphi}^{-1} = G_{\phi}^{-1} [ I + G_{\phi} \circ V ] ,$$
and
\[
\ln (G_{\varphi + \varphi}^{-1}) = \ln (G_{\varphi}^{-1}) + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} [G_{\varphi} \circ V]^k .
\] (35)

Note also that
\[
[G_{\varphi} \circ V]_{x,z} = \int dy G_{\varphi}(x,y)V(y,z) = \int dyG_{\varphi}(x,y)\delta(y-z) (ib(y)) = G_{\varphi}(x,z) (ib(z)) .
\]

Consequently,
\[
\operatorname{Tr} \ln (G_{\varphi + \varphi}^{-1}) = \operatorname{Tr} \ln (G_{\varphi}^{-1}) + \int dx_1 G_{\varphi}(x_1, x_1)(ib(x_1))
- \frac{1}{2} \int dx_1 dx_2 G_{\varphi}(x_1, x_2)G_{\varphi}(x_2, x_1)(ib(x_1))(ib(x_2))
+ \sum_{k=3}^{\infty} \frac{(-1)^{k-1}}{k} \int dx_1 \ldots dx_k G_{\varphi}(x_k, x_1) \ldots G_{\varphi}(x_{k-1}, x_k)(ib(x_1)) \ldots (ib(x_k)) .
\] (36)

Therefore,
\[
-I[\phi + \varphi] + I[\varphi] + \phi \circ \frac{\delta I[\varphi]}{\delta \varphi} = -\frac{1}{2} b \circ \tilde{D}^{-1} \circ b + \sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k
\] (37)

with
\[
\tilde{D}^{-1} = U^{-1} - D ,
\] (38)
\[
D(x, y) = G_{\varphi}(x, y) G_{\varphi}(y, x) ,
\] (39)

and
\[
I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \equiv \frac{(-1)^{k-1}}{k} \int dx_1 \ldots dx_k G_{\varphi}(x_k, x_1) \ldots G_{\varphi}(x_{k-1}, x_k) [(ib(x_1)) \ldots (ib(x_k))] .
\] (40)

As a side note, the quantity \(D(x, y)\) defined in (39) is also called the polarization associated with the Green’s function \(G_{\varphi}\), since it can be shown, by using a derivation identical to that leading to (71), that \(D(x, y) = -\delta G_{\varphi}(x, y)/\delta J(y)\) represents the reaction rate of density (given by \(n(x) \equiv -G_{\varphi}(x, x)\)) due to the influence of the potential. According to Jackiw’s results,\textsuperscript{22} Eq. (37) means that \(\beta W_{s}[\varphi]\) is given by
\[
\beta W_{s}[\varphi] = \operatorname{Tr} \ln(U) + \frac{1}{2} \operatorname{Tr} \ln \left(\tilde{D}^{-1}\right) - \sum_{n=1}^{\infty} \frac{1}{n!} \left\langle \left(\sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \right)^n\right\rangle_{\text{1PI, conn.}}.
\] (41)

where the \(\operatorname{Tr} \ln(U)\) term comes from the Jacobian of changing the variable from \(\phi\) to \(b\) in (29), the angular bracket indicates the following average
\[
\left\langle \hat{O} \right\rangle \equiv \frac{\int D[b] \hat{O} \exp \left(-\frac{1}{2} b \circ \tilde{D}^{-1} \circ b\right)}{\int D[b] \exp \left(-\frac{1}{2} b \circ \tilde{D}^{-1} \circ b\right) ,
\] (42)
and the subscript “1PI, conn.” means to include only connected, one-particle-irreducible diagrams. In our context, a one-particle-irreducible diagrams refers to a diagram that cannot be separated into two by cutting a propagator line representing $\tilde{D}$.

Substituting (22) and (41) into (30), we obtain

$$
\beta W_\phi[J] = \frac{1}{2} \varphi \circ U \varphi - \text{Tr} \ln \left( G^{-1}_\varphi \right) + iJ \varphi 
+ \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) - \sum_{n=1}^{\infty} \frac{1}{n!} \langle \sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \rangle_{\text{1PI, conn.}}^n.
$$

(43)

Note that Fukuda et al.\textsuperscript{18} obtained an expression similar to (43) and used it to derive an effective action as a functional of $i\varphi$, which coincides with $n_J$ only at $J = 0$.

We wish to keep $n_J$ as the functional variable. Let us first note that

$$
\beta W[J] = \beta W_\phi[J] - \frac{1}{2} J \circ U^{-1} \circ J.
$$

By employing the identity (25)

$$
n_J = i\varphi - U^{-1} \circ J,
$$

we can now write $\beta W[J]$ as

$$
\beta W[J] = -\text{Tr} \ln \left( G^{-1}_\varphi \right) - \frac{1}{2} n_J \circ U \circ n_J + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) 
- \sum_{n=1}^{\infty} \frac{1}{n!} \langle \sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \rangle_{\text{1PI, conn.}}^n.
$$

(44)

and

$$
\Gamma[n] = -\text{Tr} \ln \left( G^{-1}_\varphi \right) - \left[ J + \frac{1}{2} n_J \circ U \right] \circ n_J + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) 
- \sum_{n=1}^{\infty} \frac{1}{n!} \langle \sum_{k=3}^{\infty} I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \rangle_{\text{1PI, conn.}}^n.
$$

(45)

For later convenience we introduce a parameter $\lambda$ to denote the order. Specifically, we write

$$
\beta W[J] = -\text{Tr} \ln \left( G^{-1}_\varphi \right) - \frac{1}{2} n_J \circ U \circ n_J + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) 
- \lambda \sum_{n=1}^{\infty} \frac{1}{n!} \langle \sum_{k=3}^{\infty} \lambda^k I^{(k)}[\varphi] \circ b_1 \ldots \circ b_k \rangle_{\text{1PI, conn.}}^n.
$$

(46)

$$
\equiv \beta \tilde{W}_0[J] + \beta \sum_{l=1}^{\infty} \lambda^l W_l[J]
$$

(47)

The bookkeeping parameter $\lambda$ will be set to 1 in the end. The exponent associated with the parameter $\lambda$ plays the role of the number of loops introduced. For example, the term
\( \frac{1}{2} \text{Tr} \ln \left( D^{-1} U \right) \) consists of one-loop contributions. The last part of (46) contains diagrams of two loops or higher. The explicit appearance of the \( n_J U n_J \) term in (44) and (46) suggests the possibility of a connection to the Kohn-Sham decomposition of the DFT.

C. Inversion Method by Loop Order

We now come to the point of departure from typical treatments of auxiliary field approach and are ready to make a direct connection to the Kohn-Sham scheme. Let us first define a new free fermion propagator

\[
G_0^{-1}(x, x') = \left[ \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + J_0(x) \right] \delta(x - x'),
\]

where \( J_0 \) is chosen such that the free fermion system has the same particle density as the physical system (where Coulomb interactions exist) with source potential \( J \)

\[
- G_0(x, x) = n_J(x).
\]

The existence of \( J_0 \) is scrutinized below. From the perspective of the Kohn-Sham decomposition, Eq. (49) corresponds to Eq. (6). In the presence of a source term \( J \), Eq. (10) shows that it is equivalent to making \( v_{\text{ion}} \rightarrow v_{\text{ion}} + J \). Comparing with Eq. (5), we see immediately if one were to choose

\[
J_0 = J + U \cdot n_J + \frac{\delta E_{xc}[n]}{\delta n} \bigg|_{n=n_J},
\]

the requirement (49) can be fulfilled. We will therefore call the corresponding free fermion system the Kohn-Sham system. The presence of \( J_0 \), of course, depends crucially on the differentiability of \( E_{xc}[n] \), whose existence (not differentiability) was proven.\(^2\)

To bring out the Kohn-Sham quantities (orbitals and energies) in our loop expansion, let us first use a variant of (25)

\[
u_o(i \varphi) = J + U \cdot n_J
\]

and replace \( U_o(i \varphi) \) by \( J + U \cdot n_J \) in the expression of propagator \( G_{\varphi} \). Specifically, we write (34) as

\[
G_{\varphi}^{-1}(x, x') = \left[ \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + J(x) + U \cdot n_J \right] \delta(x - x').
\]

The critical step is to decompose the source \( J \) in a particular way,

\[
J \equiv (J_0 - U \cdot n_J) + J' \equiv \tilde{J}_0 + J'.
\]
Therefore, from Eqs. (25), (34) and (52) we have

$$G_{\varphi}^{-1}(x, x') = G_0^{-1}(x, x') + J'(x) \delta(x - x'),$$

(53)

and the Kohn-Sham propagator $G_0$ appears as we expected. As will be described in section III E, $G_0(x, x')$ can be expressed in terms of the Kohn-Sham quantities. Therefore, the idea is to expand $G_{\varphi}$ around $G_0$ provided that $J'$ can also be expressed via Kohn-Sham quantities. Comparing (52) with (50), we find that formally speaking $J'[n] = -\frac{\delta E_{xc}[n]}{\delta n}$.

This source decomposition is introduced here for the first time in the auxiliary field approach. (A similar decomposition has been used\textsuperscript{19,20} in the perturbative expansion in powers of $e^2$.)

The idea of inversion is to obtain $J[n]$, that is, to find the corresponding $J$ for each configuration of electron density $n$ in the domain of $\Gamma[n]$. One then substitutes $J[n]$ into $\Gamma[n] = \beta W[J[n]] - J[n] \circ n$ to express $\Gamma[n]$ using the density profile $n$ as the natural variable. For each given density profile $n$ within the domain of $\Gamma$, Eq. (49) determines the corresponding $\tilde{J}_0$. The collection of such relations forms $\tilde{J}_0[n]$. Similarly, if for every given $n$ one can find the corresponding $J'$, one obtains $J'[n]$ and the goal of inversion is achieved. When evaluating $\Gamma[n]$, one employs one density configuration at a time. That said, when we expand $W[J[n]] = W[\tilde{J}_0[n] + J'[n]]$ in powers of $J'$ within the expression $\Gamma[n] = \beta W[J] - J \circ n$, we will keep $n, J$ fixed, instead of treating it as a functional of $\tilde{J}_0$.

We now examine the loop expansion of $W[J]$ carefully. Eq. (46) tells us that

$$\beta W[J] = \beta(\tilde{W}_0 - W_0) + \beta \sum_{l=0}^{\infty} \lambda^l W_l[J + U \circ n, J],$$

(54)

where $\beta(\tilde{W}_0 - W_0) = -\frac{1}{2} n, K U \circ n, J$ and $\beta W_0[J + U \circ n, J] = -\text{Tr} \ln(G_{\varphi}^{-1})$. Note that for any $W_l$ term, its $J$ dependence is through the propagator $G_{\varphi}$, which always has $J + U \circ n, J$ as the natural variable. Our reasoning earlier indicates that when we expand $W_l[J + U \circ n, J] = W_l[\tilde{J}_0 + U \circ n, J + J'] = W_l[J_0 + J']$ in powers of $J'$ within the expression $\Gamma[n] = \beta W[J] - J \circ n$, we may write the expansion in the following way (and forget about needing to keep $n, J$ fixed)

$$W_l[J_0 + J'] = W_l[J_0] + \frac{\delta W_l[J_0]}{\delta J_0} J' + \frac{1}{2!} J' \frac{\delta^2 W_l[J_0]}{\delta J_0 \delta J_0} J' + \ldots.$$  \hspace{1cm} (55)

With (55), we may express $\beta W[J]$ as a double series

$$\beta W[J] = \beta(\tilde{W}_{00} - W_{00}) + \beta \sum_{i,k} W_{ik} J'^k \lambda^i,$$  \hspace{1cm} (56)
where each $W_{ik}$ involves the $k$'th derivative of $W_i$. In particular, $\tilde{W}_{00}$ is given by (with $n_J \rightarrow n$ hereafter)

$$\beta \tilde{W}_{00} = \beta W_{00} - \frac{1}{2} n_0 U \circ n = -\text{Tr} \ln (G^{-1}_0) - \frac{1}{2} n_0 U \circ n ,$$

(57)

and $W_{01}$ is given by

$$\beta W_{01}[J_0] = -\text{Tr} \left( \frac{\delta \ln (G^{-1}_0)}{\delta J_0(x)} \right) = -\int dz dy \ G_0(z, y) \delta(y - x) \delta(y - z) = -G_0(x, x) = n ,$$

(58)

in view of (49).

Instead of looking at the expansion of $W_i$ in powers of $J'$ within the effective action expression, we now take a moment to look at the $\tilde{W}_{00}$ term in the double series expansion of $\beta W[J]$. Consider the functional derivative of $\beta \tilde{W}_{00}$ with respect to the source term $\tilde{J}_0$. Here, one is asking the response of $\beta \tilde{W}_{00}$ with respect to change in $\tilde{J}_0$. Evidently, when $\tilde{J}_0$ changes, its corresponding density $n$ has to vary as well. Using the chain rule of differentiation and (58), we obtain

$$\frac{\delta (\beta \tilde{W}_{00})}{\delta \tilde{J}_0} = \frac{\delta (\beta W_{00})}{\delta J_0} \frac{\delta J_0}{\delta \tilde{J}_0} - n_0 U \circ \frac{\delta n}{\delta \tilde{J}_0} = n_0 \left( I + U \circ \frac{\delta n}{\delta \tilde{J}_0} \right) - n_0 U \circ \frac{\delta n}{\delta \tilde{J}_0} = n .$$

(59)

This suggests that we define

$$\tilde{\Gamma}_0[n] = \beta \tilde{W}_{00}[\tilde{J}_0] - \tilde{J}_0 \circ n = -\text{Tr} \ln (G^{-1}_0) - \frac{1}{2} n_0 U \circ n - \tilde{J}_0 \circ n ,$$

(60)

the Legendre transformation of $\beta W_{00}[\tilde{J}_0]$, leading to

$$\frac{\delta \tilde{\Gamma}_0[n]}{\delta n} = -\tilde{J}_0 .$$

(61)

Comparing (61) with (28), we find

$$\frac{\delta (\Gamma[n] - \tilde{\Gamma}_0[n])}{\delta n} = -J' .$$

(62)

The idea now is to develop a series for $\Gamma[n]$ led by $\tilde{\Gamma}_0[n]$. Subtracting (60) from $\Gamma[n] = \beta W[J] - J \circ n$, we have

$$\Gamma[n] - \tilde{\Gamma}_0[n] = \beta W[J] - \beta \tilde{W}_{00}[\tilde{J}_0] - J' \circ n ,$$

(63)

in which the last two terms on the right-hand side (RHS) exactly cancel the terms in $\tilde{W}_{00}$ and $W_{01}$ contributing to $\beta W[J]$. So the series for $\Gamma - \tilde{\Gamma}_0$ is just (56) with those two terms
removed. Next we convert the double sum in (56) into a single sum by expanding $J'$ as a series in $\lambda$. We write

$$J'[n] = \sum_{l=1}^{\infty} J_l[n] \lambda^l, \quad (64)$$

where the precise expressions for $J_1, J_2, \ldots$ are as yet undetermined since (64) is not a loop expansion. We substitute (64) formally into (63) and (56) to obtain a series

$$\Gamma[n] - \tilde{\Gamma}_0[n] = \sum_{l=1}^{\infty} \Gamma_l[n] \lambda^l, \quad (65)$$

in which each $\Gamma_l$ is defined explicitly in terms of the $J_k$, $\beta W_{k \leq l}[J_0]$, and their derivatives. Because $W_{01}$ is missing from (63), any occurrence of $J_k$ is accompanied by at least one other factor $J_{k'}$ or else by an occurrence of some $W_{i>0}$, and hence by a power of $\lambda$ higher than the $k$'th. In other words, the expression for $\Gamma_{l \geq 1}$ involves only $J_k$ with $k < l$. We finally remove the indeterminacy in (64) by imposing (62) order by order in $\lambda$, leading to (for $l \geq 1$)

$$\frac{\delta \Gamma_l[n]}{\delta n} = -J_l. \quad (66)$$

Since $\Gamma_{l \geq 1}$ involves only $J_{k<l}$, all the $J_l$ and $\Gamma_l$ can be found explicitly by applying (65) and (66) alternately. Evidently, it is the source decomposition (52) that allows us to obtain exact correspondence to the Kohn-Sham scheme. Below we will provide an explicit formula for $\Gamma_l[n]$ in terms of $W_l[J_0]$ and their functional derivatives.

To obtain an explicit expression for $\Gamma_l[n]$, let us substitute the LHS of (63) by the RHS of (65) and apply (56) as well as (64) to the RHS of (63). Then, by equating the coefficients associated with $\lambda^l$ on both sides of (63), we obtain (for $l \geq 1$)

$$\Gamma_l[n] = \beta W_l[J_0] + \sum_{k=1}^{l-1} \frac{\delta (\beta W_{l-k}[J_0])}{\delta J_0} \circ J_k + \sum_{m=2}^{l} \frac{1}{m!} \sum_{k_1+\ldots+k_m \leq l} \delta^m \left( \beta W_{l-(k_1+\ldots+k_m)}[J_0] \right) \frac{1}{\delta J_0 \ldots \delta J_0} \circ J_{k_1} \circ \ldots \circ J_{k_m}. \quad (67)$$

For $l = 1$, we see that

$$\Gamma_1[n] = \beta W_1[J_0] = \frac{1}{2} \text{Tr} \ln \left( \tilde{D}_0^{-1} \circ U \right) \equiv \text{Tr} \ln \left( \tilde{D}_0^{-1} \circ U \right). \quad (68)$$

We observe that

$$\tilde{D}_0^{-1} \equiv \tilde{D}_{J \rightarrow J_0}^{-1} = U^{-1} - D_{J \rightarrow J_0} = U^{-1} - D_0$$
We then have
\[ J_1 = -\frac{\delta \Gamma_1[n]}{\delta n} = -\frac{\delta J_0 \circ \delta (\beta W_1[J_0])}{\delta n} \cdot \]

Note that \(-\delta J_0/\delta n\) can be written as
\[ \frac{\delta J_0(x)}{\delta n(y)} = -\left( \frac{\delta n(y)}{\delta J_0(x)} \right)^{-1} = -\left( \frac{\delta^2(\beta W_0[J_0])}{\delta J_0(x) \delta J_0(y)} \right)^{-1} = \frac{\delta^2 \Gamma_0[n]}{\delta n(x) \delta n(y)} \] (69)

where
\[ \Gamma_0[n] = \beta W_0[J_0] - J_0 \circ n = \tilde{\Gamma}_0[n] - \frac{1}{2} n_0 U \circ n, \] (70)

and the inverse is in the functional matrix sense. Using (49), we can evaluate \(\delta n(x)/\delta J_0(y)\) by
\[ \frac{\delta n(x)}{\delta J_0(y)} = -\frac{\delta G_0(x, x)}{\delta J_0(y)} = \int dzdz' G_0(x, z) \frac{\delta G_0^{-1}(z, z')}{\delta J_0(y)} G_0(z', x) = G_0(x, y) G_0(y, x) = D_{J \rightarrow J_0}(x, y) \equiv D_0(x, y). \] (71)

Therefore,
\[ J_1 = -D_0^{-1} \circ \frac{\delta (\beta W_1[J_0])}{\delta J_0}. \]

Since \(-G_0(x, x) = n(x)\) represents the electron density of the KS system, we will call \(D_0(x, y)\) the polarization associated with the KS system. Note that if one were to approximate the effective action \(\Gamma[n]\) by \(\Gamma[n] = \tilde{\Gamma}_0[n] + \Gamma_1[n]\), the displayed equation above is the OEP equation for GW-OEP\(^{44}\), while eq. (68) is the corresponding exchange-correlation functional.

Once \(J_1\) is known, one can find \(\Gamma_2[n]\)
\[ \Gamma_2[n] = \beta W_2[J_0] + \frac{\delta (\beta W_1[J_0])}{\delta J_0} \circ J_1 + \frac{1}{2} J_1 \circ \frac{\delta^2 (\beta W_0[J_0])}{\delta J_0 \delta J_0} \circ J_1 = \beta W_2[J_0] - \frac{1}{2} \frac{\delta (\beta W_1[J_0])}{\delta J_0} \circ D_0^{-1} \circ \frac{\delta (\beta W_1[J_0])}{\delta J_0}, \] (72)

and \(J_2\) now can be computed via \(-\delta \Gamma_2[n]/\delta n\)
\[ J_2 = D_0^{-1} \circ \frac{\delta (\beta W_2[J_0])}{\delta J_0} + D_0^{-1} \circ \frac{\delta^2 (\beta W_1[J_0])}{\delta J_0 \delta J_0} \circ J_1 + \frac{1}{2} D_0^{-1} \circ \frac{\delta^3 (\beta W_0[J_0])}{\delta J_0 \delta J_0 \delta J_0} \circ J_1 \circ J_1. \] (73)

The explicit expression of \(J_2\) leads to \(\Gamma_3[n]\) and so on. It should now be clear how the strategy goes. We are assuming that the functionals \(\{W_l[J_0]\}\) and their derivatives with respect to \(J_0\) are known. This information can indeed be obtained by standard, albeit tedious, many-body perturbation method. One then uses Eq. (67) to express \(\Gamma_l\) in terms of the known functionals and \(J_k\) with \(k < l - 1\). Once \(\Gamma_l\) is obtained, one can then use Eq. (66) to obtain \(J_l\), which then facilitates the calculation of \(\Gamma_{l+1}\) via (67) and so on.
We now take a moment to organize the terms of effective action \( \Gamma[n] \). From (65) and (70), we know that

\[
\Gamma[n] = \tilde{\Gamma}_0[n] + \sum_{l=1}^{\infty} \Gamma_l[n] = \Gamma_0[n] + \frac{1}{2} n o U o n + \sum_{l=1}^{\infty} \Gamma_l[n].
\] (74)

The first term on the RHS of (74) indeed corresponds to the effective action of the free KS system, the second term is exactly the Hartree energy. It is thus natural for us to define the last part, sum of \( \Gamma_l[n] \), as

\[
\Gamma_{xc}[n] \equiv \sum_{l=1}^{\infty} \Gamma_l[n].
\] (75)

At the physical condition (i.e., when the source is absent), we should have \( \delta \Gamma / \delta n = -J = 0 \). Knowing that

\[
\frac{\delta \tilde{\Gamma}_0[n]}{\delta n} = -\tilde{J}_0 = -J_0 + U o n ,
\]

we conclude that at the physical condition,

\[
\frac{\delta \Gamma_{xc}[n]}{\delta n} = \tilde{J}_0 = J_0 - U o n .
\] (76)

Note that the potential \( J_0 \) together with the original non-interacting part of the Hamiltonian leads to the exact particle density of the interacting system. This implies that \( J_0 \) contains both the Hartree term and the exchange-correlation potential. Since \( J_0 = \tilde{J}_0 + U o n_T \), with \( U o n_T \) being the Hartree term, the term \( \tilde{J}_0 \) plays the role of exchange-correlation potential, as evidenced by (76). The quantum mechanical effects are completely contained in \( \Gamma_{xc}[n] \), defined in (75).

Note that a different density profile other than that corresponding to the physical ground state can be induced by introducing a nonzero \( J \). Let us again call the corresponding density profile \( n_J \). When \( J \neq 0 \), we learn from (10) that it is equivalent to replacing \( v \) by \( v + J \). Eq. (5) then tells us that \( J_0 \) must contain \( J \), the Hartree term and the exchange-correlational potential as shown in (50). In this case, one writes \( J_0 = J + (\tilde{J}_0 - J) + U o n_J \). With \( U o n_J \) being the Hartree term, \( (\tilde{J}_0 - J) \) must represent the exchange-correlation potential corresponding to the configuration \( n_J \), and

\[
\frac{\delta (\Gamma_{xc}[n])}{\delta n} = \tilde{J}_0 - J .
\] (77)

This then leads to

\[
\frac{\delta \Gamma[n]}{\delta n} = -J ,
\]
what we expected when $J \neq 0$.

In terms of real computation, since the $n$ dependence is through $J_0$, we may rewrite Eq. (76) as

$$\frac{\delta J_0}{\delta n} \frac{\delta (\Gamma_{xc}[J_0[n]])}{\delta J_0} = \tilde{J}_0 = J_0 - U \circ n$$

or

$$0 = D_0 \circ \tilde{J}_0 - \frac{\delta (\Gamma_{xc}[J_0[n]])}{\delta J_0} D_0 \circ (J_0 - U \circ n) - \frac{\delta (\Gamma_{xc}[J_0[n]])}{\delta J_0},$$

and the condition $\delta \Gamma[n]/\delta n = 0$ is turned into $\delta \Gamma[J_0[n]]/\delta J_0 = 0$. Since the effective action is a strictly convex function of the electron density $n$, there exists no local minima. One can therefore solve $\delta \Gamma[J_0[n]]/\delta n = 0$ by steepest descent. Effectively, we may define the direction of steepest descent $\kappa(x)$ by

$$\kappa(x) \equiv -\frac{\delta \Gamma[J_0[n]]}{\delta J_0(x)} = D_0 \circ (J_0 - U \circ n) - \frac{\delta (\Gamma_{xc}[J_0[n]])}{\delta J_0}$$

and then update $J_0(x)$ by $J_0(x) \to J_0(x) + \zeta \kappa(x)$, with $\zeta > 0$ being the step size, till convergence is reached, that is, when $\kappa(x) \to 0$. Note that eq. (78) is the standard OEP-equation for consistency. The iterative procedure described after (78) is largely identical to the Kuemmel-Perdew\textsuperscript{37} procedure used for solving the exchange-only OEP equation.

D. Diagrammatic Expansion of the Density Functional

We now examine how one computes the effective action via diagrams. From Eqs. (65), (68) and (70), we have

$$\Gamma[n] = \tilde{\Gamma}_0[n] + \sum_{i=1}^{\infty} \Gamma_i[n] = \Gamma_0[n] + \frac{1}{2} n \circ U \circ n + \sum_{i=1}^{\infty} \Gamma_i[n]$$

$$= -\text{Tr} \ln (G_0^{-1}) - J_0 \circ n + \frac{1}{2} n \circ U \circ n + \frac{1}{2} \text{Tr} \ln (\tilde{D}_0^{-1} U) + \sum_{i=2}^{\infty} \Gamma_i[n],$$

where

$$\tilde{D}_0^{-1} = U^{-1} - D_0$$

$$D_0(x,y) = G_0(x,y) G_0(y,x).$$

Evidently, we need diagrammatic symbols for $U$, $G_0$ and $\tilde{D}_0$. To get to higher-order terms $\Gamma_i \geq 2$ of the effective action, we see from Eqs. (71-73) and the text afterwards that it is necessary to incorporate into the diagrams the inverse density correlator $D_0^{-1}$ and to evaluate
functional derivatives with respect to \( n \) (or \( J_0 \)). We define the symbols for each line type below

\[
\begin{align*}
\text{x'} & \quad \ldots \quad x \quad U(x, x') \quad x' \quad \overrightarrow{U(x, x')} \quad x \quad D_0^{-1}(x, x') \\
\text{x'} & \quad \overrightarrow{x} \quad G_0(x, x') \quad x' \quad \overrightarrow{G_0(x, x')} \quad \tilde{D}_0(x, x') .
\end{align*}
\]

The smaller dots associated with the \( U, D_0^{-1} \), and \( G_0 \) propagators are introduced to guide the eyes regarding the starting and ending points of these propagators. The \( \tilde{D}_0 \) propagator comes from contracting two \( b \) fields, see (33), and thus the bigger dots associated with \( \tilde{D}_0 \) denote the coordinates/locations of those \( b \) fields. We will also use the bigger dots to indicate the space-time coordinate of a point of interest.

To evaluate functional derivatives of \( W_l[J_0[n]] \) with respect to \( n \) (or \( J_0 \)), we note from Eqs. (25), (34), (40) and (46) that the \( J_0 \) dependence comes from \( G_0(x, y) \) and the functional derivatives associated with the formalism using Eqs. (67-79) necessarily require evaluations of \( \delta G_0(x, x')/\delta J_0(y) \). Using a derivation similar to that in (71), we find that

\[
\frac{\delta G_0(x, x')}{\delta J_0(y)} = -G_0(x, y)G_0(y, x') .
\] (83)

The propagators \( D_0^{-1} \) and \( \tilde{D}_0 \) also contain \( G_0 \) and thus may be differentiated with respect to \( J_0 \). Note that \( \tilde{D}_0 = (I - U \circ D_0)^{-1} \circ U \) and \( D_0(x, y) = G_0(x, y)G_0(y, x) \). Employing the identity

\[
\frac{\delta M^{-1}}{\delta J_0} = -M^{-1} \frac{\delta M}{\delta J_0} M^{-1} ,
\]

we let \( M = (I - U \circ D_0) \) for the case of \( \tilde{D}_0 \) and \( M = D_0 \) for the case of \( D_0^{-1} \) to obtain

\[
\frac{\delta \tilde{D}_0}{\delta J_0} = \tilde{D}_0 \frac{\delta D_0}{\delta J_0} \circ \tilde{D}_0 ,
\] (84)

\[
\frac{\delta D_0^{-1}}{\delta J_0} = -D_0^{-1} \frac{\delta D_0}{\delta J_0} \circ D_0^{-1} .
\] (85)
Eq. (83-85) may be expressed diagrammatically as follows

\[
\frac{\delta \mathcal{G}_0(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} \quad = - \quad y,
\]

\[
\frac{\delta \tilde{\mathcal{D}}_0(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} \quad = - y - y,
\]

\[
\frac{\delta D_0^{-1}(x, x')}{\delta J_0(y)} = \frac{\delta}{\delta J_0(y)} \quad = + y + y,
\]

where the \(\mp\) signs come from

\[
\frac{\delta}{\delta J_0(y)} D_0(z, z') = \frac{\delta}{\delta J_0(y)} \quad = - \quad z - z.
\]

When combined with the inverse density correlator, the graphs above yield

\[
\frac{\delta \mathcal{G}_0(x, x')}{\delta n(z)} = - \int dy \ D_0^{-1}(z, y) \mathcal{G}_0(x, y) \mathcal{G}_0(y, x') ,
\]

\[
\frac{\delta \tilde{\mathcal{D}}_0(x, x')}{\delta n(z)} = - \int dy dx_1 dx_2 D_0^{-1}(z, y) \tilde{\mathcal{D}}_0(x, x_1) \left[ \mathcal{G}_0(x_2, x_1) \mathcal{G}_0(x_1, y) \mathcal{G}_0(y, x_2) + \mathcal{G}_0(x_1, x_2) \mathcal{G}_0(x_2, y) \mathcal{G}_0(y, x_1) \right] \tilde{\mathcal{D}}_0(x_2, x') ,
\]

\[
\frac{\delta D_0^{-1}(x, x')}{\delta n(z)} = \int dy dx_1 dx_2 D_0^{-1}(z, y) D_0^{-1}(x, x_1) \left[ \mathcal{G}_0(x_2, x_1) \mathcal{G}_0(x_1, y) \mathcal{G}_0(y, x_2) + \mathcal{G}_0(x_1, x_2) \mathcal{G}_0(x_2, y) \mathcal{G}_0(y, x_1) \right] D_0^{-1}(x_2, x') ,
\]
which are shown diagrammatically below

\[
\frac{\delta G_0(x, x')}{\delta n(z)} = \frac{\delta}{\delta n(z)} \left| \begin{array}{ccc} x & \delta & x' \\ x' & \delta n(z) & z \\ \end{array} \right|,
\]

\[
\frac{\delta \tilde{D}_0(x, x')}{\delta n(z)} = \frac{\delta}{\delta n(z)} \left| \begin{array}{ccc} x & \delta & x' \\ x' & \delta n(z) & z \\ \end{array} \right| - \frac{\delta}{\delta n(z)} \left| \begin{array}{ccc} x & \delta & x' \\ x' & \delta n(z) & z \\ \end{array} \right|,
\]

\[
\frac{\delta D_0^{-1}(x, x')}{\delta n(z)} = \frac{\delta}{\delta n(z)} \left| \begin{array}{ccc} x & \delta & x' \\ x' & \delta n(z) & z \\ \end{array} \right| + \frac{\delta}{\delta n(z)} \left| \begin{array}{ccc} x & \delta & x' \\ x' & \delta n(z) & z \\ \end{array} \right|.
\]

The diagrammatic differential rules of \(\delta/\delta J_0\) and \(\delta/\delta n\) are needed not only for the calculations of higher-order terms \(\Gamma_{i \geq 2}\) of the effective action but also for the calculations of excitations, which we will discuss in section V.

Before formally introducing the diagrammatic expansion, let us first set the convention that we will use. In general, each Feynman graph will carry with it a symmetry factor, which is inversely proportional to the number of ways to label this graph without changing the topology of the graph. The convention in quantum field theory usually leaves out the symmetry factor, as it may be deduced from the graph. To avoid enumeration of the symmetry factors needed, however, we will explicitly provide the symmetry factors for Feynman diagrams to be investigated later.

Let us now look at the effective action (80) term by term. The Hartree term \(n \circ U \circ n/2\) is expressed diagrammatically below

\[
\Gamma_{\text{Hartree}} = \frac{1}{2} \circ \cdots \circ.
\]

As remarked by Jackiw, each term in the effective action expansion represents an infinite number of Feynman diagrams in regular perturbative field theoretic calculations. We use
the $\frac{1}{2} \text{Tr} \ln (\tilde{D}_0^{-1} U)$ term as an explicit example

$$\frac{1}{2} \text{Tr} \ln (\tilde{D}_0^{-1} U) = \frac{1}{2} \text{Tr} \ln [I - D_0 U] = - \sum_{n=1}^{\infty} \frac{\text{Tr} (D_0 U)^n}{2n},$$

where each term in the summation corresponds to a vacuum diagram, see Fig 1.

Figure 1: Feynman diagrams corresponding to $\frac{1}{2} \text{Tr} \ln (\tilde{D}_0^{-1} U)$. The first term corresponds to $-\frac{1}{2} \text{Tr} (D_0 U)$, the second term corresponds to $-\frac{1}{2} \text{Tr} (D_0 U)^2$, the third term corresponds to $-\frac{1}{2} \text{Tr} (D_0 U)^3$, and the fourth term corresponds to $-\frac{1}{2} \text{Tr} (D_0 U)^4$. In general, the diagram corresponding to $-\text{Tr} (D_0 U)^n$ contains $n$ bubbles strung by $n$ $U$ propagators with the symmetry factor $\frac{1}{2n}$.

If we pull together the lowest order diagrams in $\epsilon^2$, we find the combination

$$\frac{1}{2} n_0 U_{n0} - \frac{1}{2} \text{Tr} (D_0 U)$$

that corresponds to the Feynman diagrams in Fig. 2.

Figure 2: The Feynman diagrams corresponding to the Hartree term (a) and the lowest order exchange term (b), the first graph from Fig. 1. The numerical factor associated with each diagram is shown explicitly.

To compute $\Gamma_2$, we need to first calculate $J_1$. Since $\Gamma_1[n] = \beta W_1[J_0] = \frac{1}{2} \text{Tr} \ln (I - D_0 U)$

$$J_1(z) = - \frac{\delta \Gamma_1}{\delta n(z)} = - \frac{1}{2} \text{Tr} \left[ (I - D_0 U)^{-1} \left( - \frac{\delta D_0}{\delta n(z)} \right) \circ U \right]$$

$$= \frac{1}{2} \text{Tr} \left[ U \circ (I - D_0 U)^{-1} \frac{\delta D_0}{\delta n(z)} \right] = \frac{1}{2} \text{Tr} \left[ \tilde{D}_0 \frac{\delta D_0}{\delta n(z)} \right]$$

$$= - \int dy \, dx \, dx' \, D_0^{-1}(z,y) \tilde{D}_0(x,x') \mathcal{G}_0(x,x') \mathcal{G}_0(x',y) \mathcal{G}_0(y,x), \quad (86)$$
which can also be expressed diagrammatically as

\[ J_1(z) = - \frac{1}{z} \]

From Eq. (72), we know that \( \Gamma_2[n] = \beta W_2[J_0] - \frac{1}{2} J_1 \circ D_0^{-1} \circ J_1 \). We note from Eq. (46) and (47) that \( \beta W_2[J_0] \) corresponds to the \( \lambda^2 \) diagrams in

\[ -\lambda \sum_{n=1}^{\infty} \frac{1}{n!} \left[ \frac{1}{\lambda} \sum_{k=3}^{\infty} \lambda^k I^{(k)}[\varphi] \circ b_1 \cdots \circ b_k \right]^n \]

the last part of Eq. (46). There are two combinations of \( n \) and \( k \) that can give rise to \( \lambda^2 \). The first one is to have \( n = 1 \) and \( k = 4 \), while the second one is to have \( n = 2 \) and \( k = 3 \). The first possibility generates two distinct graphs, while the second possibility generates three distinct diagrams. For \( n = 1 \) and \( k = 4 \), we have the following diagrams with their symmetry factors specified

\[(a) \quad -\frac{(i)^4 (-1)^3}{1!} \frac{3}{4}
(b) \quad -\frac{(i)^4 (-1)^3}{1!} \frac{3}{4} \frac{2}{3}
\]

For \( n = 2 \) and \( k = 3 \), we have the following diagrams with their symmetry factors specified

\[(a) \quad -\frac{3(i)^6 (-1)^2}{2!} \frac{3}{3} \frac{1}{3} \\
(b) \quad -\frac{3(i)^6 (-1)^2}{2!} \frac{3}{3} \frac{1}{3} \\
(c) \quad -\frac{3(i)^6 (-1)^2}{2!} \frac{3}{3} \frac{1}{3} \]

The first diagram (a) among the three will be discarded since one can cut a \( \tilde{D}_0 \) line and then separate it into two diagrams. Let us display below the diagram corresponding to \( J_1 \circ D_0 \circ J_1 \),

\[ J_1 \circ D_0 \circ J_1 = (-J_1) \circ D_0 \circ (-J_1) = \]

Therefore, the diagrammatic expression for \( \Gamma_2[n] \) is given by
\[ \Gamma_2[n] = \frac{1}{4} \left( \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array} \right) + \frac{1}{2} \left( \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array} \right) - \frac{1}{2} \left( \begin{array}{cccc} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array} \right). \]

Note that each \( \tilde{D}_0 \) propagator line contains the sum of infinitely many terms

\[ \tilde{D}_0 = (U^{-1} - D_0)^{-1} = (I - U \circ D_0)^{-1} \circ U = U + U \circ D_0 \circ U + U \circ D_0 \circ U \circ D_0 \circ U + \ldots \quad (87) \]

Since each \( U \) carries a factor of \( e^2 \), the above expansion may be viewed as the \( e^2 \) expansion of \( \tilde{D}_0 \) with \( U \) being the leading order. Therefore, in the diagrams corresponding to \( \Gamma_2 \) (Fig. 3), if one were to expand \( \tilde{D}_0 \) in \( e^2 \), the first three diagrams are of order \( e^4 \) or higher, while the last two diagrams contain terms of order \( e^6 \) or higher only.

It is now instructive to compare with the perturbative methods which use \( e^2 \) as the expansion parameter. Among those methods, the approach of Valiev and Fernando\(^{20} \) is the closest to ours. Let us pull out the diagrams contributing to order \( e^4 \) in \( \Gamma_{i \leq 2} \) and compare to the results of reference 20. From \( \Gamma_1[n] \), we see that the second diagram in Fig. 1 corresponding to \(-\frac{1}{4} \text{Tr} [(D_0 \circ U)^2] \) will contribute to this order. The first three diagrams representing \( \Gamma_2[n] \) will contribute to the same order if we replace the \( \tilde{D} \) propagator by \( U \). Thus, one obtains the diagrams shown in Fig. 4, which are identical to the results in reference 20.

We use this example to illustrate the difference between our diagrammatic rules and those of reference 20. In order to obtain \( e^4 \) diagrams, the diagrammatic rules of reference 20
require the generation of all $e^4$ diagrams of $\beta W[J]$, each of which is shown in Fig. 5.

![Feynman diagrams](image)

Figure 5: The Feynman diagrams of order $U^2$ (or $e^4$) of $\beta W[J]$. The correct symmetry factors are also provided.

Then one deletes diagrams that can be cut into two parts by cutting a Coulomb line $u$. This means that the last two diagrams above will be deleted from consideration. One then needs to find in the remaining diagrams the two-particle reducible (in the sense of fermion propagator) ones followed by an iterative operation to construct $D_0^{-1}$ lines. In this case, the only two-particle-reducible diagram is the third one and the iterative procedure generates exactly the only diagram containing a $D_0^{-1}$ line in $\Gamma_2$, with $\tilde{D}$ replaced by $U$. Therefore, the diagrammatic rules of reference 20 require first one-particle-irreducibility of the Coulomb line followed by searching for diagrams that are two-particle-reducible (in fermion propagators sense).

For our case, when considering a diagram’s reducibility, we only consider the $\tilde{D}_0$ lines. Let us denote $I^{(k)}[\phi] \circ b_1 \ldots \circ b_k$ by $B^{(k)}$, and call it blob $k$. The one-particle-irreducible criterion simply means that when one joins any two blobs, say $B^{(k_1)}$ and $B^{(k_2)}$, one must make sure that at least two or more $\tilde{D}_0$ lines are connecting $B^{(k_1)}$ and $B^{(k_2)}$ due to contraction of $b$ fields. Therefore, it is very easy to find and exclude one-particle-reducible diagrams in our method. For this particular example, only the diagrams surviving in the end are present in our formalism. Since the leading order of $\tilde{D}_0$, in terms of expansion of $e^2$, is $U$ itself, our one-particle-irreducibility in $\tilde{D}_0$ lines covers the one-particle-irreducibility of the Coulomb lines in reference 20. Although one may show that the rule of inserting $D_0^{-1}$ for two-particle-reducible (in terms of fermion propagators) diagrams still applies, it is not essential to have. However, one may choose to use this rule as a tool to ensure correct generation of all distinct diagrams. Equipped with the diagrammatic expansion rules, one may construct
consider \( \Gamma_{t \geq 2} \) following the inversion method described in section III C.

E. Evaluation of \( G_0 \) using single particle orbitals

To calculate \( G_0(x, x') \), we define \( v(x) \equiv v_{\text{ion}}(x) - \mu + J_0(x) \). Since the evaluation of the Green’s function is general, we use the symbol \( G(x, x') \) in place of \( G_0(x, x') \) in the following derivation.

Consider first a generic free fermion Hamiltonian,

\[
H[\hat{\psi}^\dagger, \hat{\psi}] = \int dx \hat{\psi}^\dagger(x) \left(-\frac{\nabla^2}{2m} + v(x)\right) \hat{\psi}(x) = \hat{\psi}^\dagger \hat{h} \hat{\psi}
\]

where

\[
\hat{h}(x, y) = \left(-\frac{\nabla^2}{2m} + v(x)\right) \delta(x - y)
\]

and the corresponding Green’s function (with \( Z \equiv \text{Tr} e^{-\beta H} \))

\[
G(x, y) = \langle T \hat{\psi}(x) \hat{\psi}^\dagger(y) \rangle = Z^{-1} \text{Tr} \left[ e^{-\beta H} T(\hat{\psi}(x) \hat{\psi}^\dagger(y)) \right]
\]

\[
= \theta(\tau_x - \tau_y - \eta) Z^{-1} \text{Tr} \left[ e^{-\beta H} \hat{\psi}(x) \hat{\psi}^\dagger(y) \right] - \theta(\tau_y - \tau_x + \eta) Z^{-1} \text{Tr} \left[ e^{-\beta H} \hat{\psi}^\dagger(y) \hat{\psi}(x) \right].
\]

The positive infinitesimal quantity \( \eta \) is introduced to ensure that in the limit \( \tau_x = \tau_y \), the time ordered product corresponds to normal ordering (represented by the second term at equal time). Note that \( 0 < \tau_x, \tau_y < \beta, -\beta < \tau_x - \tau_y < \beta \) and \( \hat{\psi}(x) = e^{\tau_x H} \hat{\psi}(x) e^{-\tau_x H} \) and \( \hat{\psi}^\dagger(y) = e^{\tau_y H} \hat{\psi}^\dagger(y) e^{-\tau_y H} \). When \( \tau_x - \tau_y < 0 \), one must have \( \tau_x - \tau_y + \beta > 0 \). Observe that

\[
G(\tau_x - \tau_y < 0) = -\text{Tr} \left[ e^{-\beta H} e^{\tau_y H} \hat{\psi}^\dagger(y) e^{-\tau_x H} e^{\tau_x H} \hat{\psi}(x) e^{-\tau_x H} \right] / Z
\]

\[
= -\text{Tr} \left[ e^{\tau_x H} \hat{\psi}(x) e^{-\tau_x H} e^{-\beta H} e^{\tau_y H} \hat{\psi}^\dagger(y) e^{-\tau_y H} \right] / Z
\]

\[
= -\text{Tr} \left[ e^{-\beta H} e^{(\tau_x + \beta) H} \hat{\psi}(x) e^{-\tau_x H} e^{\tau_y H} \hat{\psi}^\dagger(y) e^{-\tau_y H} \right] / Z
\]

\[
= -G(\tau_x - \tau_y + \beta > 0), \quad (89)
\]

where the first equality results from \( \text{Tr}(AB) = \text{Tr}(BA) \), while the final equality results from the definition of the Green’s function with positive time argument \( \tau_x + \beta - \tau_y > 0 \). Similarly, one may easily show that \( G(\tau_x - \tau_y > 0) = -G(\tau_x - \tau_y - \beta < 0) \). Therefore, the Green’s function is antiperiodic in the imaginary time \( \tau \).

Letting \( M(x, y) \equiv \left( \partial_{\tau_x} \delta(x - y) + \hat{h}(x, y) \delta(\tau_x - \tau_y) \right) = \left( \partial_{\tau_x} - \frac{\nabla^2}{2m} + v(x) \right) \delta(x - y) \), we
find

\[ G(x, y) = \langle T \hat{\psi}(x) \hat{\psi}^\dagger(y) \rangle = -\frac{i}{\hbar} \frac{\delta}{\delta \xi(x)} \frac{\delta}{\delta \xi(y)} \langle T e^{i \int \xi \hat{\psi} + \hat{\psi}^\dagger} \rangle_{\xi \to 0, \xi \to 0} \]

\[ = -\frac{\delta}{\delta \xi(x)} \frac{\delta}{\delta \xi(y)} \int \mathcal{D}[\psi^\dagger, \psi] e^{-\psi^\dagger \tau_0 \hbar \psi + \xi \psi + \psi^\dagger \xi} \bigg|_{\xi \to 0, \xi \to 0} \]

\[ = -\frac{1}{\delta \xi(x) \delta \xi(y)} \left[ e^{\xi \tau_0 - \xi} \right]_{\xi \to 0, \xi \to 0} = M^{-1}(x, y). \]

This implies that \(\int dx' M(x, x') G(x', y) = (\partial_{x'} + \hat{h}_x) G(x, y) = \delta(x - y)\) with \(\hat{h}_x\) being a one particle first quantized Hamiltonian \(\hat{h}_x = -\frac{\nabla^2}{2m} + v(x)\). Note that \(\delta(x - y) = \delta(x - y) \delta(\tau_x - \tau_y)\) and the latter delta function in time is defined via \(\int_0^\beta g(\tau_x) \delta(\tau_x - \tau_y) d\tau_x = g(\tau_y)\) for any antiperiodic function \(g(\tau)\). With this understanding, one may express \(\delta(x - y)\) in the following way to obtain \(G(x, y)\). Observing that

\[ (\partial_{x'} + \hat{h}_x) G(x, y) = \langle x | y \rangle = \sum_{\omega_n, \alpha} \langle x | \omega_n, \alpha \rangle \langle \omega_n, \alpha | y \rangle \]

\[ = \sum_{\omega_n, \alpha} \phi_\alpha(x) \phi_\alpha^*(y) e^{-i \omega_n (\tau_x - \tau_y)} \beta, \]

one sees that the action of \((\partial_{x'} + \hat{h}_x)\) may be compensated, leading to

\[ G(x, y) = \sum_{\alpha} \phi_\alpha(x) \phi_\alpha^*(y) \left[ \frac{1}{\beta} \sum_{\omega_n} \frac{e^{-i \omega_n (\tau_x - \tau_y)}}{-i \omega_n + \epsilon_\alpha - \mu} \right], \]

where

\[ \langle x | \omega_n, \alpha \rangle = \phi_\alpha(x) \frac{e^{-i \omega_n \tau_x}}{\sqrt{\beta}}, \]

\[ \omega_n = \frac{\pi (2n + 1)}{\beta}, \]

and

\[ \hat{h}_x \phi_\alpha(x) = \left[ -\frac{\nabla^2}{2m} + v(x) \right] \phi_\alpha(x) = (\epsilon_\alpha - \mu) \phi_\alpha(x). \]

Eq. (93) implies that

\[ \left[ -\frac{\nabla^2}{2m} + v_{\text{ion}}(x) + J_0(x) \right] \phi_\alpha(x) = \epsilon_\alpha \phi_\alpha(x). \]

Only frequencies of the type \(\frac{\pi (2n + 1)}{\beta}\) is included in the expansion to ensure the antiperiodicity of the fermionic Green’s function. To proceed further in (90), one may sum the frequency by introducing a function \(-\beta/(e^{\beta \omega} + 1)\) which has poles at \(\omega = \frac{\pi (2n + 1)}{\beta}\) with residue 1.
Evidently, poles for the function $-\beta/(e^{\beta \omega} + 1)$ occur whenever $e^{\beta \omega} + 1 = 0$. To investigate the strength of each pole, let's rewrite $e^{\beta \omega} + 1$ in the limit when $\omega \to i\pi (2n + 1)/\beta$ as

$$1 + \exp \left( i\pi(2n + 1) + \beta (\omega - \frac{i\pi(2n + 1)}{\beta}) \right) = 1 - \exp \left( \beta (\omega - \frac{i\pi(2n + 1)}{\beta}) \right)$$

$$= -\beta \left( \omega - \frac{i\pi(2n + 1)}{\beta} \right) + O \left( \left( \omega - \frac{i\pi(2n + 1)}{\beta} \right)^2 \right).$$

Therefore, $-\beta/(e^{\beta \omega} + 1)$ indeed has residue strength 1 at each of the allowable frequencies.

To evaluate $\frac{1}{\beta} \sum_{\omega_n} \frac{e^{-i\omega_n (\tau_x - \tau_y)}}{-i\omega_n + \varepsilon_{\alpha} - \mu}$ when $\tau_x < \tau_y$, one integrates over a circular contour (with radius $|\omega| \to \infty$) on the complex $\omega$-plane

$$\frac{1}{\beta} \oint_{|\omega| \to \infty} \frac{e^{-\omega (\tau_x - \tau_y)}}{-\omega + \varepsilon_{\alpha} - \mu e^{\beta \omega} + 1} d\omega.$$

Because the line integral along the infinite circle vanishes, the sum of residues must vanish, meaning that

$$\frac{1}{\beta} \sum_{\omega_n} \frac{e^{-i\omega_n (\tau_x - \tau_y)}}{-i\omega_n + \varepsilon_{\alpha} - \mu} + e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} \frac{1}{e^{\beta (\varepsilon_{\alpha} - \mu)} + 1} = 0.$$

Thus, when $\tau_x \leq \tau_y$ (because when $\tau_x = \tau_y$, it must agree with $\tau_x - \tau_y \to 0^-$) one finds

$$G(x, y) = \sum_\alpha \phi_\alpha(x) \phi_\alpha^*(y) e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} (-n_\alpha).$$

On the other hand, when $\tau_x > \tau_y$, one considers

$$\frac{1}{\beta} \oint_{|\omega| \to \infty} \frac{e^{\omega (\tau_x - \tau_y)}}{\omega + \varepsilon_{\alpha} - \mu e^{\beta \omega} + 1} d\omega.$$

The residue sum then turns into

$$\frac{1}{\beta} \sum_{\omega_n} \frac{e^{-i\omega_n (\tau_x - \tau_y)}}{-i\omega_n + \varepsilon_{\alpha} - \mu} - e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} \frac{1}{e^{-\beta (\varepsilon_{\alpha} - \mu)} + 1} = 0.$$

Thus, when $\tau_x > \tau_y$ one obtains

$$G(x, y) = \sum_\alpha \phi_\alpha(x) \phi_\alpha^*(y) e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} (1 - n_\alpha).$$

Therefore, we have

$$G(x, y) = \sum_\alpha \phi_\alpha(x) \phi_\alpha^*(y) e^{-(\varepsilon_{\alpha} - \mu)(\tau_x - \tau_y)} \begin{cases} (-n_\alpha) & \text{if } \tau_x \leq \tau_y, \\ (1 - n_\alpha) & \text{if } \tau_x > \tau_y, \end{cases}$$

(95)
where \( n_\alpha = 1/(e^{\beta(\varepsilon_\alpha - \mu)} + 1) \). Note that in the expression involving \( \varepsilon_\alpha \), it is always \( \varepsilon_\alpha \) minus the chemical potential \( \mu \).

To evaluate \( G_0(x, y) \), we need to solve the eigen-system (93). It requires evaluations of the RHS of Eq. (79) and self-consistency is reached when \( \kappa(x) \to 0 \). Of course, one cannot evaluate all the terms and must truncate the series on the RHS of Eq. (79) at some stage. This implies that the density profile obtained through the self-consistency condition in this manner depends on the number of terms one includes on the RHS of Eq. (79). Nevertheless, the self-consistent solution obtained when keeping \( k \) terms on the RHS of Eq. (79) can be used as the starting point when one wishes to include \( k + 1 \) terms on the RHS of Eq. (79).

F. Functional derivative of \( G_0(x, x') \) and \( \int d\tau_y G_0(x, y)G_0(y, x') \)

Especially when \( J_0 \) is time-independent, we need to evaluate

\[
\frac{\delta G_0(x, x')}{\delta J_0(y)} = -\int G_0(x, z) \left[ \frac{\delta G_0^{-1}(z, z')}{\delta J_0(y)} \right] G_0(z', x') \, dz \, dz'
\]

\[
= -\int G_0(x, z) \delta(z - z') \delta(y - z) \, G_0(z', x') \, dz \, dz'
\]

\[
= -\int_0^\beta G_0(x, y) G_0(y, x') \, d\tau_y,
\]

where the central expression \( \int_0^\beta G_0(x, y) G_0(y, x') \, d\tau_y \) may be re-expressed by single-particle orbitals as will be shown below.

From Eq. (90), we see that

\[
G(x, y) = \frac{1}{\beta} \sum_{n, \alpha} \frac{e^{-i\omega_n(\tau_x - \tau_y - \eta)}}{-i\omega_n + \varepsilon_\alpha - \mu} \phi_\alpha(x) \phi_\alpha^*(y),
\]

and

\[
G(y, x') = \frac{1}{\beta} \sum_{n', \rho} \frac{e^{-i\omega_n'(\tau_y - \tau_{x'} - \eta)}}{-i\omega_n' + \varepsilon_\rho - \mu} \phi_\rho(y) \phi_\rho^*(x'),
\]

and therefore

\[
\int_0^\beta d\tau_y G(x, y) G(y, x') = \frac{1}{\beta^2} \sum_{n, n', \alpha, \rho} \frac{\phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x')}{-i\omega_n + \varepsilon_\alpha - \mu} \delta_{n, n'} e^{-i\omega_n(\tau_x - \tau_{x'} - 2\eta)}
\]

\[
= \sum_{\alpha, \rho} \left( \frac{1}{\beta} \sum_n \frac{e^{-i\omega_n(\tau_x - \tau_{x'} - 2\eta)}}{-i\omega_n + \varepsilon_\alpha - \mu} \right) \phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x') .
\]

Let us now concentrate on the portion inside the parentheses. Assuming that there is no energy degeneracy, we rewrite the denominator of this factor when \( \alpha \neq \rho \)

\[
\frac{1}{-i\omega_n + \varepsilon_\alpha - \mu} = \frac{1}{\varepsilon_\rho - \varepsilon_\alpha} \left( \frac{1}{-i\omega_n + \varepsilon_\alpha - \mu} - \frac{1}{-i\omega_n + \varepsilon_\rho - \mu} \right)
\]
and when $\alpha = \rho$

\[
\frac{1}{(-i\omega_n + \varepsilon\alpha - \mu)(-i\omega_n + \varepsilon\rho - \mu)} \rightarrow \frac{1}{(-i\omega_n + \varepsilon\alpha - \mu)^2} = -\frac{\partial}{\partial\varepsilon\alpha} \left(\frac{1}{(-i\omega_n + \varepsilon\alpha - \mu)}\right).
\]

Therefore, we need to evaluate $\sum_n \frac{e^{i\omega_n(\tau_x - \tau_x')}}{(-i\omega_n + \varepsilon\alpha - \mu)}$.

We distinguish the two cases: $\tau_x \leq \tau_x'$ and $\tau_x > \tau_x'$. When $\tau_x \leq \tau_x'$, we consider the following integral over the infinite circle

\[
\oint \frac{e^{\omega(\tau_x - \tau_x')}}{-\omega + \varepsilon\alpha - \mu} \frac{-\beta}{e^{\beta\omega} + 1} \frac{d\omega}{2\pi i} = \sum_n \frac{e^{i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu} + \frac{\beta e^{(\varepsilon\alpha - \mu)(\tau_x - \tau_x')}}{e^{\beta(\varepsilon\alpha - \mu)} + 1}.
\]

Since the integral over the infinite circle vanishes, we have

\[
\frac{1}{\beta} \sum_n \frac{e^{i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu} = -\frac{e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')}}{e^{\beta(\varepsilon\alpha - \mu)} + 1} = -e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} n_\alpha.
\]

To evaluate the expression $\frac{1}{\beta} \sum_n \frac{e^{i\omega_n(\tau_x - \tau_x')}}{(-i\omega_n + \varepsilon\alpha - \mu)}$, we consider

\[
-\frac{\partial}{\partial\varepsilon\alpha} \left(\frac{1}{\beta} \sum_n \frac{e^{i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu}\right) = e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} \left[-\beta n_\alpha (1 - n_\alpha) - (\tau_x - \tau_x') n_\alpha\right].
\]

Therefore, when $\tau_x \leq \tau_x'$,

\[
\int_0^\beta d\tau_y G(x, y) G(y, x') = \sum_\alpha \phi_\alpha(x)n_\alpha(y)\phi_\alpha^*(x') e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} \left[-\beta n_\alpha (1 - n_\alpha) - (\tau_x - \tau_x') n_\alpha\right]
\]

\[
+ \sum_{\alpha \neq \rho} \phi_\alpha(x)\phi_\alpha^*(y)\phi_\rho(y)\phi_\rho^*(x') \left[\frac{e^{-(\varepsilon\rho - \mu)(\tau_x - \tau_x')} n_\rho - e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} n_\alpha}{\varepsilon_\rho - \varepsilon_\alpha}\right],
\]

where $n_\alpha(y) = \phi_\alpha^*(y)\phi_\alpha(y)$.

On the other hand, when $\tau_x > \tau_x'$, we consider the integral

\[
\oint \frac{e^{\omega(\tau_x - \tau_x')}}{\omega + \varepsilon\alpha - \mu} \frac{-\beta}{e^{\beta\omega} + 1} \frac{d\omega}{2\pi i} = \sum_n \frac{e^{-i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu} - \frac{\beta e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')}}{e^{-\beta(\varepsilon\alpha - \mu)} + 1},
\]

and obtain (since the integral over the infinite circle vanishes)

\[
\frac{1}{\beta} \sum_n \frac{e^{-i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu} = e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} \left[-\beta n_\alpha (1 - n_\alpha) + (\tau_x - \tau_x') (1 - n_\alpha)\right].
\]

Similarly,

\[
-\frac{\partial}{\partial\varepsilon\alpha} \left(\frac{1}{\beta} \sum_n \frac{e^{-i\omega_n(\tau_x - \tau_x')}}{-i\omega_n + \varepsilon\alpha - \mu}\right) = e^{-(\varepsilon\alpha - \mu)(\tau_x - \tau_x')} \left[-\beta n_\alpha (1 - n_\alpha) + (\tau_x - \tau_x') (1 - n_\alpha)\right].
\]
Therefore, when $\tau_x > \tau_x'$,
\[
\int_0^\beta d\tau_y \, G(x, y) \, G(y, x') = \sum_\alpha \phi_\alpha(x) n_\alpha(y) \phi_\alpha^*(x') e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_x')} \left[ -\beta n_\alpha(1 - n_\alpha) + (\tau_x - \tau_x')(1 - n_\alpha) \right] \\
+ \sum_{\alpha \neq \rho} \phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x') \left[ \frac{e^{-(\varepsilon_\rho - \mu)(\tau_x - \tau_x')n_\rho} - e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_x')n_\alpha}}{\varepsilon_\rho - \varepsilon_\alpha} \right]. \tag{100}
\]

We may now write down the full expression for $\delta G_0(x, x')/\delta J_0(y)$ as
\[
\frac{\delta G_0(x, x')}{\delta J_0(y)} = -\int_0^\beta G_0(x, y) \, G_0(y, x') \, d\tau_y \\
= \sum_\alpha \phi_\alpha(x) n_\alpha(y) \phi_\alpha^*(x') e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_x')} \left[ \beta n_\alpha(1 - n_\alpha) + (\tau_x - \tau_x')n_\alpha \right] \\
- (\tau_x - \tau_x') \theta(\tau_y - \tau_x' - \eta) \sum_\alpha \phi_\alpha(x) n_\alpha(y) \phi_\alpha^*(x') e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_x')} \\
- \sum_{\alpha \neq \rho} \phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x') \left[ \frac{e^{-(\varepsilon_\rho - \mu)(\tau_x - \tau_x')n_\rho} - e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_x')n_\alpha}}{\varepsilon_\rho - \varepsilon_\alpha} \right]. \tag{101}
\]

In the absence of time-dependence, we have
\[
n(x) = \frac{1}{\beta} \frac{\delta (\beta W[J_0])}{\delta J_0(x)} = -\frac{1}{\beta} \int dz dy \, G_0(z, y) \delta(y - x) \delta(y - z) = -G_0(x, x).
\]

Therefore, using Eq. (101) we have
\[
D_0(x, y) = \frac{\delta n(x)}{\delta J_0(y)} = \sum_{\alpha \neq \rho} \phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x) \left[ \frac{n_\rho - n_\alpha}{\varepsilon_\rho - \varepsilon_\alpha} \right] \\
+ \sum_\alpha n_\alpha(x) n_\alpha(y) \left[ \beta n_\alpha(1 - n_\alpha) \right].
\]

Note that the expression $\beta n_\alpha(1 - n_\alpha)$ vanishes as $\beta \to \infty$, because $n_\alpha(1 - n_\alpha)$ decays exponentially with $\beta$ when $\mu \neq \varepsilon_\alpha$. That is, at the zero temperature limit, one has
\[
D_0(x, y) \to \sum_{\alpha \neq \rho} \phi_\alpha(x) \phi_\alpha^*(y) \phi_\rho(y) \phi_\rho^*(x) \left[ \frac{n_\rho - n_\alpha}{\varepsilon_\rho - \varepsilon_\alpha} \right]
\]
as long as $\mu$ is not equal to any eigenenergy of the orbital.

G. The Computational Procedure

The recipe for computation goes as follows. Starting with a reasonably guessed $J_0(x)$, one first obtains single particle wave functions $\phi_\alpha$ and energies $\varepsilon_\alpha$ through (94). Note that the occupation number of state $\alpha$ is given by
\[
n_\alpha = \frac{1}{e^{\beta(\varepsilon_\alpha - \mu)} + 1}
\]
and the chemical potential is chosen such that
\[ g_s \sum_{\alpha} n_{\alpha} = N_e , \]
where \( g_s \) denotes the spin degeneracy (\( g_s = 2 \) for spin 1/2 electrons).

Through eqs. (95), (82), and (81), one constructs respectively the \( G_0, D_0^{-1}, \) and \( \tilde{D}_0 \) propagators. Combined with their differentiation rules (83-85) with respect to \( J_0 \), these propagators are used to compute \( \delta \Gamma / \delta J_0 \).

As the third step, one obtains a new estimate of \( J_0 \) given by \( J_0 - \varsigma \delta \Gamma / \delta J_0 \) with \( \varsigma > 0 \) being the step size. See eq. (79) and the text nearby for details.

Finally, one starts again with the new \( J_0 \) and goes through the other steps, iteratively until the convergence condition \( \delta \Gamma / \delta J_0 = 0 \) is reached. This simultaneously determines \( J_0 \) (sum of the Hartree potential and the KS potential), the ground state charge density and the ground state energy, as well as the KS orbitals and energies.

IV. CASE STUDIES

A. The Universal Functional \( \mathcal{F}[n] \) at Arbitrary Temperature

There are vast discussions\(^{18,20,21}\) on the equivalence between \( E_\nu[n] \) in (1-2) and \( \lim_{\beta \to \infty} \frac{1}{\beta} \Gamma[n] \). However, not much attention was given to the emergence of the universal functional \( \mathcal{F}[n] \) (at any given temperature) resulting from the effective action formalism. We address here for the first time how \( \mathcal{F}[n] \) arises naturally from our effective action formulation.

Fukuda et al.\(^{18}\) showed that it is possible to eliminate the \( \nu \) dependence in the functional to obtain (when translated into our terms)
\[ \Gamma_\nu[i\varphi] = \Gamma_{\nu=0}[i\varphi] + \nu_0(i\varphi) + \frac{1}{2} \nu_0 U^{-1} \nu_0. \]
They interpret \( i\varphi \) as some sort of electron density since it coincides with the real electron density when \( J = 0 \). The appearance of the quadratic term in \( \nu \), however, disagrees with (2) where it is clearly stated that in addition to a term that is linear in \( \nu \), the remainder should be \( \nu \)-independent. We settle this discrepancy below by showing that the appearance of the quadratic \( \nu \) dependence is due to the fact that reference 18 did not use the system’s electron density as the natural variable. Once the system’s electron density is used as the natural variable, the universal functional \( \mathcal{F}[n] \) emerges naturally.
Note that (10) indicates that one may view $\nu_{\text{ion}}(x)$ as a nonvanishing source term. In the change of variable $\phi \to \phi + i U^{-1} \circ J$ right after (17), if we make $\phi \to \phi + i U^{-1} \circ (J + \nu)$ instead, we see that $\nu$ is then bonded with $J$ from that point on. That said, we may view $W[J] \equiv W'[J + \nu]$. That is, the generating functional in the presence of the one-body potential $\nu$ with source $J$ is equivalent to the generating functional of a system without a one-body potential but with source $J + \nu$. Following the algebra in Eqs. (21-46), one sees that

$$
\beta W[J] = \beta W'_\phi[J + \nu] - \frac{1}{2} (J + \nu) \circ U^{-1}(J + \nu),
$$

where

$$
\beta W'_\phi[J + \nu] = \frac{1}{2} \varphi \circ U \circ \varphi - \text{Tr} \ln \left( G^{-1}_\varphi \right) + i (J + \nu) \circ \varphi 
$$

$$
+ \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) - \sum_{n=1}^{\infty} \frac{1}{n!} \left\{ \sum_{k=3}^{\infty} I^{(k)} \circ b_1 \ldots \circ b_k \right\}_{1\text{PI, conn.}}^n 
$$

$$
G^{-1}_\varphi(x, x') = \left( \partial - \frac{\nabla^2}{2m} - \mu + i (U \circ \varphi) \right) \delta(x - x').
$$

Upon using the following variant of (25)

$$
n = i \varphi - U^{-1} \circ (J + \nu),
$$

the quadratic term in $J + \nu$ in (102) gets absorbed into the density of the electron and one arrives at the following variant of (44)

$$
\beta W[J] = \beta W'[J + \nu] = - \text{Tr} \ln \left( \tilde{G}^{-1}_\varphi \right) - \frac{1}{2} n \circ \nu \circ n + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}^{-1} \circ U \right) 
$$

$$
- \sum_{n=1}^{\infty} \frac{1}{n!} \left\{ \sum_{k=3}^{\infty} I^{(k)} \circ b_1 \ldots \circ b_k \right\}_{1\text{PI, conn.}}^n.
$$

Note that here $n = n = n'_{J + \nu}$ represents the electron density of the system.

The effective action $\Gamma[n] = \beta W[J] - J \circ n$ can thus be rewritten as

$$
\Gamma[n] = \beta W'[J + \nu] = \nu \circ n + \beta W'[J + \nu] - (J + \nu) \circ n,
$$

where the first term on the RHS represents $\beta \int n(x) \nu(x) d\mathbf{x}$, and the last two terms represent the effective action, $\Gamma'[n] = \beta W'[J + \nu] - (J + \nu) \circ n$, of a system in the absence of one-body potential. We thus identify $\mathcal{F}[n]$ as

$$
\mathcal{F}[n] = \frac{1}{\beta} \{ \beta W'[J + \nu] - (J + \nu) \circ n \}.
$$

This also serves as an alternative exposition of what Mermin proved.3
B. Effective Potential near Zero Temperature

The effective potential divided by $\beta$ is the ground state energy plus $\mu N_e$ in the $T \to 0$ limit. Below, we will show how the Hartree-Fock terms appear in this formulation.

Equations (47-73) provide a systematic expansion for calculating the effective potential. In the expression (60), the term $-\text{Tr} \ln(G^{-1})$ is equivalent to $-\ln[\det(G^{-1})]$. There are many ways to obtain $\det(G^{-1})$: one may obtain the results directly through the definition of $e^{-\beta W_0[J_0]}$ or one may express $e^{-\beta W_0[J_0]}$ as a path integral to obtain the determinant in discrete time. We shall denote $-\text{Tr} \ln(G^{-1})$ by $\beta W_0[J_0]$ with

$$e^{-\beta W_0[J_0]} = \text{Tr} \left\{ e^{-\beta \left[ \hat{\psi}^\dagger (\hat{h}+J_0) \hat{\psi} \right]} \right\} = \int D[\psi^\dagger, \psi] e^{-\int dx \psi^\dagger (x) \left[ \partial_x + \hat{h} + J_0(x) \right] \psi(x)}$$

$$= \int D[\psi^\dagger, \psi] e^{-\psi^\dagger \phi_0^{-1} \psi} = \det(G^{-1}).$$

Direct evaluation using the trace definition leads to

$$\det(G^{-1}) = \prod_\alpha (1 + e^{-\beta (\epsilon_\alpha - \mu)}),$$

and consequently

$$W_0[J_0] = -\frac{1}{\beta} \text{Tr} \ln(G^{-1}) = -\frac{1}{\beta} \sum_\alpha \ln (1 + e^{-\beta (\epsilon_\alpha - \mu)}) = \frac{1}{\beta} \sum_\alpha \ln (1 - n_\alpha).$$

Note that the energy is measured with respect to the chemical potential $\mu$. Therefore, in the limit of $\beta \to \infty$, we have

$$\lim_{\beta \to \infty} W_0[J_0] = -\frac{1}{\beta} \text{Tr} \ln(G^{-1}) = \sum_{\alpha=1}^{N_e} (\epsilon_\alpha - \mu),$$

with $\epsilon_\alpha \leq \mu$ for $1 \leq \alpha \leq N_e$.

Using Eqs. (80) and (103), we obtain the low temperature limit of the effective action

$$\lim_{\beta \to \infty} \left( \frac{1}{\beta} \Gamma[n] \right) = \sum_{\alpha=1}^{N_e} (\epsilon_\alpha - \mu) - J_0 \cdot n + \frac{1}{2} n \cdot U \cdot n$$

$$+ \lim_{\beta \to \infty} \left[ \frac{1}{2\beta} \text{Tr} \ln(\tilde{D}_0^{-1} U) + \frac{1}{\beta} \sum_{i=2}^{\infty} \Gamma_i[n] \right].$$

The first term in (104) can be expressed in a different way if we multiply both sides of Eq. (93) by $\phi_\alpha^\dagger(x)$, sum $\alpha$ over the lowest $N_e$ states, and integrate over $x$. Upon doing this,
we obtain
\[ N_e \sum_{\alpha=1}^{N_e} (\varepsilon_{\alpha} - \mu) = \sum_{\alpha=1}^{N_e} \int d\mathbf{x} \phi_\alpha^*(\mathbf{x}) \left[ -\frac{\nabla^2}{2m} + v_{\text{ion}}(\mathbf{x}) - \mu + J_0(\mathbf{x}) \right] \phi_\alpha(\mathbf{x}) \]
\[ \equiv T_0[n] - \mu N_e + \int d\mathbf{x} [v_{\text{ion}}(\mathbf{x}) + J_0(\mathbf{x})] n(\mathbf{x}) , \]
where
\[ n(\mathbf{x}) = \sum_{\alpha=1}^{N_e} \phi_\alpha^*(\mathbf{x}) \phi_\alpha(\mathbf{x}) , \]
and
\[ T_0[n] \equiv \sum_{\alpha=1}^{N_e} \int d\mathbf{x} \phi_\alpha^*(\mathbf{x}) \left[ -\frac{\nabla^2}{2m} \right] \phi_\alpha(\mathbf{x}) . \]

Therefore, the first two terms in (104) give us
\[ \sum_{\alpha=1}^{N_e} (\varepsilon_{\alpha} - \mu) - J_0 \cdot n = T_0[n] - \mu N_e + \int d\mathbf{x} v_{\text{ion}}(\mathbf{x}) n(\mathbf{x}) . \]

Evidently, the third term in (104) is nothing but the Hartree energy
\[ \frac{1}{2} n \cdot U \cdot n = \frac{1}{2} \int d\mathbf{x} d\mathbf{y} n(\mathbf{x}) \frac{e^2}{|\mathbf{x} - \mathbf{y}|} n(\mathbf{y}) . \]

Therefore, we have
\[ \lim_{\beta \to \infty} \left( \frac{1}{\beta} \Gamma[n] \right) = T_0[n] + \int v_{\text{ion}}(\mathbf{x}) n(\mathbf{x}) d\mathbf{x} - \mu N_e + \frac{1}{2} \int d\mathbf{x} d\mathbf{y} \frac{e^2}{|\mathbf{x} - \mathbf{y}|} n(\mathbf{y}) \]
\[ + \lim_{\beta \to \infty} \frac{1}{2\beta} \text{Tr} \ln (\mathbf{I} - D_0 U) + \lim_{\beta \to \infty} \left[ \frac{1}{\beta} \sum_{i=2}^{\infty} \Gamma_i[n] \right] , \quad (105) \]

with the last two terms combined to form the exchange-correlation energy functional when compared with the Kohn-Sham decomposition (4).

If \( D_{0^\circ} U \) (or \( e^2 \)) may be treated as a small quantity, one may expand \( \frac{1}{2\beta} \text{Tr} \ln (\mathbf{I} - D_0 U) \) as
\[ \frac{1}{2\beta} \text{Tr} \ln (\mathbf{I} - D_0 U) = -\frac{1}{2\beta} \sum_{n=1}^{\infty} \frac{\text{Tr} [(D_0 U)^n]}{n} , \quad (106) \]

with the leading term (in the static limit)
\[ -\frac{1}{2\beta} \int d\mathbf{x} d\mathbf{y} D_0(x, y) u(y, x) = \frac{-e^2}{2} \int d\mathbf{x} d\mathbf{y} \frac{n(\mathbf{x}, \mathbf{y}) n(\mathbf{y}, \mathbf{x})}{|\mathbf{x} - \mathbf{y}|} , \]
where \( n(x, y) = \sum_{m=1}^{N_e} \phi_m(x) \phi_m^*(y) = -G_0(x, \tau; y, \tau) \). Consequently, when \( D_0 \circ U \) (or \( e^2 \)) can be treated as a small quantity, we may write the leading terms of the effective potential as

\[
\lim_{\beta \to \infty} \frac{1}{\beta} \Gamma[n] = T_0[n] + \int \psi_{\text{ion}}(x)n(x)dx - \mu N_e + \frac{e^2}{2} \int dx dy \frac{n(x)n(y) - n(x,y)n(y,x)}{|x - y|}
\]

\[
+ \lim_{\beta \to \infty} \left[ -\frac{1}{2\beta} \sum_{n=2}^{\infty} \frac{1}{n} \text{Tr} \left[ (D_0 \circ U)^n \right] + \frac{1}{\beta} \sum_{i=2}^{\infty} \Gamma_i[n] \right],
\]

where the fourth term is nothing but the Hartree-Fock term. The higher-order terms inside the square brackets encode the remaining contributions of exchange and correlation. In the case when the Coulomb interaction is strong, one may choose not to use the expansion in Eq. (106), but to use (105) for the zero temperature limit and (80) for finite temperature.

### C. Single Electron at Zero Temperature

When the system contains only one electron and when the energy difference between the first excited state and the ground state is much larger than \( k_B T \), there will be no particle-hole pairs. Consequently, there should be no exchange-correlation energy as well as the Hartree energy. When one employs empirical density functionals, this feature is unlikely to be preserved – an issue known as the self-interaction problem. It is customary to define the exchange-correlation energy \( E_{xc} \) as the sum of the Fock exchange energy \( E_x \) and the correlation energy \( E_c \). Since it is easy to show that the exchange energy \( E_x \) exactly cancels the Hartree energy in the case of one electron, one easily concludes that \( E_c = 0 \) for the one electron case. This argument has been used, for example, by Perdew and Zunger. However, from the diagrammatic expansion point of view, the Hartree term and the Fock exchange term correspond only to the first order (in terms of \( e^2 \)) diagrams. The cancellation of the first order terms does not imply that the higher order diagrams, making up \( E_c \), will give no contribution. That is, although the fact that \( E_c = 0 \) for one electron system can be argued, a formal diagrammatic exposition incorporating all higher orders is needed to justify the asymptotic exactness of the proposed functional.

The purpose of this section is to illustrate how \( E_c = 0 \) can be derived formally within our formalism. It should be noted, however, that the self-interaction will remain if one truncate the series in eq. (80). While the exchange-only functional will have no self-interaction problem, as we will show below it is not because the exchange-only functional is an approach with more correct physics, but because the simplification it makes is equivalent to completely
ignoring the correlation energy.

When \( N_e = 1 \) and when \( T \to 0 \), we find from Eq. (95) that the Green’s function \( G_0(x, y) \) takes the following form

\[
G_0(x, y) = \begin{cases} 
\phi_1(x)\phi_1^*(y)e^{-(\varepsilon_1 - \mu)(\tau_x - \tau_y)}(-1) & \text{if } \tau_x \leq \tau_y \\
\sum_{\alpha \geq 2} \phi_\alpha(x)\phi_\alpha^*(y)e^{-(\varepsilon_\alpha - \mu)(\tau_x - \tau_y)} & \text{if } \tau_x > \tau_y
\end{cases}
\]

(108)

where \( \varepsilon_1 < \mu < \varepsilon_{\alpha \geq 2} \) and \( \phi_{1(\rho)}(x) \) is the ground \((\rho^{th})\) state wave function of the single particle Hamiltonian

\[
\hat{h}(x) = -\frac{\nabla^2}{2m} + v_{\text{ion}}(x) + J_0(x) - \mu
\]

with eigenvalue \( \varepsilon_{1(\rho)} - \mu \).

The disappearance of the Hartree energy and the exchange-correlation energy is best seen by grouping terms with the same number of Coulomb lines \( U \). We will explicitly show the first few calculations followed by a sketch of the general proof.

Let us first show that the first term \((n = 1)\) on the RHS of (106) cancels the Hartree term exactly. When there is only one electron, the Hartree term becomes

\[
\frac{e^2}{2} \int dxdy n(x)n(y) \frac{\phi_1(x)\phi_1^*(y)}{|x - y|} = \frac{e^2}{2} \int dxdy \phi_1(x)\phi_1^*(x)\phi_1(y)\phi_1^*(y) |x - y|
\]

The Fock term \((n = 1 \text{ term of order } U \text{ in (106)})\), when there is only one electron, reads,

\[
\frac{-1}{2\beta} \text{Tr} [D_0^\circ U] = \frac{-1}{2\beta} \int dxdy D_0(x, y)U(y, x) = \frac{-e^2}{2} \int dxdy \phi_1(x)\phi_1^*(x)\phi_1(y)\phi_1^*(y) |x - y|
\]

The cancellation between the Fock term and the Hartree term is thus apparent. If one were to approximate the exchange-correlation functional by the Fock exchange functional, correlation energy can never be accounted for. That is, this approximation coincidently leads to the expected result \( E_c = 0 \) at the single electron limit simply because it never takes \( E_c \) into account.

In terms of diagrammatic expression, the Hartree term is given by diagram (a) of Fig. 2, while the lowest order exchange term \((n = 1 \text{ term of (106)})\) corresponds to diagram (b) of Fig. 2. That is, the order \( U \) diagrams in \( \frac{1}{\beta} \Gamma[n] \) are identical to the order \( U \) diagrams in \( W[J_0] \) at zero temperature. The perfect cancellation between the Hartree term and the lowest order exchange term implies that the sum of these two terms remains zero when one makes a derivative with respect to either \( J_0 \) or \( n \). Diagrammatically speaking, this means
that when the system contains only one electron, we have

\[
\begin{align*}
0 = \frac{\delta}{\delta J_0} & = \left\{ \frac{\delta}{\delta n} \left[ \frac{1}{2} \quad \cdots 
\quad \cdot \quad - \frac{1}{2} \right] \right\}, \\
0 = \frac{\delta}{\delta n} & = \left\{ \frac{\delta}{\delta n} \left[ \frac{1}{2} \quad \cdots 
\quad \cdot \quad - \frac{1}{2} \right] \right\}.
\end{align*}
\]

(109)

Terms of the next order in \( U \) are contained in \( \Gamma_{i \leq 2} \). See Fig. 4 for a diagrammatic expression of \( \Gamma_{i \leq 2} \) of order \( U^2 \) (or of order \( e^4 \)). We show below that in Fig. 4 the first two graphs cancel each other and the last two diagrams also cancel each other. For illustration, we will work out the explicit cancellation of the first two graphs by labelling the space-time points. The cancellation of the the last two graphs require additional operations which we will turn to later. The first two graphs in Fig. 4 with the space-time points labelled appear to be

\[
\frac{1}{4} \quad x_1 \quad \cdots \quad x_2 \quad - \frac{1}{4} \quad y_1 \quad \cdots \quad y_2
\]

\[
= \int \! d\tau_x d\tau_y \prod_{i=1}^{2} d \mathbf{x}_i d \mathbf{y}_i \frac{\mathcal{G}_0(x_1, y_1)(\mathcal{G}_0(x_2, y_2)}{4|x_1 - x_2| |y_1 - y_2|} \times \times [\mathcal{G}_0(y_1, x_2)\mathcal{G}_0(y_2, x_1) - \mathcal{G}_0(y_1, x_1)\mathcal{G}_0(y_2, x_2)]
\]

(110)

We have used \( \tau_x \) to denote the time associated with both \( x_1 \) and \( x_2 \), while denoting by \( \tau_y \) the time associated with both \( y_1 \) and \( y_2 \). When \( \tau_y \leq \tau_x \), the quantity inside the square brackets of Eq. (110) vanishes because

\[
\mathcal{G}_0(y_i, x_j) \propto \phi_1(y_i)\phi_1^*(x_j),
\]

and thus \( \mathcal{G}_0(y_1, x_2)\mathcal{G}_0(y_2, x_1) = \mathcal{G}_0(y_1, x_1)\mathcal{G}_0(y_2, x_2) \). When \( \tau_y > \tau_x \), we simply swap the dummy variable \( y_1 \) and \( y_2 \) in the second graph above to arrive at

\[
\int \! d\tau_x d\tau_y \prod_{i=1}^{2} d \mathbf{x}_i d \mathbf{y}_i \frac{\mathcal{G}_0(y_1, x_2)(\mathcal{G}_0(y_2, x_1)}{4|x_1 - x_2| |y_1 - y_2|} [\mathcal{G}_0(x_1, y_1)\mathcal{G}_0(x_2, y_1) - \mathcal{G}_0(x_1, y_2)\mathcal{G}_0(x_2, y_1)].
\]

And again the quantity inside the square brackets vanishes due to the same reason as before.

As for the cancellation of the last two graphs in Fig. 4, we first use the bottom portion of (109) to obtain

\[
0 = \frac{\delta}{\delta n} \left[ \frac{1}{2} \quad \cdots 
\quad \cdot \quad - \frac{1}{2} \right] = - \cdots + \quad \cdot,
\]

\[
0 = \frac{\delta}{\delta n} \left[ \frac{1}{2} \quad \cdots 
\quad \cdot \quad - \frac{1}{2} \right] = - \cdots + \quad \cdot,
\]

\[
0 = \frac{\delta}{\delta n} \left[ \frac{1}{2} \quad \cdots 
\quad \cdot \quad - \frac{1}{2} \right] = - \cdots + \quad \cdot,
\]
and then

\[ 0 = \frac{1}{2} \left[ - \begin{array}{c} \circ \ldots \circ \\ - \end{array} + \begin{array}{c} \circ \ldots \circ \\ + \end{array} \right] (\equiv)^{-1} \left[ - \begin{array}{c} \circ \ldots \circ \\ - \end{array} + \begin{array}{c} \circ \ldots \circ \\ + \end{array} \right], \]

or

\[ -\frac{1}{2} \begin{array}{c} \circ \ldots \circ \\ - \end{array} = \frac{1}{2} \begin{array}{c} \circ \ldots \circ \\ - \end{array}, \]  

(111)

when there is only one electron in the system.

Equation (111) means that at the single electron limit, the last two graphs in Fig. 4 are equivalent to the last three graphs in Fig. 5. In other words, at the single electron limit and at zero temperature, the set of order \( U^2 \) diagrams in \( \Gamma[n] \) is equivalent to the set of order \( U^2 \) diagrams in \( \beta W[J_0] \). We shall pause at this point and elucidate the general situation by looking at these cancellations via Hugenholtz diagrams.\(^{29}\)

With a two-body interaction term such as the Coulomb interaction, typical Feynman diagrams treat the direct (Coulomb) and exchange matrix elements separately. It is not surprising that one may simplify the calculation by combining the direct and exchange matrix elements into a single antisymmetrized matrix element. The basic idea is to combine the following two scenarios into one

\[ \begin{array}{c} \gamma \\ \alpha \end{array} \rightarrow \begin{array}{c} \delta \\ \rho \end{array} - \begin{array}{c} \gamma \\ \alpha \end{array} \rightarrow \begin{array}{c} \delta \\ \rho \end{array} \equiv \begin{array}{c} \gamma \\ \alpha \end{array} \rightarrow \begin{array}{c} \delta \\ \rho \end{array} \]

\[ (\gamma \delta | v | \alpha \rho) - (\gamma \delta | v | \rho \alpha) \equiv \{ \gamma \delta | v | \alpha \rho \}, \]  

(112)

where

\[ (\gamma \delta | v | \alpha \rho) \equiv \int d\tau_x d\tau_y d\mathbf{x} d\mathbf{y} \phi^*_\gamma(x) \phi^*_\delta(y) v(x, y) \phi_\alpha(x) \phi_\rho(y), \]

and

\[ \{ \gamma \delta | v | \alpha \rho \} \equiv \int d\tau_x d\tau_y d\mathbf{x} d\mathbf{y} \phi^*_\gamma(x) \phi^*_\delta(y) v(x, y) [\phi_\alpha(x) \phi_\rho(y) - \phi_\rho(x) \phi_\alpha(y)], \]

with \( \phi_\alpha(x) \) being the single-particle wave function described earlier in Eq. (93). The resulting diagrams with bullet dots as the new vertices are called Hugenholtz diagrams. The appearance of those vertex matrix elements comes from the following. When one evaluates a Feynman diagram, a propagator \( G_0(x, x') \) going from \( x' \) to \( x \) connects two vertices located at \( x' \) and \( x \) respectively. From Eq. (95), we know that

\[ G_0(x, x') = \sum_\alpha \phi_\alpha(x) \phi^*_\alpha(x') e^{-(\epsilon_\alpha - \mu)(\tau_x - \tau_{x'})} \left\{ \begin{array}{ll} -n_\alpha & \text{if } \tau_x \leq \tau_{x'} \\ 1 - n_\alpha & \text{if } \tau_x > \tau_{x'} \end{array} \right. \]
Upon integration of the space-time coordinates, we see that \( \phi_\alpha(x) \) will be integrated with vertex \( x \), whither the propagator leads, while \( \phi_\alpha^*(x') \) will be integrated with vertex \( x' \), whence the propagator originates. Therefore, when evaluating a Feynman diagram, one may associate each propagator going from time \( \tau' \) to time \( \tau \) with a state index \( \alpha \) with

\[
G_0(\alpha, \tau - \tau') = e^{-(\varepsilon_\alpha - \mu)(\tau - \tau')} \left[ (1 - n_\alpha) \theta(\tau - \tau - \eta) - n_\alpha \theta(\tau' - \tau + \eta) \right].
\]

Each vertex will contribute a numerical factor equivalent to its vertex matrix element. Note that each vertex carries a time index. At zero temperature, for a vertex with time index \( \tau \), if the two incoming lines originate from vertices with times larger than or equal to \( \tau \), the vertex matrix element associated with \( \tau \) becomes zero in the single electron limit. This is because both incoming lines each carry only the \( \alpha = 1 \) index. Upon antisymmetrization, the Hugenholtz vertex matrix element becomes zero.

For an arbitrary Hugenholtz diagram with \( n \) vertices, one may always name their time index such that \( \tau_1 \leq \tau_2 \leq \tau_3 \leq \cdots \leq \tau_n \). In this case, the vertex associated with \( \tau_1 \) gives zero matrix element since its two incoming lines must come from two other time indices that are larger than or equal to \( \tau_1 \). Consequently, each Hugenholtz diagram yields value zero at zero temperature when there is only one electron present. As a matter of fact, the order \( U \) diagrams of \( W[J_0] \) are represented by the Hugenholtz diagram \( \text{H} \). On the other hand, the first two graphs of Fig. 4 (order \( U^2 \) terms of \( \Gamma[n] \)) correspond to the Hugenholtz diagram \( \text{H} \), while the last two graphs of Fig. 4 (order \( U^2 \) terms of \( \Gamma[n] \)) are equivalent to the last three graphs of Fig. 5 (order \( U^2 \) terms of \( \beta W[J_0] \)) and correspond to the Hugenholtz diagram \( \text{H} \) (see reference 29). Therefore, we see that all the order \( U^2 \) terms cancel each other out in the effective action \( \Gamma[n] \).

If one were to expand the effective action (80) in powers of \( U \), our approach reduces to performing the inversion method using \( e^2 \) as the expansion parameter.\(^{19,20}\) In this case, \( W_{l \geq 1}[J_0] \) in Eqs. (47-73) contains exactly all the order \( U^l \) diagrams in \( W[J_0] \) and can be expressed as Hugenholtz diagrams of order \( U^l \) as well. Since all the Hugenholtz diagrams give value zero, all the derivatives of \( W_l \) (all the order \( u^l \) diagrams) with respect to the density vanish as well. This implies that all the \( J_{l \geq 1} \) vanish and consequently in the effective action the sum of Hartree energy and the exchange-correlation energy equals zero at zero temperature when there is only one electron present.

The perfect cancellation of the Hartree energy and exchange-correlation energy means
that one is the negative of the other. This means that \( \sum_{i=1}^{\infty} \Gamma_i = -\frac{1}{2} n_0 U \cdot n \). Employing Eq. (77) for the most general case, we obtain

\[
\tilde{J}_0 - J = - \frac{1}{2} \frac{\delta (n_0 U \cdot n)}{\delta n} = -U \cdot n.
\]

Since \( J_0 = \tilde{J}_0 + U \cdot n \), we find that \( J_0 = J \) at the single electron limit at zero temperature. The fact that \( J_0 = J \) means that the final effective potential \( \varepsilon_1 - \mu - J \cdot n \) is nothing but the lowest eigenenergy of the following single-particle Hamiltonian

\[
\hat{h}(x) = -\frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + J
\]

less the expectation value of \( J \), which is exactly what one expected.

**D. Screening of Coulomb Interaction**

In the physical limit, \( n = i \varphi \). In our formulation, lumps of charge fluctuation around the configuration \( i \varphi \) interact with each other via

\[
U \circ D_0^{-1} U = (U - U \circ D_0 \circ U).
\]

As will be described in the discussion section, \( U \circ (i \phi) = ib \) plays the role of the photon field here. Therefore,

\[
-(\varphi_0 (U - U \circ D_0 \circ U) \circ \phi = (i \phi_0 U) \circ D_0^{-1} \circ (U \circ i \phi) = (ib) \circ (U^{-1} - D_0) \circ (ib).
\]

Since \( U(x, y) = \delta(\tau_x - \tau_y)U(x, y) \) and \( G_0(x, y) \) only depends on the relative time difference \( \tau_x - \tau_y \), we expect \( D_0(x, y) \) to depend only on \( \tau \equiv \tau_x - \tau_y \). Furthermore, since \( G_0(x, y) \) is antiperiodic in \( \tau_x, \tau_y \), and \( \tau_x - \tau_y \), one expects that \( G_0(x, y)G_0(y, x) \) to be periodic in \( \tau_x - \tau_y \).

Introducing the spatial momenta \( p \) and \( q \) conjugate to the spatial variables \( x \) and \( y \), we may write

\[
[U^{-1} - D_0](\nu_n, p, q) = \int e^{ipx + iqv} dx dy \int_0^\beta d\tau e^{i\nu_n \tau} [U^{-1}(x, y) \delta(\tau) - G_0(x, y)G_0(y, x)].
\]

When \( U(x, y) = \frac{\varepsilon^2}{|x-y|} \), we find that \( U^{-1}(x, y) = -\frac{1}{4\pi \varepsilon^2} \delta(\tau_x - \tau_y) \nabla_x^2 \delta(x - y) \) and

\[
U^{-1}(\nu_n, p, q) = \frac{(2\pi)^3}{4\pi \varepsilon^2} q^2 \delta(p + q) = \frac{L^3}{4\pi \varepsilon^2} q^2 \delta(p + q),
\]

where \( L^3 \) is the spatial volume of the system. Let us now write \( D_0(\nu_n, p, q) \) as

\[
D_0(\nu_n, p, q) = \int e^{ipx + iqv} dx dy \int_0^\beta d\tau e^{i\nu_n \tau} G_0(x, y)G_0(y, x).
\]
In momentum space, \( U^{-1} \propto q^2 \delta(p + q) \) and it is well known that this type of Coulomb interaction leads to infrared divergence (that occurs near \( q \to 0 \)). In the presence of \(-D_0\), one may wish to calculate the zero momentum contribution of \(-D_0\). Let us define \( D_0(\nu_n) \equiv D_0(\nu_n, p = 0, q = 0) \). Using Eq. (95), we find

\[
D_0(\nu_n) = -\sum_{\alpha, \alpha'} \delta_{\alpha, \alpha'} \int_0^\beta d\tau e^{i\nu_n \tau} [n_\alpha(1 - n_{\alpha'})] = -\beta \delta_{\nu_n, 0} \sum_\alpha n_\alpha(1 - n_\alpha) .
\]

(113)

From Eq. (101), we see that when \( x = x' \),

\[
\beta \sum_\alpha n_\alpha(1 - n_\alpha) = -\int dx \frac{\partial G_0(x, x)}{\partial \mu} = \frac{\partial N_e}{\partial \mu} .
\]

We therefore have

\[
D_0(\nu_n) = -\delta_{\nu_n, 0} L^3 \frac{\partial \bar{n}}{\partial \mu} ,
\]

where \( \bar{n} = N_e / L^3 \) is the average electron density.

Therefore at the stationary limit, where \( \nu_n = 0 \), the inverse propagator with nearly zero momentum behaves as

\[
L^3 \left[ \frac{q^2}{4\pi \varepsilon^2} + \frac{\partial \bar{n}}{\partial \mu} \right] \Rightarrow \frac{L^3}{4\pi \varepsilon^2} \left[ q^2 + 4\pi \varepsilon^2 \frac{\partial \bar{n}}{\partial \mu} \right] ,
\]

analogous to the Thomas-Fermi results for electric charge screening.

Except during the intermediate steps of computing the excitation spectrum, one deals with the time independent system. Note that \( 4\pi \varepsilon^2 \frac{\partial \bar{n}}{\partial \mu} \) plays the role of \( m^2 \) in the screened potential \( e^{-mr}/r \). This shows that the static interaction between charge fluctuations in the long wave length limit is a screened one instead of the bare Coulomb interaction. It should be noted that the use of this screened propagator dates back half a century. DuBois\(^{46}\) replaced the bare Coulomb interaction by the screened interaction in his study of electron interactions. Hedin\(^{31}\) also used it to replace the bare Coulomb interaction in the expansion of the Luttinger-Ward functional,\(^{25}\) resulting in the so-called GW approximation. The differences among the three mentioned approaches should be described. In both DuBois’s and Hedin’s formalism, they use the \textit{full} polarization of the interacting system. The difference between their formalism is in the electron propagators employed. In DuBois’s approach, the free electron propagator is used, while in Hedin’s method, similar to the Luttinger-Ward functional,\(^{25}\) the \textit{full} electron propagator is employed. In our approach, it is the polarization of the KS system that enters the calculation and the electron propagator entering the diagrammatic calculation is the noninteracting KS Green’s function.
E. Homogeneous Electron Gas

Being the foundation for the LDA of the DFT, the homogeneous electron gas (HEG) is also a simplified model for a metal or a plasma. The HEG system is an interacting electron gas placed in a uniformly distributed positive background chosen to ensure that the total system is neutral. Due to the translational symmetry of the HEG system, the one-particle propagator functions only depend on the coordinate difference between two variables (space-time points) instead of on both variables. Consequently, each propagator (Green’s function) carries a definite momentum even if the Coulomb interaction among electrons is fully taken into consideration.

Investigation of the HEG system dates back to 1930s by Wigner, who coined the term “correlation energy” to represent the ground state energy per electron after subtracting away the average kinetic and exchange energy. (The Hartree energy is cancelled exactly by the interaction between electrons and the positive background, and by the Coulomb energy among the uniform positive charges.) Apparently, after choosing the Rydberg (the negative of the Hydrogen atom ground state energy) as the energy unit, one may express either the correlation energy or the ground state energy of the HEG system in terms of the dimensionless quantity $r_s \equiv r_0/r_B$, where $\frac{4\pi}{3}r_0^3 = \frac{V}{N_e}$, $V$ being the volume of the system considered, $N_e$ being the total number of electrons, and $r_B = \frac{\hbar^2}{me^2}$ representing the Bohr radius. In fact, efforts have been invested to express the correlation energy as a power series in $r_s$ (and $r_s \ln r_s$ as well) at both the high density and low density limits. Lacking real experimental results to compare with, however, it is hard to assess how much improvement each increasing order of $r_s$ (or $1/r_s$) can bring.

Since $r_s \propto 1/r_B \propto e^2$, a small $r_s$ expansion is most naturally performed by treating the Coulomb interaction as a perturbation. Equivalent to the method of computing the vacuum amplitude, the time-ordered perturbative expansion developed by Goldstone formalized the Brueckner theory and made a direct connection to diagrammatic expansion in calculation of the ground state energy. The electron propagator in diagrams under this formalism is that of the noninteracting electrons. An alternative formalism to compute the ground state energy (or the grand potential) is to utilize the full propagator (i.e., the one with self-energy included) in diagrammatic calculation. Under this alternative formalism, only two-particle irreducible diagrams contribute. Indeed, the work of Luttinger and Ward...
(as well as that of Klein\textsuperscript{52}) was exactly along this line. Since the self-energy is not known \textit{a priori}, this type of energetic expression is a functional of the self-energy (or the full Green’s function), which must be determined via a stationary condition.\textsuperscript{25}

An equivalent of the Brueckner-Goldstone formalism\textsuperscript{50,53} was used by Gell-Mann and Brueckner\textsuperscript{54} to compute the correlation energy of the HEG system. Given the long-range nature of the Coulomb interaction, it is not surprising that Gell-Mann and Brueckner identified the occurrence of divergence as early as in the second order of $e^2$-based perturbative calculation. To circumvent this unphysical divergence, DuBois\textsuperscript{46} replaced the bare Coulomb interaction by the screened one. Starting with calculating the vacuum amplitude, he expressed the ground state energy in terms of integration of the \textit{full} electronic polarization over the Coulomb coupling strength, using a version of the Feynman-Hellmann theorem. While the full polarization is used, the electron propagator entering DuBois’s formalism is the free electron propagator instead of the full propagator. Unfortunately, DuBois made a mistake in extracting the higher order terms of the ground state energy at the high density (small $r_s$) limit. Although this error was later corrected by Carr and Maradudin,\textsuperscript{55} according to Hedin,\textsuperscript{31} this high density expansion violated at moderate $r_s$ values Ferrell’s condition,\textsuperscript{56} which is based on the simple fact that the second order perturbation contribution to the ground state energy is always negative.

Except for using the screened Coulomb interaction to replace the bare one and working directly at zero temperature, Hedin’s approach is largely similar to the finite-temperature formalism of Luttinger and Ward\textsuperscript{25} in the sense that the \textit{full} electron propagator is used as the fundamental variable. As a consequence, the higher order diagrams contributing to the full polarization appear different in DuBois’s work and in Hedin’s formalism. Instead of solving his own self-consistent equations, however, Hedin approximated the \textit{full} Green’s function within his formalism by the \textit{non-interacting} Green’s function to compute the energetics of the HEG system. Nevertheless, it is still possible to maintain the exactness within Hedin’s approach if two-particle reducible diagrams are properly included. We will provide an example of such a two-particle reducible diagram that would not be included in Hedin’s approximate calculation but should be incorporated for theoretical soundness.

Another important issue in obtaining the ground state energy of a many-electron system has to do with whether the finite temperature formalism (setting $V \to \infty$ first followed by
$T \to 0$) or the zero temperature formalism (setting $T \to 0$ and then followed by $V \to \infty$) is used. In terms of diagrammatic expansion, there exist diagrams (termed anomalous diagrams by Luttinger et al.\textsuperscript{25,57}) that are present (giving finite contribution) within the finite temperature formalism but are absent (giving zero contribution) within the zero temperature formalism. To be specific, a diagram is anomalous if within it there exist two electron propagators linking two different times (say $\tau_1$, $\tau_2$ and of course $\tau_1 \neq \tau_2$) in the opposite orders: $\mathcal{G}(x, \tau_1, y, \tau_2)\mathcal{G}(w, \tau_2, z, \tau_1)$.

Zero temperature methods typically rely on the Gell-Mann and Low theorem,\textsuperscript{58} which assures that adiabatic transformation of the noninteracting ground state by gradually switching on the interaction leads to an eigenstate of the interacting system.\textsuperscript{29,48} The energetic difference of this eigenstate and the noninteracting ground state is what the zero temperature formalism obtains. This approach therefore makes sense only if the adiabatically transformed state is the ground state of the interacting system, which occurs only if the noninteracting Fermi surface is identical to that of the interacting system.\textsuperscript{49} For the HEG system, the perturbed Fermi surface remains spherical (identical to that of the unperturbed one) since the Coulomb interaction respects spherical symmetry and the background positive charge distribution also has spherical symmetry. Consequently, for the HEG system, the anomalous diagrams should end up giving no contribution. Indeed, Luttinger et al.\textsuperscript{25,57} illustrated how the contributions from the anomalous diagrams in this case are cancelled by the chemical potential shift. Luttinger and Ward\textsuperscript{25} also showed how one may avoid anomalous contributions from appearing by expressing the grand potential as a sum of all possible linked diagrams (including two-particle reducible ones). The key step there is to subtract from each self-energy part a number, which is given by that self-energy part evaluated at the Fermi surface. As we will illustrate later, under our finite temperature formalism it is not necessary to implement such an elaborate subtraction scheme because each two-particle reducible diagram is automatically accompanied by another appropriate diagrammatic subtraction.

What sets our self-consistent equation (78) apart from that of Luttinger and Ward and of Hedin is the variable to be solved for. It is the KS potential, instead of the physical Green’s function, that enters our exact, self-consistent equation. In general, one needs to first solve $\tilde{J}_0$ self-consistently using eq. (78) prior to the evaluation of the grand potential (or the ground state energy). When limiting to a homogeneous system with constant electron density,
However, $\tilde{J}_0 = \text{const.}$ becomes the only possibility. Whether or not such a choice satisfies the self-consistent equation (78) depends on whether a uniform electron density truly represents the lowest energy configuration. For the present purpose of considering a high density HEG, we assume a constant $\tilde{J}_0$ to proceed. Because a constant $\tilde{J}_0$ can be easily absorbed into the chemical potential, the resulting KS Green's function carries a corresponding energy that consists of kinetic energy only. That is, rather than being an approximation as in Hedin's case, the single-particle Green's function carrying only kinetic energy represents exactly the self-consistent KS Green's function under our formalism. Consequently, for the HEG system, the grand potential (or the ground state energy) may be calculated using eq. (80).

In the remaining part of this section, we will first show how our formalism naturally avoids divergence and how one may use it to obtain the ground state energy of the HEG as a series in $r_s$ (and $\ln r_s$). We will then illustrate with an explicit example how the anomalous contributions are cancelled within our formalism, followed by a brief description of diagrams that would be missed within Hedin's approximation in computing the ground state energy of the HEG system. To provide an easier comparison with existing results, we restore in this section the electron spins that have been suppressed thus far to simplify the exposition.

In our definition of the energy functional $E_\nu$, see eq. (4), the $-\mu N_e$ term is included but the interaction among background charges is not included. Since most zero temperature formalism does not include the $-\mu N_e$ term and for the HEG system the interaction between background charges is also included, the ground state energy in the literature will correspond to

$$E_g = \lim_{\beta \to \infty} \left[ \frac{1}{\beta} \Gamma[n] + \mu N_e + \frac{1}{2} m_{bg} \cdot U \cdot m_{bg} \right]$$

in our formalism. Eq. (104) can then be used to arrive at

$$E_g = \lim_{\beta \to \infty} \left[ \frac{1}{\beta} \Gamma[n] + \mu N_e + \frac{1}{2} m_{bg} \cdot U \cdot m_{bg} \right]$$

$$= \sum_{\alpha=1}^{N_e} \epsilon_\alpha - J_0 \cdot n + \frac{1}{2} n \cdot U \cdot n + \frac{1}{2} m_{bg} \cdot U \cdot m_{bg} + \lim_{\beta \to \infty} \left[ \frac{1}{2\beta} \text{Tr} \ln \left( \tilde{D}_0^{-1} U \right) + \frac{1}{\beta} \sum_{i=2}^{\infty} \Gamma_i[n] \right]$$

$$= \sum_{\alpha=1}^{N_e} \left( \epsilon_\alpha - \tilde{J}_0 \right) + \lim_{\beta \to \infty} \left[ \frac{1}{2\beta} \text{Tr} \ln \left( \tilde{D}_0^{-1} U \right) + \frac{1}{\beta} \sum_{i=2}^{\infty} \Gamma_i[n] \right],$$

where $J_0 = \tilde{J}_0 + U \cdot n$ is used and $m_{bg} = n$ for the HEG system is also employed. Note that the state label $\alpha = (p, \sigma)$ includes both momentum and spin. For the HEG system, $v_{\text{ion}} + U \cdot n = 0$ and thus eq. (94) leads to $\epsilon_\alpha = p^2/2m + \tilde{J}_0$. Therefore, the ground state
energy of the HEG system may be written as

\[
E_g = 2 \sum_{\mathbf{p}} \frac{|\mathbf{p}|^2}{2m} + \lim_{\beta \to \infty} \frac{1}{\beta} \left[ \frac{1}{2} \text{Tr} \ln \left( \mathbf{D}_0^{-1} U \right) + \sum_{i=2}^{\infty} \Gamma_i[n] \right],
\]

(115)

where \( p_F \) indicates the Fermi momentum and the factor of 2 in the first term of the right hand side comes from noting that there are two spin states associated with each momentum. Furthermore, the KS Green’s function in this case may be written as

\[
G_0(x,\sigma;y,\sigma') = \frac{1}{\beta V} \sum_{p,n} \frac{e^{-i\omega_n(\tau_x-\tau_y)}e^{-ip(x-y)}}{-i\omega_n + \varepsilon_p + \tilde{J}_0 - \mu} \delta_{\sigma,\sigma'},
\]

(116)

where \( \varepsilon_p = p^2/2m \) is the kinetic energy of an electron carrying momentum \( p \). By absorbing the constant \( \tilde{J}_0 \) into the chemical potential in (116), one sees that the KS Green’s function in the HEG system is indeed the free electron propagator and at the zero temperature, the new chemical potential (the original one subtracted by \( \tilde{J}_0 \)) simply becomes \( p_F^2/2m \). The diagrammatic expression of our first correction term \( \Gamma_1[n] = \frac{1}{2} \text{Tr} \ln \left( \mathbf{D}_0^{-1} U \right) = \frac{1}{2} \text{Tr} \ln \left( \mathbf{I} - D_0 \circ U \right) \) is shown in Fig. 1. It can be seen that, upon being divided by the inverse temperature \( \beta \), our \( \Gamma_1[n] \) contains the exchange energy \( \varepsilon_x \) and all the ring-like correlation energy \( \varepsilon' \) discussed by Gell-Mann and Brueckner\(^{54}\) via the relation \( \Gamma_1[n]/\beta = N_e(\varepsilon_x + \varepsilon') \), with \( N_e \) being the total number of electrons. Since both \( D_0 \) and \( U \) are diagonal in momentum space for the HEG system, we may write

\[
\frac{1}{\beta} \Gamma_1[n] = \frac{1}{2\beta} \sum_{q,\nu_0} \ln \left[ 1 - D_0(q,\nu_0) U(q) \right] = \frac{V}{2\beta} \int \frac{dq}{(2\pi)^3} \sum_{\nu_0} \ln \left[ 1 - D_0(q,\nu_0) U(q) \right].
\]

(117)

By comparing this equation to a derived result (eq. (30.16) of reference 48), it is also evident that our \( \Gamma_1[n]/(\beta N_e) \) indeed gives \( \varepsilon_x + \varepsilon' \) of reference 54 as \( \beta \to \infty \). In Fig. 1, except for the first diagram, all other diagrams when evaluated individually exhibit infrared divergence due to the piling up of \( 1/|q|^2 \) propagators.\(^{54}\) To obtain the leading contribution, one must pay particular attention to the small \(|q|\) region.

The polarization \( D_0 \equiv \delta n(x)/\delta J_0(y) \) is defined in eq. (71). When the electron spins are included, \( n(x) = -\sum_{\sigma} G_0(x,\sigma;x,\sigma) \). Because the Coulomb interaction does not flip spins, the KS propagator is diagonal in the electron spins and thus

\[
D_0(x, y) = \sum_{\sigma} G_0(x, \sigma; y, \sigma) G_0(y, \sigma; x, \sigma) = 2 G_0(x, y) G_0(y, x).
\]

(118)
We therefore have

\[ D_0(q, \nu_n) = 2 \int d(x - y)d(\tau_x - \tau_y)e^{i q \cdot (x - y)}d^\nu_n(\tau_x - \tau_y) \left[ G_0(x, y)G_0(y, x) \right] \]

\[ = \frac{2}{\beta} \sum_{n'} \int \frac{d p}{(2\pi)^3} \frac{1}{(-i \omega_{n'} - i \nu_n + \epsilon_{p+q} - \epsilon_p)(-i \omega_{n'} + \epsilon_p - \mu)} \]

\[ = 2 \int \frac{d p}{(2\pi)^3} \frac{n_{p+q} - n_p}{-i \nu_n + \epsilon_{p+q} - \epsilon_p} \]

\[ = -2 \int \frac{d p}{(2\pi)^3} n_p(1 - n_{p+q}) - n_{p+q}(1 - n_p) \]

\[ = -2 \int \frac{d p}{(2\pi)^3} n_p \left[ \frac{1}{-i \nu_n + \epsilon_{p+q} - \epsilon_p} + \frac{1}{i \nu_n + \epsilon_{p+q} - \epsilon_p} \right] \]

\[ = -2 \int \frac{d p}{(2\pi)^3} n_p \left[ \frac{1}{(\epsilon_{p+q} - \epsilon_p) + \nu_n^2} \right] = -4 \int \frac{d p}{(2\pi)^3} n_p(\epsilon_{p+q} - \epsilon_p) \]

where the third line of the above equation is obtained using the technique described in section III E, the fourth line is obtained by rewriting the numerator of the third line as 

\[-n_p(1 - n_{p+q}) + n_{p+q}(1 - n_p), \]

the fifth line is obtained by a change of variable \((p + q \rightarrow -p)\) in the second half and assuming the spherical property of \(n_p\), and the sixth line comes from the fact that \(n_p n_{p+q}\) is symmetric with respect to \((p + q) \leftrightarrow p\) while the quantity inside the square bracket is antisymmetric with respect to \((p + q) \leftrightarrow p\). Since \(\epsilon_p \propto |p|^2\) is a monotonic increasing function of \(|p|\), while both \(n_p = 1/(e^{\beta |p|^2} + 1)\) and \(1 - n_p\) are nonnegative, we see that \(D_0(q, \nu_n)\) is a negative definite quantity.

It turns out that for the HEG system one can further simplify the expression of \(D_0(q, \nu)\) by introducing a new variable \(u\) via \(\nu \equiv u|q|/m\). We then have (by choosing \(\hat{q}\) as the \(\hat{z}\) direction in \(p\) and using the fact that \(n_p = n(|p|) = n(p)\))

\[ D_0(q, \frac{u q}{m}) = -2 \int \frac{d p}{(2\pi)^3} n_p \left[ \frac{1}{-i u q/m + \epsilon_{p+q} - \epsilon_p} + \frac{1}{i u q/m + \epsilon_{p+q} - \epsilon_p} \right] \]

\[ = -2 \frac{m}{q} \int_0^\infty \frac{n(p) p^2 dp}{(2\pi)^2} \int_{-1}^1 d \cos \theta \left[ \frac{1}{-i u q/2 + p \cos \theta} + \frac{1}{i u q/2 + p \cos \theta} \right] \]

\[ = -2 \frac{m}{q} \int_0^\infty \frac{n(p) dp}{(2\pi)^2} p \left[ \ln \left( \frac{q}{2} + p + i u \right) + \ln \left( \frac{q}{2} + p - i u \right) \right. \]

\[ - \ln \left( \frac{q}{2} - p + i u \right) - \ln \left( \frac{q}{2} - p - i u \right) \]

\[ = \frac{2m}{(2\pi)^2} \int_0^\infty \frac{\partial n(p)}{\partial p} dp \left[ p + \frac{1}{2q} \left( p^2 + u^2 - \frac{q^2}{4} \right) \ln \left( \frac{p + \frac{q}{2}}{p - \frac{q}{2}} \right)^2 + u^2 \right. \]

\[ - u \tan^{-1} \frac{q}{2} + p + u \tan^{-1} \frac{q}{2} - p \left. \right] \].

(120)
As $\beta \to \infty$, $n(p) = \theta(p_F - p)$ and therefore $\partial n(p)/\partial p = -\delta(p - p_F)$, leading to

$$D_0(q, \frac{uq}{m}) \xrightarrow{\beta \to \infty} -\frac{2m}{(2\pi)^2} \left[ p_F + \frac{1}{2q} \left( p_F^2 + u^2 - \frac{q^2}{4} \right) \ln \left( \frac{p_F + \frac{q}{2} + u^2}{p_F - \frac{q}{2} + u^2} \right) \right.$$  

$$\left. -u \tan^{-1} \left( \frac{q + p_F}{u} \right) + u \tan^{-1} \left( \frac{q - p_F}{u} \right) \right].$$  \hspace{1cm} (121)

The exact expression (121) allows one to extract the limits of $q \to \infty$ and $q \to 0$, both of which are important for determining the convergence properties of the energy expansion. We have

$$D_0(q \gg 1, \frac{uq}{m}) \xrightarrow{\beta \to \infty} -\frac{4m p_F^3}{3\pi^2 q^2 + 4u^2} + \mathcal{O} \left( (q^2 + 4u^2)^{-2} \right) ,$$  \hspace{1cm} (122)

$$D_0(q \ll 1, \frac{uq}{m}) \xrightarrow{\beta \to \infty} -\frac{m}{\pi^2} \left[ R_0(u) + R_1(u) q^2 + R_2(u) q^4 \right] + \mathcal{O} \left( q^6 \right) ,$$  \hspace{1cm} (123)

where

$$R_0(u) \equiv p_F - u \tan^{-1} \frac{p_F}{u} ,$$  \hspace{1cm} (124)

$$R_1(u) = -\frac{p_F^3}{12(p_F^2 + u^2)^2} ,$$  \hspace{1cm} (125)

$$R_2(u) = -\frac{p_F^3 (p_F^2 - 5u^2)}{240(p_F^2 + u^2)^4} .$$  \hspace{1cm} (126)

With these asymptotic behaviors, we see from eq. (117) that $\Gamma_1[n]$ is finite. Methods for extracting coefficients associated with the $e^2$-based expansion for $\epsilon'$ can be found in references 54 and 55. The $\epsilon' = \lim_{\beta \to \infty} \Gamma_1[n]/(N_e \beta) - \epsilon_x$ part contains in general $r_s^{n \geq 0} \ln r_s$ and $r_s^{n \geq 0}$ terms when the energy is expressed in Rydbergs and expanded in power of $r_s$ (or $e^2$).

We now turn our attention to $\Gamma_2[n]$, whose diagrammatic expression is given in Figure 3. As mentioned earlier, within our formalism, $\Gamma_{i \geq 2}[n]$ correspond to diagrams containing only $\tilde{D}_0$ propagator and the KS electron propagator. Since the $\tilde{D}_0$ propagator retains a finite value even when its associated momentum approaches zero, each of the diagrams corresponding to $\Gamma_{i \geq 2}[n]$ takes a finite value. The absence of divergence no longer holds when one perform high density (small $r_s$) expansion, as we will illustrate explicitly later. To make easy comparison with existing HEG studies, one employs Dyson’s equation,

$$\tilde{D}_0 = U + U \circ D_0 \circ \tilde{D}_0$$  \hspace{1cm} (127)
to decompose the propagator $\tilde{D}_0$ (of order $e^2$ and higher) into the sum of a bare Coulomb propagator $U$ (of order $e^2$) and $U \circ D_0 \circ \tilde{D}_0$ (of order $e^4$ and higher). The reason that one should not expand further and write $\tilde{D}_0 = U + U \circ D_0 \circ U + U \circ D_0 \circ U \circ D_0 \circ \tilde{D}_0$ is because the $U \circ D_0 \circ U$ term causes infrared divergence due to the momentum integral $\int dq / q^4$. In fact, this is exactly what causes (in the second diagram of Figure 1) the infrared divergence, motivating the summation of the ring diagrams.

To illustrate the main points, let us begin by examining the first three diagrams of $\Gamma_2[n]$ and employ the decomposition rule mentioned above:

\begin{equation}
\frac{1}{4} \begin{pmatrix} p_1 + q \\ -p_2 \\ -p_2 - q \end{pmatrix} = \frac{1}{4} \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \frac{1}{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \frac{1}{4} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (128)
\end{equation}

\begin{equation}
\frac{1}{2} \begin{pmatrix} -p_1 - q \\ -p_2 - q \\ -p_1 - q \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \frac{1}{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (129)
\end{equation}

\begin{equation}
-\frac{1}{2} \begin{pmatrix} p_2 \\ q \\ p_2 \\ p_1 \\ p_1 \\ q \end{pmatrix} = \frac{1}{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} - \frac{1}{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (130)
\end{equation}

Let us start with the diagrams to the left of the equal signs in (128-130). We will for now keep the bosonic propagators general, that is, allowing them to carry frequencies. After that, we will discuss the (a) diagrams in (128-130), followed by the (b) diagrams and then the (c) diagrams.

In (128), let the vertical boson propagator, denoted by $B_1$, carry momentum $q$ (upward) and frequency $\nu$. Let the horizontal boson propagator, denoted by $B_2$, carry momentum $q' \equiv -(p_1 + p_2 + q)$ (leftward) and frequency $\nu'$. Using techniques described in section III E
for frequency summation, one obtains the following generic result

\[
\beta V \sum_{\nu,\nu'} \frac{1}{2} \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \frac{dq}{(2\pi)^3} B_1(q, \nu) B_2(q', \nu') \left\{ \frac{n_{p_2} - n_{p_1}}{\epsilon_{p_2} - \epsilon_{p_1} - i(\nu + \nu')} + \frac{n_{p_1} - n_{p_1+q'}}{\epsilon_{p_1+q'} - \epsilon_{p_1} - i\nu'} + \frac{n_{p_2+q'} - n_{p_1+q'}}{\epsilon_{p_2+q'} - \epsilon_{p_1+q'} + i(\nu - \nu')} \right\},
\]

or equivalently,

\[
\beta V \sum_{\nu,\nu'} \frac{1}{2} \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \frac{dq}{(2\pi)^3} B_1(q, \nu) B_2(q', \nu') \left\{ \frac{n_{p_2} - n_{p_1}}{\epsilon_{p_2} - \epsilon_{p_1} - i(\nu + \nu')} + \frac{n_{p_1} - n_{p_1+q'}}{\epsilon_{p_1+q'} - \epsilon_{p_1} - i\nu'} + \frac{n_{p_2+q'} - n_{p_1+q'}}{\epsilon_{p_2+q'} - \epsilon_{p_1+q'} + i(\nu - \nu')} \right\}.
\]

Note that the factor 2 associated with \( \frac{2}{\beta^2} \) comes from the two possible spin states for an electron.

In (129), let the boson propagator on top, denoted by \( B_1 \), carry momentum \( q \) (towards lower-right) and frequency \( \nu \). Let the boson propagator at the bottom, denoted by \( B_2 \), carry momentum \( q' \equiv (p_1 - p_2) \) (towards upper-left) and frequency \( \nu' \). Using techniques described in section III E for frequency summation, one obtains the following generic result

\[
\beta V \sum_{\nu,\nu'} \frac{1}{2} \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \frac{dq}{(2\pi)^3} B_1(q, \nu) B_2(q', \nu') \left\{ \frac{n_{p_1+q} - n_{p_1+q'}}{\epsilon_{p_1+q} - \epsilon_{p_1} - i\nu'} + \frac{n_{p_1-q} - n_{p_2+q'}}{\epsilon_{p_1-q} - \epsilon_{p_1} + i(\nu - \nu')} \right\}.
\]

In (130), let the boson propagator at the right hand side, denoted by \( B_1 \), carry momentum \( q \) (downwards) and frequency \( \nu \). Let the boson propagator at the left hand side, denoted by \( B_2 \), carry momentum \( q' \) (also downwards) and frequency \( \nu' \). Using techniques described in section III E for frequency summation, one obtains the following generic result

\[
-\beta V \sum_{\nu,\nu'} \frac{1}{2} \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \frac{dq}{(2\pi)^3} B_1(q, \nu) B_2(q', \nu') \left\{ \beta n_{p_1+q}(1 - n_{p_1+q}) + n_{p_1+q} - n_{p_2+q'} + \frac{n_{p_1+q} - n_{p_1}}{\epsilon_{p_1+q} - \epsilon_{p_1} + i(\nu - \nu')} \right\}.
\]

where the factor \(-1/\left\{2\beta \int \frac{dp}{(2\pi)^3} n_p (1 - n_p)\right\}\) arises from the fact that in a translationally invariant system, momentum conservation at each vertex demands that the inverse density correlator must carry zero momentum and frequency.
For the diagram (a) on the right hand side of eq. (128), \(B_1(q, \nu) = 4\pi e^2/q^2\) and \(B_2(q', \nu') = 4\pi e^2/(p_1 + p_2 + q)^2\) are both frequency independent. Thus, one may sum over both \(\nu\) and \(\nu'\). And upon doing so, we obtain

\[
\frac{1}{4\beta} \int = V \int \frac{dp_1 dp_2 dq}{(2\pi)^3 (2\pi)^3 (2\pi)^3} \frac{(4\pi e^2)^2}{q^2} (p_1 + p_2 + q)^2 n_{p_1}.n_{p_2}(1 - n_{p_1 + q})(1 - n_{p_2 + q}).
\]

If we divide the quantity above by \(N_e\) and then take the zero temperature limit, it gives rise to (using \(p_F\) as the unit for momentum)

\[
\frac{m p_F^2}{N_e(2\pi)^9} (4\pi e^2)^2 \int_{|p_i|<|p_i+q|>1} dq dp_1 dp_2 \frac{1}{q^2 (p_1 + p_2 + q)^2 q^2 + q \cdot (p_1 + p_2)} = \left[ \frac{3}{16\pi^3} \int_{|p_i|<|p_i+q|>1} dq dp_1 dp_2 \frac{1}{q^2 (p_1 + p_2 + q)^2 q^2 + q \cdot (p_1 + p_2)} \right]_{\text{Rydberg}},
\]

which is exactly the \(\epsilon_b^{(2)}\) term of Gell-Mann and Brueckner.\(^{54}\)

Diagram (a) on the right hand side of eq. (129) is one of the anomalous diagrams\(^{25,57}\) that give rise to finite contribution as the \(T \to 0\) limit is taken within finite temperature formalism but are absent within zero temperature formalism. For this diagram, \(B_1(q, \nu) = 4\pi e^2/q^2\) and \(B_2(q', \nu') = 4\pi e^2/(p_1 - p_2)^2\) are both frequency independent. Thus, one may evaluate its zero temperature contribution by summing over both \(\nu\) and \(\nu'\). Upon doing so, one obtains from diagram (a) of (129) the following anomalous contribution

\[
\frac{1}{2\beta} \int = -(V) \int \frac{dp_1 dp_2 dq}{(2\pi)^9} \frac{4\pi e^2}{q^2} (p_1 - p_2)^2 \beta n_{p_1 + q}(1 - n_{p_1 + q}) n_{p_2 + q} n_{p_1}.
\]

where the last expression is obtained via the following change of variables: \(p_1(2) \to -p_1(2) - q\), eliminating \(p_2\) by \(q' \equiv p_1 - p_2\), and \(q' \to -q'\). This expression can be further simplified via the following definition

\[
f(p) \equiv \int \frac{dq}{(2\pi)^3} \frac{1}{q^2} n_{p + q},
\]

leading to

\[
\frac{1}{2\beta} \int = -(V)(4\pi e^2)^2 \int \frac{dp_1}{(2\pi)^3} \beta n_{p_1}(1 - n_{p_1}) f^2(p_1),
\]

As mentioned earlier, each two-particle reducible diagram within our formalism is accompanied by a corresponding diagram that will eliminate anomalous contribution when
applicable. Diagrams in eq. (130), appearing only under the effective action formalism, are such diagrams. They are neither present in the zero temperature formalism of Goldstone\textsuperscript{50} and Brueckner\textsuperscript{51} nor in the finite temperature formalism of Luttinger and Ward.\textsuperscript{25} Diagram (a) on the right hand side of (130) corresponds to the case $B_1(q, \nu) = 4\pi e^2/q^2$ and $B_2(q', \nu') = 4\pi e^2/(q')^2$, both being frequency independent. Thus, upon summing over both $\nu$ and $\nu'$, one obtains

\[
-\frac{1}{2\beta} \begin{array} {c}
\end{array} = \frac{2(-1)^2V(4\pi e^2)^2}{2\beta \int \frac{dp}{(2\pi)^3} n_p (1 - n_p) \int \frac{dp_1 dp_2 dq dq'}{(2\pi)^4} \frac{4\pi e^2}{q^2} \frac{4\pi e^2}{q'^2} \times \beta^2 n_{p_1}(1 - n_{p_1}) n_{p_2}(1 - n_{p_2}) n_{p_1+q} n_{p_2+q'} \quad (137)
\]

\[
= \frac{V(4\pi e^2)^2}{\int \frac{dp}{(2\pi)^3} \frac{\partial n_p}{\partial \mu} f(p)} \left[ \int \frac{dp}{(2\pi)^3} \frac{\partial n_p}{\partial \mu} f(p) \right]^2 \quad (138)
\]

When combined with eq. (136), one obtains

\[
\frac{1}{2\beta} \begin{array} {c}
\end{array} - \frac{1}{2\beta} \begin{array} {c}
\end{array} = -V(4\pi e^2)^2 \left( \int \frac{dp}{(2\pi)^3} \frac{\partial n_p}{\partial \mu} \right) (f - \bar{f})^2, \quad (139)
\]

where the overline symbol is defined as $\bar{f} \equiv \int \frac{dp}{(2\pi)^3} \frac{\partial n_p}{\partial \mu} f(p)$. Apparently, the expression (139) is in general negative unless $f = \bar{f}$. We will show that this happens only at zero temperature and only if the system has spherical symmetry.

In order to have $f(p) = \bar{f}$, $p$ can only have support at a constant $f(p)$ surface. This is achieved when $T \to 0$, where $n_p \to \theta(\mu - \varepsilon_p)$ and $\partial n_p/\partial \mu = \delta(\mu - \varepsilon_p)$ forcing $p$ to lie on a constant $\varepsilon_p$ surface. Furthermore, $f(p) = \bar{f}$ demands that $f(p)$ depends only on the magnitude of $p$, i.e., $f(p) = f(p)$. This can only be achieved if $n_p$ depends only on $|p| = p$. For the HEG system, $\varepsilon_p = p^2/2m$, thus $n_p = n(p)$ and $\mu = p_F^2/2m$. We therefore have $\partial n_p/\partial \mu = m\delta(p - p_F)/p_F$, fixing the length of $p$. Now $n_{p+q} = \theta(\mu - (p + q)^2/2m)|_{p=p_F} = \theta(-\cos \vartheta - \frac{q}{2p_F})$, with $\vartheta$ being the angle between $q$ and $p$. Thus, in the integral defining $f(p)$, although $\hat{p}$ defines the $\hat{z}$ direction of vector $q$ the integral is independent of the choice of $\hat{p}$. Therefore, the anomalous contribution (136) may be written as (when $T \to 0$)

\[
-(V) \left[ \int \frac{dp_1}{(2\pi)^3} \frac{m}{p_F} \delta(p_1 - p_F) \right] \left[ \int_{-1}^{1} dx \int_{0}^{\infty} \frac{q^2 dq}{(2\pi)^2} \frac{4\pi e^2}{q^2} \theta(-x - \frac{q}{2p_F}) \right]^2, \quad (140)
\]
while the corresponding subtraction term (138) may be written as

\[
\frac{V}{\beta(2\pi)^3} \frac{m}{p_F} \delta(p_1 - p_F) \left[ \int_0^{p_F} \frac{d\mathbf{p}_1}{(2\pi)^3} \frac{m}{p_F} \delta(p_1 - p_F) \right]^2 \left[ \int_{-1}^{1} dx \int_0^{\infty} \frac{q^2 dq}{(2\pi)^2} \frac{4\pi e^2}{q^2} \theta \left( -x - \frac{q}{2p_F} \right) \right]^2 = V \left[ \int_0^{p_F} \frac{d\mathbf{p}_1}{(2\pi)^3} \frac{m}{p_F} \delta(p_1 - p_F) \right] \left[ \int_{-1}^{1} dx \int_0^{\infty} \frac{q^2 dq}{(2\pi)^2} \frac{4\pi e^2}{q^2} \theta \left( -x - \frac{q}{2p_F} \right) \right]^2 ,
\]

cancelling exactly the anomalous contribution (140) in the HEG case.

Within the framework of Luttinger et al., the anomalous contribution is cancelled by the chemical potential shift, the difference between \( \mu(T \to 0) \), under finite temperature formalism, and \( \mu(T = 0) = p_F^2 / 2m \), under zero temperature formalism. Within the current finite temperature framework, however, the \( \mu(T \to 0) \) is identical to \( \mu(T = 0) \) and the cancellation of anomalous contribution is explicit. As we will show later, however, diagram (b) of (129) can’t be cancelled by diagram (b) of (130). This is because diagram (b) of (129) is not an anomalous diagram.

Before moving onto (b) diagrams in (128-130), let us remark that diagrams within our formalism, i.e., diagrams on the left hand side of (128-130) with \( B_{1(2)} \to \mathcal{D}_0 \) yield only finite contribution. The decomposition made in (128-130), however, may introduce divergence as we will illustrate using the (b) diagrams that correspond to the main results of DuBois.

For the (b) diagram of (128), \( B_2(q', \nu') = 4\pi e^2/(p_1 + p_2 + q)^2 \) while \( B_1(q, \nu) = (4\pi e^2)^2 D_0(q, \nu) / \{ q^2[q^2 - 4\pi e^2 D_0(q, \nu)] \} \). Therefore, one may sum over \( \nu' \) to simplify the expression. Using again the methods described in section III E for frequency summation, one obtains

\[
\frac{1}{2\beta} \int \frac{dp_2}{(2\pi)^3} \frac{dp_1}{(2\pi)^3} \frac{dq}{(2\pi)^3} D_0(q, \nu) \frac{1}{q^2(q^2 - 4\pi e^2 D_0(q, \nu)) (p_1 + p_2 + q)^2} \times \\
\times \frac{n_{p_1+q} - n_{p_1}}{-i\nu + \varepsilon_{p_1+q} - \varepsilon_{p_1}} \frac{n_{p_2+q} - n_{p_2}}{i\nu + \varepsilon_{p_2+q} - \varepsilon_{p_2}} \\
= \frac{V}{\beta(2\pi)^3} \sum_{\nu} \int \frac{dp_1}{(2\pi)^3} \frac{dp_2}{(2\pi)^3} \frac{dq}{(2\pi)^3} D_0(q, \nu) \frac{1}{q^2(q^2 - 4\pi e^2 D_0(q, \nu)) (p_1 - p_2)^2} \times \\
\times \frac{n_{p_1+q} - n_{p_1}}{-i\nu + \varepsilon_{p_1+q} - \varepsilon_{p_1}} \frac{n_{p_2+q} - n_{p_2}}{-i\nu + \varepsilon_{p_2+q} - \varepsilon_{p_2}} ,
\]

where the last expression is obtained by changing variables: \( p_2 + q \to -p_2' \) followed by \( p_2' \to p_2 \). For the high density expansion, where \( e^2 \) is treated as a small parameter, the major contribution in (142) comes from the region \( q \to 0 \). One thus writes

\[
n_{p+q} - n_p \bigg|_{q \to 0} (\varepsilon_{p+q} - \varepsilon_p) \frac{\partial n_p}{\partial \varepsilon_p} = -\beta n_p (1 - n_p)(\varepsilon_{p+q} - \varepsilon_p) \bigg|_{T \to 0} \to -q \cos \vartheta \delta(p - p_F) ,
\]
where $\vartheta$ is the angle between $p$ and $q$. As $T \to 0$, $\frac{1}{\beta} \sum_n F(\nu_n) \to \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} F(\nu)$ if $F(\nu)$ does not have pole strength greater than one. Making a change of variable $\nu \equiv u|q|/m$ and treating $q$ as a small quantity, the major contribution of the (b) diagram of (128) is given by

$$\frac{1}{2\beta} \approx \frac{V(4\pi e^2)^3}{m(2\pi)^9} \int_{-\infty}^{\infty} \frac{du}{2\pi} \int dp_1 dp_2 \frac{m\delta(p_1 - p_F) \cos \vartheta_1 m\delta(p_2 - p_F) \cos \vartheta_2}{-iu + p_F \cos \vartheta_1} \frac{iu + p_F \cos \vartheta_2}{\times}$$

$$\frac{1}{(p_1 - p_2)^2} \int_0^{q_c} 4\pi q dq \frac{\cos \vartheta_1 d \cos \vartheta_1 \cos \vartheta_2 d \cos \vartheta_2}{q^2 - 4\pi e^2 D_0(q, uq/m)}$$

$$\approx \frac{Vm(4\pi e^2)^3}{(2\pi)^9} \int_{-\infty}^{\infty} \frac{du}{2\pi} \int_{-1}^{1} \frac{\cos \vartheta_1 d \cos \vartheta_1 \cos \vartheta_2 d \cos \vartheta_2}{-iu + p_F \cos \vartheta_1} \frac{iu + p_F \cos \vartheta_2}{\times}$$

$$\frac{(2\pi)^2 p_F^2/2}{|\cos \vartheta_1 - \cos \vartheta_2|} \int 4\pi q dq \frac{\cos \vartheta_1 d \cos \vartheta_1 \cos \vartheta_2 d \cos \vartheta_2}{q^2 - 4\pi e^2 D_0(q, uq/m)}. \quad (143)$$

Apparently, the $1/|\cos \vartheta_1 - \cos \vartheta_2|$ factor in the integrand causes an undesirable divergence in the $\vartheta$ integral that is absent if one does not decompose the diagrams using (127). A finite result emerges only when one combines (143) with the (b) diagram of (129), which we soon turn to.

Before elaborating on the evaluation of the (b) diagram of (129), we wish to point out that this is the type of diagram (two-particle reducible ones) that was missed in Hedin’s approximation but should have been included for the exactness of the theory. For this diagram, $B_2(q', \nu') = 4\pi e^2/(p_1 - p_2)^2$ while $B_1(q, \nu) = (4\pi e^2)^2 D_0(q, \nu)/\{q^2 - 4\pi e^2 D_0(q, \nu)\}$. 

Summing over \( \nu’ \) via methods described in section III E, one obtains

\[
\frac{1}{\beta} = \frac{V (4\pi e^2)^3 2}{(2\pi)^9} \sum_{\nu} \int d\mathbf{p}_1 d\mathbf{p}_2 dq \frac{1}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu))} \times \left[ \frac{-n_{p_2+q}(n_{p_1+q} - n_{p_1})}{(-i\nu + \varepsilon_{p_1+q} - \varepsilon_{p_1})^2} - \frac{\beta n_{p_1}(1 - n_{p_1})n_{p_2}}{-i\nu + \varepsilon_{p_1} - \varepsilon_{p_1+q}} \right] \times \frac{D_0(q,\nu)}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu))} \times \frac{1}{(2\pi)^9} \sum_{\nu} \int d\mathbf{p}_1 d\mathbf{p}_2 dq \frac{1}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu))} \times \left[ \frac{(n_{p_2+q} - n_{p_2})(n_{p_1+q} - n_{p_1})}{(-i\nu + \varepsilon_{p_1+q} - \varepsilon_{p_1})^2} + \frac{2\beta n_{p_1}(1 - n_{p_1})n_{p_2}}{-i\nu + \varepsilon_{p_1+q} - \varepsilon_{p_1}} \right] \times \frac{D_0(q,\nu/m)}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu/m))} \times + (2V) \frac{(4\pi e^2)^3}{(2\pi)^3} \sum_{\nu} \int d\mathbf{p}_1 d\mathbf{p}_2 dq \frac{1}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu/m))} \times \left[ \frac{q^2 dq'dq}{(2\pi)^2} \right] \theta(-\cos \vartheta' - \frac{q'}{2p_F}) \right] \quad (144)
\]

where the first term inside the square brackets after the second equal sign is obtained by adding to it an equivalent expression with \( \mathbf{p}_1 + q \to -\mathbf{p}_1, \mathbf{p}_2 + q \to -\mathbf{p}_2, \nu \to -\nu \), and then taking the average, while the second term inside the same square brackets results from changing \( \nu \to -\nu \). The \( L_2 \) part, where the dummy variable of the integral is switched from \( \mathbf{p}_2 \) to \( \mathbf{q'} \equiv \mathbf{p}_2 - \mathbf{p}_1 \), can be cancelled by one of the terms contributing to the (b) diagram of (130). The \( L_1 \) part, however, upon taking the \( T \to 0 \) and \( q \to 0 \) limits, may be combined with (143) to yield a finite expression

\[
\frac{Vm p_F^2 (4\pi e^2)^3}{2 (2\pi)^7} \sum_{\nu} \int d\mathbf{p}_1 d\mathbf{p}_2 dq \frac{1}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu/m))} \times \left[ \frac{\cos \vartheta_1 - \cos \vartheta_2}{\cos \vartheta_1 - \cos \vartheta_2} \right] \int 2\pi d\vartheta_1 \cos \vartheta_1 \cos \vartheta_2 \cos \vartheta_2 \cos \vartheta_1 \cos \vartheta_1 \cos \vartheta_2 \cos \vartheta_2 \times \frac{D_0(q,\nu/m)}{(p_1 - p_2)^2 q^2 (q^2 - 4\pi e^2 D_0(q,\nu/m))} \right. \quad (145)
\]

Note that this expression, in agreement with Carr and Maradudin,\(^{55}\) carries a different sign when compared to the original result of DuBois.\(^{46}\)

It was conjectured before\(^{20}\) that cancellation of diagrams of the following form always hold true for HEG

\[
+ \quad = 0 .
\]
Here, black circles denote parts of the diagram that are connected to each other via two propagators. If this is the case, then the contributions of the (b) diagrams of (129) and (130) will cancel each other. We don’t expect this to happen since the (b) diagram of (129) is not anomalous. To illustrate that the (b) diagram of (130) does not eliminate the (b) diagram of (129), we now proceed to evaluate the (b) diagram of (130).

Here, $B_2(q', \nu') = 4\pi e^2/(q')^2$ while $B_1(q, \nu) = (4\pi e^2)^2 D_0(q, \nu) / \{q^2 [q^2 - 4\pi e^2 D_0(q, \nu)]\}$.

Summing over $\nu'$ via methods described in section III E, one obtains

$$\frac{1}{\beta} \longrightarrow \frac{1}{\beta} \sum_{\nu} \int dp dp dq \frac{d^2 \nu p_2 + q'}{(q')^2} \times$$

The contribution of (146) can be easily divided in two by explicitly expanding the two parts inside the round parentheses. It is obvious that the contribution associated with 1 cancels exactly the $(2V) L_2$ part of (144) while the contribution associated with $\frac{p_F \cos \vartheta_1}{-iu + p_F \cos \vartheta_1}$ cannot cancel the $(-V m) L_1$ part of (144).

For the (c) diagrams of (128-130), both $B_1$ and $B_2$ are of order $(4\pi e^2)^2$, leading to contributions of order $(e^2)^4$ and higher. The (c) diagrams thus already lead us beyond what was studied by DuBois$^{46}$ and by Carr and Maradudin.$^{55}$ The last two diagrams of $\Gamma_2[n]$
(shown in Figure 3) gives rise to the $E'_3$ term of Carr and Maradudin$^{55}$ when the $\tilde{D}_0$ lines are each replaced by $U$, the first term in the decomposition of $\tilde{D}_0$. In principle, one may go on to study terms of order $(e^2)^4$; we will not, however, delve into this endeavor since this is not the primary aim here. We would like to emphasize the following points. First, unlike conventional $e^2$ based perturbation theory, the formalism presented here naturally avoids divergence. This is shown by the fact that each diagram in our formalism contains no singularity while attempts to perform $e^2$ based perturbation necessarily require further re-grouping, such as combining the (b) diagrams of (128) and (129), to tame the divergence. Second, even if one were to pursue $e^2$ expansion, using Dyson’s equation (127) within our formalism still makes the task straightforward. In fact, as shown in this section, the $\Gamma_0[n] + \Gamma_1[n] + \Gamma_2[n]$ part when applied to the HEG already contain the celebrated results of Carr and Maradudin.$^{55}$ Third, the removal of anomalous contributions that required special attention within the formalism of Luttinger et al.$^{25,57}$ becomes automatic under this formalism.

V. EXCITATIONS

To obtain information regarding the excitations, one needs a time-dependent probe, although one with infinitesimal amplitude is sufficient. Runge and Gross$^{59}$ extended the correspondence between the external probe potential and the ground state charge density of the DFT to the time-dependent case. This relationship provides the foundation for studying excitation energies under DFT. Fukuda et al.$^{18}$ expressed the excitation energy condition using effective action formalism, without explicit connection to the Kohn-Sham formalism. By introducing time-dependent Kohn-Sham orbitals while assuming time independence of the orbital occupation numbers, Casida$^{60}$ derived via linear response theory a self-consistent condition on the density matrix response that leads to determination of excitation energies. Along a similar line, Petersilka et al.$^{36}$ proposed the so-called optimized effective potential (expanded in time-dependent Kohn-Sham orbitals) to tackle the problem of excitation energies. Since there exist formalisms to extract the excitation energies of the system provided that the UDF is known, our result for excitation energies should not be considered novel. The reasons for this section are twofold. First, we would like to explicitly show that the excitation energies can be obtained using the formalism of section III without introducing time-dependent orbitals. Second, although it is possible to find derivations of formulas$^{20}$
similar to those that will be shown here, they do appear slightly different and thus a self-contained exposition may be helpful.

Intuitively speaking, by varying the frequency of the probe, one seeks the frequency/energy where the amplitude of the response function diverges. Indeed, it is known that the spectral representation of the correlation function has poles at the excitation energies of the system\textsuperscript{61}. Having obtained the effective action $\Gamma[n]$, we also note that the second (functional) derivative of $\Gamma[n]$ with respect to the local electron density is the inverse of the density-density correlation function. Therefore, any pole associated with the correlation function becomes a root of the effective action. It can be shown that upon analytic continuation the correlation function, obtained using the imaginary time (finite temperature) formalism, can be turned into the response function of the real time. Below we briefly illustrate this point. Readers interested in more details can find an extensive exposition in reference 48.

From Eqs. (13) and (28), we know that
\[ n(x) = \frac{\delta(\beta W[J])}{\delta J(x)}, \]
and
\[ J(x) = -\frac{\delta\Gamma[n]}{\delta n(x)}. \]

One then considers
\[ \delta(x - y) = \frac{\delta J(x)}{\delta J(y)} = -\int dz \frac{\delta^2 \Gamma[n]}{\delta n(x) \delta n(z)} \frac{\delta n(z)}{\delta J(y)} = -\int dz \frac{\delta^2 \Gamma[n]}{\delta n(x) \delta n(z)} \frac{\delta^2 (\beta W[J])}{\delta J(z) \delta J(y)}. \] (147)

Although a time-dependence of $J$ is introduced to probe the excitations, in the end we will return to a time-independent source ($J(x) \to J(x)$) while computing the excitation energies. As we will show below, it is most convenient to go to the zero temperature limit to compute the excitation energies.

Note that
\[ \frac{\delta^2 (\beta W[J])}{\delta J(x) \delta J(y)} = -[\hat{n}(x)\hat{n}(y)]_T + [\hat{n}(x)]_T [\hat{n}(y)]_T = -[\hat{n}(x)\hat{n}(y)]_T + n(x)n(y) \]
\[ = -[(\hat{n}(x) - n(x))(\hat{n}(y) - n(y))]_T \equiv -[\tilde{n}(x)\tilde{n}(y)]_T \] (148)

where $\hat{n}(x) = \psi_\dagger(x)\psi(x)$ is the electron density operator and the square bracket $[]_T$ indicates an (imaginary) time-ordered thermal average such that
\[ \left[ \hat{O}_1(t_1)\hat{O}_2(t_2) \right]_T = \frac{\text{Tr} \left[ e^{-\beta H[J]} T \left( \hat{O}_1(t_1)\hat{O}_2(t_2) \right) \right]}{\text{Tr} \left[ e^{-\beta H[J]} \right]} = \frac{\text{Tr} \left[ e^{-\beta H[J]} T \left( \hat{O}_1(t_1)\hat{O}_2(t_2) \right) \right]}{Z[J]}. \]
Let us denote by \( \{ |\ell\rangle_{\text{ex}} \}_{\ell=0}^{\infty} \) the eigenstates of the Hamiltonian \( H[J] \) with the corresponding eigenenergies \( \{ \mathcal{E}_\ell \}_{\ell=0}^{\infty} \). The spectral representation is obtained by first writing the time-ordered product (assuming that operators \( \hat{O}_1(t_1) \) and \( \hat{O}_2(t_2) \) are bosonic) as

\[
\exp\ell \!\! \langle \hat{O}_1(t_1) \hat{O}_2(t_2) \rangle |\ell\rangle_{\text{ex}} = \theta(t_1-t_2) \exp\ell \!\! \langle \hat{O}_1(t_1) \hat{O}_2(t_2) \rangle |\ell\rangle_{\text{ex}} + \theta(t_2-t_1) \exp\ell \!\! \langle \hat{O}_2(t_2) \hat{O}_1(t_1) \rangle |\ell\rangle_{\text{ex}} ,
\]

then by inserting the identity operator \( \sum_{\ell'} |\ell'\rangle_{\text{ex}} \!\! \langle \ell'| \) between the two operators, and finally by multiplying by \( e^{i\omega(t_1-t_2)} \) and then integrating over the time variable \( t_1-t_2 \). Proceeding in this way, one will then obtain information on \( \mathcal{E}_{\ell'} - \mathcal{E}_\ell \). Since knowing \( \Omega_{\ell'} \equiv \mathcal{E}_{\ell'} - \mathcal{E}_0 \) also provides complete information on \( \mathcal{E}_{\ell'} - \mathcal{E}_\ell \), one may also focus on \( \ell = 0 \) by taking the limit \( \beta \to \infty \). Let

\[
-W^{(2)}(x,y) \equiv -\frac{\delta^2(\beta W[J])}{\delta J(x) \delta J(y)} ,
\]

and

\[
-W^{(2)}(x,y,\imath\nu_n) \equiv \int_0^\beta d(\tau_x - \tau_y) e^{\imath \nu_n (\tau_x - \tau_y)} W^{(2)}(x,y) \equiv \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\omega') ,
\]

with \( \nu_n = 2\pi n/\beta \) and

\[
A(\omega) = e^{\beta W[J]} \sum_{\ell,m} e^{-\beta \mathcal{E}_\ell} (e^{-\beta \omega} - 1) 2\pi \delta(\omega + \mathcal{E}_\ell - \mathcal{E}_m) \exp\ell \!\! \langle \hat{n}(x) | m \rangle_{\text{ex}} \exp\ell \!\! \langle m | \hat{n}(y) \rangle |\ell\rangle_{\text{ex}} .
\]

Note that \( \hat{n}(x) \) measures the deviation from the thermally averaged electronic density \( n_T(x) \). Since the expression (149) is evaluated at static \( J(x) \), the Hamiltonian contains no time dependence. We may thus write \( \hat{n}(x) = e^{\imath H_T} \hat{n}(x) e^{-\imath H_T} \).

Let’s now express using real time the retarded correlation function (\( \mathcal{R} \)), also called the response function, and the advanced correlation function (\( \mathcal{A} \)) as follows (with \( n(x) = e^{\imath H_T} \hat{n}(x) e^{-\imath H_T} \))

\[
\begin{pmatrix}
\mathcal{R}(x,y) \\
\mathcal{A}(x,y)
\end{pmatrix} = \begin{pmatrix}
-i\theta(t_x - t_y) \\
i\theta(t_y - t_x)
\end{pmatrix} e^{\beta W[J]} \text{Tr} \left( e^{-\beta H} [\hat{n}(x), \hat{n}(y)] \right) 
\]

\[
= \begin{pmatrix}
-i\theta(t_x - t_y) \\
i\theta(t_y - t_x)
\end{pmatrix} \sum_{\ell,m} e^{\beta (W[J] - \mathcal{E}_\ell)} \left[ e^{\imath \theta(t_x - t_y)(\mathcal{E}_\ell - \mathcal{E}_m)} \exp\ell \!\! \langle \hat{n}(x) | m \rangle_{\text{ex}} \exp\ell \!\! \langle m | \hat{n}(y) \rangle |\ell\rangle_{\text{ex}} 
- e^{-\imath \theta(t_x - t_y)(\mathcal{E}_\ell - \mathcal{E}_m)} \exp\ell \!\! \langle \hat{n}(y) | m \rangle_{\text{ex}} \exp\ell \!\! \langle m | \hat{n}(x) \rangle |\ell\rangle_{\text{ex}} \right] .
\]

(152)
Taking the Fourier transform of the response function, we consider

$$\begin{align*}
\left( R(x, y, \omega) \right) & \equiv \int_{-\infty}^{\infty} d(t_x - t_y) \ e^{i\omega(t_x - t_y)} \left( R(x, y) \right) \\
\left( A(x, y, \omega) \right) & \equiv \int_{-\infty}^{\infty} d(t_x - t_y) \ e^{i\omega(t_x - t_y)} \left( A(x, y) \right)
\end{align*}$$

$$\begin{align*}
\left( \mathcal{R}(x, y, \omega) \right) & = \int_{-\infty}^{\infty} d(t_x - t_y) \ e^{i\omega(t_x - t_y)} \left( \mathcal{R}(x, y) \right) \\
& = e^{\beta W[J]} \sum_{\ell, m} e^{-\beta \epsilon_{\ell}} \frac{e^{\beta (\epsilon_{\ell} - \epsilon_{m})} - 1}{\omega + \epsilon_{\ell} - \epsilon_{m} \pm i\eta} \ ex(\ell)|\tilde{n}(x)|m \ ex(m)|\tilde{n}(y)|\ell \ ex
\end{align*}$$

$$\begin{align*}
& = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\omega') - i\eta .
\end{align*}$$

Comparing Eqs. (150) and (153), one finds that substituting $i\nu_n \rightarrow \omega + i\eta$ ($\omega - i\eta$) in the imaginary time-ordered correlation function leads to the retarded (advanced) correlation function. The validity of this analytic continuation was discussed by Baym and Mermin.\(^{62}\)

As $T \rightarrow 0$, $e^{-\beta W[J]} = e^{-\beta \epsilon_0} \left[ 1 + O(e^{-\beta (\epsilon_1 - \epsilon_0)}) \right]$, and $e^{\beta W[J]} = e^{\beta \epsilon_0} \left[ 1 - O(e^{-\beta (\epsilon_1 - \epsilon_0)}) \right]$.

Under this limit, we may rewrite the spectral weight $A(\omega)$ as

$$\begin{align*}
\lim_{\beta \rightarrow \infty} \frac{A(\omega)}{2\pi} & = \sum_{\ell, m} \left( e^{-\beta (\epsilon_m - \epsilon_0)} - e^{-\beta (\epsilon_{\ell} - \epsilon_0)} \right) \delta(\omega + \epsilon_{\ell} - \epsilon_{m}) \ ex(\ell)|\tilde{n}(x)|m \ ex(m)|\tilde{n}(y)|\ell \ ex
\end{align*}$$

$$- \delta(\omega - (\epsilon_{\ell} - \epsilon_0)) \ ex(\ell)|\tilde{n}(x)|0 \ ex - \delta(\omega - (\epsilon_{\ell} - \epsilon_0)) \ ex(\ell)|\tilde{n}(y)|0 \ ex$$

$$\equiv \sum_{\ell} \left[ \delta(\omega + \epsilon_{\ell} - \epsilon_0) n_{\ell, e}^*(y) n_{\ell, e}(x) - \delta(\omega - (\epsilon_{\ell} - \epsilon_0)) n_{\ell, e}^*(x) n_{\ell, e}(y) \right] \ (154)$$

where $n_{\ell, e}(y) \equiv ex(\ell)|\tilde{n}(y)|0 \ ex$.

When continued to the retarded correlation function (response function), the density correlation function $W^{(2)}$ reads

$$\begin{align*}
\lim_{\beta \rightarrow \infty} W^{(2)}(x, y, \omega) & = \sum_{\ell} \left[ \frac{n_{\ell, e}^*(x) n_{\ell, e}(y)}{\omega - \Omega_{\ell} + i\eta} - \frac{n_{\ell, e}^*(y) n_{\ell, e}(x)}{\omega + \Omega_{\ell} + i\eta} \right] ,
\end{align*}$$

with

$$\Omega_{\ell} \equiv \epsilon_{\ell} - \epsilon_0 .$$

(156)

Provided that the amplitudes $ex(\ell)|\tilde{n}|\ell \ ex$ are nonzero, we see from Eq. (155) that $\omega + i\eta = \pm (\epsilon_{\ell} - \epsilon_0)$ are simple poles of $W^{(2)}(x, y, \omega)$. Furthermore, we also see that

$$\left( W^{(2)}(x, y, \omega) \right)^* = W^{(2)}(x, y, -\omega^*) ,$$

(157)

and when $\omega$ is real

$$\left( W^{(2)}(x, y, \omega) \right)^* = W^{(2)}(x, y, -\omega) .$$
Let us also define
\[ \Gamma^{(2)}(x, y) \equiv \frac{\delta^2 \Gamma[n]}{\delta n(x) \delta n(y)}. \]

Eq. (147) may thus be rewritten as
\[ -\delta(x - y) = \int dz \, \Gamma^{(2)}(x, z) \, W^{(2)}(z, y). \quad (158) \]

Since eventually, \( \tau_x \) must agree with \( \tau_y \) in the equation above, if \( \tau_z > \tau_y \), we must have \( \tau_z > \tau_x \) as well. Similarly to Eq. (150), the Fourier transform for \( \Gamma^{(2)} \) can be written as
\[ \Gamma^{(2)}(x, z, i\nu_n) \equiv \int_0^\beta d(\tau_z - \tau_x) \, e^{i\nu_n(\tau_z - \tau_x)} \, \Gamma^{(2)}(x, z). \quad (159) \]

The inverse transform of (150) and (159) can be written as
\[ W^{(2)}(z, y) = \frac{1}{\beta} \sum_n e^{-i\nu_n(\tau_z - \tau_y)} W^{(2)}(z, y, i\nu_n) \]
\[ \Gamma^{(2)}(x, z) = \frac{1}{\beta} \sum_n e^{-i\nu_n(\tau_z - \tau_x)} \Gamma^{(2)}(x, z, i\nu_n) \]

and
\[ \int_0^\beta \int dz \, \Gamma^{(2)}(x, z) \, W^{(2)}(z, y) = \int dz \, \frac{1}{\beta} \sum_n e^{-i\nu_n(\tau_z - \tau_y)} \Gamma^{(2)}(x, z, -i\nu_n) \, W^{(2)}(z, y, i\nu_n). \]

Since \( \delta(\tau_z - \tau_y) = \frac{1}{\beta} \sum_n e^{-i\nu_n(\tau_z - \tau_y)} \), one obtains
\[ -\delta(x - y) = \int dz \, \Gamma^{(2)}(x, z, -i\nu_n) W^{(2)}(z, y, i\nu_n) = \int dz \, W^{(2)}(x, z, -i\nu_n) \Gamma^{(2)}(z, y, i\nu_n), \]

which under analytic continuation becomes
\[ -\delta(x - y) = \int dz \, \Gamma^{(2)}(x, z, -\omega) W^{(2)}(z, y, \omega) = \int dz \, W^{(2)}(x, z, -\omega) \Gamma^{(2)}(z, y, \omega). \quad (160) \]

From Eqs. (157) and (161), one has
\[ (\Gamma^{(2)}(x, z, \omega))^* = \Gamma^{(2)}(x, z, -\omega^*). \quad (162) \]

Multiplying the LHS and the middle expression of Eq. (161) by \( (\omega \mp \Omega_\ell + i\eta) \) and then setting \( \omega \rightarrow \pm \Omega_\ell - i\eta \), we see that
\[ \int dz \, \Gamma^{(2)}(x, z, -\omega \rightarrow -\Omega_\ell - i\eta) \, n_{\ell,e}^*(z) = 0, \quad (163) \]
\[ \text{and} \quad \int dz \, \Gamma^{(2)}(x, z, -\omega \rightarrow +\Omega_\ell - i\eta) \, n_{\ell,e}(z) = 0. \quad (164) \]
That is, \( n_{\ell}^{(s)}(y) \) become eigenvectors of \( \Gamma^{(2)}(x, y, -\omega) \) with zero eigenvalues. The matter of finding excitation energies and the corresponding electronic densities thus reduces to finding for \( \Gamma^{(2)} \) the eigenvectors with zero eigenvalue.\(^{18} \) Since we are interested in obtaining the excitation energy under the physical condition, \( J(x) \rightarrow 0 \), this also means that the derivatives of \( \Gamma \) above are evaluated at the ground state electronic density in the zero temperature limit.

From the expressions (65) and (70), one sees that the effective action is split into the free particle part \( \Gamma_0 \), the Hartree functional and the exchange-correlational functional

\[
\Gamma[n] = \Gamma_0[n] + \frac{1}{2} n_0 U_0 n + \Gamma_{xc}[n] \equiv \Gamma_0[n] + \Gamma_{\text{int}}[n],
\]

(165)

where \( \Gamma_{xc}[n] = \sum_{l=1}^{\infty} \Gamma_l[n] \). Letting \( \Delta(x) \) be the eigenvector, the excitation condition becomes

\[
\int d\mathbf{z} \Gamma^{(2)}(x, \mathbf{z}) \Delta(\mathbf{z}) = 0.
\]

(166)

After splitting the effective action into \( \Gamma_0 \) and \( \Gamma_{\text{int}} \) the eigenvalue equations (163-164) may be expressed as

\[
-\int d\mathbf{z} \Gamma^{(2)}_0(y, \mathbf{z}, -\omega) \Delta(\mathbf{z}) = \int d\mathbf{z} \Gamma^{(2)}_{\text{int}}(y, \mathbf{z}, -\omega) \Delta(\mathbf{z}).
\]

(167)

Multiplying both sides of (167) by \( W^{(2)}_0(x, y, \omega) \) and then integrating over \( dy \), one obtains

\[
\Delta(\mathbf{x}) = \int dy dz W^{(2)}_0(x, y, \omega) \Gamma^{(2)}_{\text{int}}(y, \mathbf{z}, -\omega) \Delta(\mathbf{z}).
\]

(168)

Note that \( W_0[J_0] \) describes our Kohn-Sham system, a constructed non-interacting system that produces the same ground state electron density as that of the physical system considered. From Eq. (155), one can write down \( W^{(2)}_0(x, y, \omega) \) in terms of the excitation energies associated with the Kohn-Sham non-interacting system:

\[
W^{(2)}_0(x, y, \omega) = \sum_{\ell} \left[ \frac{n^*_\ell(x) n^{}_{\ell}(y)}{\omega - \omega_{\ell} + i\eta} - \frac{n^*_{\ell}(y) n^{}_{\ell}(x)}{\omega + \omega_{\ell} + i\eta} \right],
\]

(169)

where

\[
\omega_{\ell} \equiv E_{\ell} - E_0,
\]

(170)

and \( E_{\ell} \) is the energy of \( |\ell\rangle_{ks} \), the \( \ell \)th state of the many-particle Kohn-Sham system with \( J_0(\mathbf{x}) \) chosen to generate the correct ground state electron density. Therefore, for any \( \ell \), \( E_{\ell} \) is simply the sum of single-particle energies \( \varepsilon_m \). Note that in Eq. (169), \( n^{}_{\ell}(x) \) is defined by
ks, \ell|\tilde{n}(x)|0\rangle_{ks}$ except that $|\ell\rangle_{ks}$ now describes the \ellth state of the Kohn-Sham system, not the physical system considered.

We seek a general solution for $\Delta(x)$ of the form

$$\Delta(x) = \sum_{\ell} \left[ a_\ell n_\ell(x) + b_\ell n_\ell^*(x) \right].$$  \hspace{1cm} (171)

Evidently, if a frequency $\hat{\omega}$ leads to a solution $\{b_\ell\}$, then $-\hat{\omega}^*$ should lead to a solution $\{a_\ell\}$, which plays the role of $\{b_\ell^*\}$. Substituting Eqs. (169) and (171) into Eq. (168), we find that

$$\sum_{\ell} \left[ a_\ell n_\ell(x) + b_\ell n_\ell^*(x) \right] = \sum_{\ell,\ell'} \int dy\,dz \left[ \frac{n_\ell^*(x)n_\ell(y)}{\omega - \omega_\ell + i\eta} - \frac{n_\ell(x)n_\ell^*(y)}{\omega + \omega_\ell + i\eta} \right] \Gamma_{\text{int}}^{(2)}(y, z, -\omega) \left[ a_\ell n_\ell(z) + b_\ell n_\ell^*(z) \right].$$  \hspace{1cm} (172)

Equating the coefficients associated with $n_\ell(x)$ and $n_\ell^*(x)$, we find that

$$a_\ell = -\sum_{\ell'} \int dy\,dz \frac{n_{\ell'}^*(y)}{\omega + \omega_{\ell'} + i\eta} \Gamma_{\text{int}}^{(2)}(y, z, -\omega) \left[ a_{\ell'} n_{\ell'}(z) + b_{\ell'} n_{\ell'}^*(z) \right],$$

$$b_\ell = \sum_{\ell'} \int dy\,dz \frac{n_{\ell'}(y)}{\omega - \omega_{\ell'} + i\eta} \Gamma_{\text{int}}^{(2)}(y, z, -\omega) \left[ a_{\ell'} n_{\ell'}(z) + b_{\ell'} n_{\ell'}^*(z) \right].$$

Let us define

$$Y_{\ell,\ell'}(\omega) = \int dy\,dz \, n_{\ell'}^*(y) \Gamma_{\text{int}}^{(2)}(y, z, -\omega) n_{\ell'}(z) + \omega_\ell \delta_{\ell,\ell'},$$  \hspace{1cm} (173)

$$K_{\ell,\ell'}(\omega) = \int dy\,dz \, n_{\ell'}(y) \Gamma_{\text{int}}^{(2)}(y, z, -\omega) n_{\ell'}^*(z),$$  \hspace{1cm} (174)

and we obtain the following matrix equation

$$\begin{pmatrix} Y(\omega) & K(\omega) \\ K^*(-\omega^*) & Y^*(-\omega^*) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = (\omega + i\eta) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix},$$  \hspace{1cm} (175)

where $(A)_\ell = a_\ell$ and $(B)_\ell = b_\ell$. Evidently, one seeks $\hat{\omega}$ such that

$$\det \left[ \begin{pmatrix} Y(\hat{\omega}) & K(\hat{\omega}) \\ K^*(-\hat{\omega}^*) & Y^*(-\hat{\omega}^*) \end{pmatrix} - (\hat{\omega} + i\eta) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right] = 0.$$  \hspace{1cm} (176)

As mentioned earlier, one anticipates $(A(\hat{\omega})) = (B^*(-\hat{\omega}^*))$. To see this, we perform the change $\omega \leftrightarrow -\omega^*$ in (175) and find that one can then rearrange the resulting equation into

$$\begin{pmatrix} Y(\omega) & K(\omega) \\ K^*(-\omega^*) & Y^*(-\omega^*) \end{pmatrix} \begin{pmatrix} B^*(-\omega^*) \\ A^*(-\omega^*) \end{pmatrix} = (\omega + i\eta) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} B^*(-\omega^*) \\ A^*(-\omega^*) \end{pmatrix},$$  \hspace{1cm} (177)
which is identical to Eq. (175) except with \( B*(-\hat{\omega}^*) \) playing the role of \( A(\hat{\omega}) \) and \( A*(-\hat{\omega}^*) \) playing the role of \( B(\hat{\omega}) \).

We now compare Eq. (175) with similar existing results. In references 63 and 20, equations similar to (175) were obtained, and those will be identical to Eq. (175) provided that \( \mathbf{K}^*(-\omega^*) = \mathbf{K}^*(\omega) \). This will happen if \( \Gamma(x, y, -\omega) = \Gamma(x, y, \omega) \) for real \( \omega \).

VI. SADDLE-POINT AS AN ALTERNATIVE FORMALISM

Below, we will obtain the effective action using a classical variable \( i\varphi_c \) that corresponds to the saddle-point of the auxiliary field path integral. At the physical condition \( J = 0 \), \( i\varphi_c \) is interpreted as the electron density of a self-consistent Hartree solution. Our Hartree problem is not of the conventional type, but rather similar to what Kohn described in his Nobel lecture.\(^1\) In the conventional Hartree calculation, the wave functions obtained may not be orthogonal to each other due to the fact that each particle’s wave function is solved with a different potential.\(^64\) In the method below and mentioned by Kohn\(^1\), the electric potential experienced by every electron is the same. Another difference between the method below and the aforementioned Hartree methods\(^1,64\) is that the integral of the Hartree density in our method is not necessarily an integer due to the possibility that the density correction term may have a nonzero integral.

The saddle-point method below is quite different from what was described in the previous sections. First, although the diagrams in the saddle-point method are all connected diagrams, they are not one-particle irreducible (1PI). Second, unlike the method presented in previous sections, the computation of the effective action now requires no further functional derivatives of \( \beta W[J] \) with respect to \( J \) evaluated at \( J_c \), while in the formalism mentioned in previous sections, one needs to compute higher order derivatives of \( \beta W[J_0] \) with respect to \( J_0 \) (see Eqs. (67-73)).

A. Evaluation of \( e^{-\beta W[J]} \) via expansion around the saddle-point

The path integral (23)

\[
e^{-\beta W[J]} \equiv \int D\phi \exp\{-I[\phi] - iJ_0\phi\}
\]
may be evaluated by the saddle point method. The extrema condition gives

$$\frac{\delta I[\phi]}{\delta \phi(x)|_{\varphi_c}} = -iJ(x).$$

Since

$$\frac{\delta I[\phi]}{\delta \phi(x)|_{\varphi_c}} = (U \circ \varphi_c)_x - \text{Tr} \left( G_\phi \frac{\delta G_\phi^{-1}}{\delta \phi(x)} \right)_{\phi \rightarrow \varphi_c}$$

$$= (U \circ \varphi_c)_x - \int dy \, G_c(y, y) (iU(y, x)),$$  \hspace{1cm} (178)

where $G_c(y, y) \equiv G_{\phi \rightarrow \varphi_c}(y, y)$, we obtain with $U(x, y) = U(y, x)$

$$J(x) = (U \circ (i\varphi_c))_x + \int dy \, U(x, y) G_c(y, y) = \int dy \, U(x, y) [i\varphi_c(y) + G_c(y, y)].$$  \hspace{1cm} (179)

As $J \to 0$ (the physical condition), when $U$ is invertible such as Coulomb interaction, one must have $i\varphi_c(x) = -G_c(x, x)$. Note that the negative of the diagonal element of the Green’s function $-G_c(x, x)$ is the particle density corresponding to the following Hamiltonian

$$\int dx \, \hat{\psi}^\dagger(x) \left[ -\frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + i(U \circ \varphi_c)_x \right] \hat{\psi}(x).$$

The saddle-point equation therefore produces a Hartree-like equation: the Green’s function depends on the input particle density $i\varphi_c(x)$ and is required to produce the same particle density $i\varphi_c(x)$ in the end.

When $J \neq 0$, one can still view (179) as a generalized Hartree equation in the following sense. Remember that the inverse Green’s function $G_c^{-1}(x, y)$ is given by (with $\delta(x - x') = \delta(\tau - \tau')\delta(x - x')$)

$$G_c^{-1}(x, x') = \left[ \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) - \mu + U \circ (i\varphi_c) \right] \delta(x - x'),$$  \hspace{1cm} (180)

and may be rewritten as

$$G_c^{-1}(x, x') = \left[ \partial_\tau - \frac{\nabla^2}{2m} + v_{\text{ion}}(x) + J(x) - \mu + U \circ n_H \right] \delta(x - x').$$  \hspace{1cm} (181)

That is, we now view the potential as given by $v_{\text{ion}}(x) + J(x)$ and the Hartree particle density $n_H(x) = i\varphi_c(x) - (U^{-1} \circ J)_x$. This interpretation indeed agrees with our equation (179) which can be written as

$$0 = \int dy \, U(x, y) \left[ (i\varphi_c(y) - \int dz \, U^{-1}(y, z) J(z)) + G_c(y, y) \right].$$  \hspace{1cm} (182)
That is, for a given \( J(x) \neq 0 \), one will solve as before the Hartree equation but with \( v_{\text{ion}}(x) \to v_{\text{ion}}(x) + J(x) \). Once the Hartree particle density \( n_H \) is obtained, one obtains \( i\varphi_c = n_H + U^{-1} \circ J \). Since \( U \circ (i\varphi_c) \) always appears as a unit inside the Green’s function \( G_c(x,x') \), for convenience, we define

\[
J_c \equiv U \circ (i\varphi_c) = J + U \circ n_H .
\]

Once \( \varphi_c(x) \) is obtained, we shift \( \phi \) by \( \varphi_c \) and re-express the exponent in the integrand as

\[-I[\phi] - iJ \circ \phi \Rightarrow -I[\varphi_c + \phi] - iJ \circ (\varphi_c + \phi),\]

and then expand around \( \varphi_c \). To do the expansion, we first rewrite (20) as

\[
G_{\phi}^{-1}(x,x') = G_c^{-1}(x,x') + i b(x) \delta(x - x') \equiv G_c^{-1}(x,x') + V(x,x'), \quad (183)
\]

where \( b = U \circ \phi \). We may then write down

\[
G_{\phi}^{-1} = G_c^{-1} [I + G_c \circ V] ,
\]

and

\[
\ln (G_{\phi}^{-1}) = \ln (G_c^{-1}) + \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} [G_c \circ V]^k . \quad (184)
\]

Note that

\[
[G_c \circ V]_{x,z} = \int dy G_c(x,y)V(y,z) = \int dy G_c(x,y)\delta(y-z) \left. (i b(y)) \right| = G_c(x,z) \left. (ib(z)) \right| .
\]

Consequently,

\[
\begin{align*}
\text{Tr} \ln (G_{\phi}^{-1}) &= \text{Tr} \ln (G_c^{-1}) + \int dx_1 G_c(x_1,x_1)(ib(x_1)) \\
&- \frac{1}{2} \int dx_1 dx_2 G_c(x_1,x_2)G_c(x_2,x_1)(ib(x_1))(ib(x_2)) \\
&+ \sum_{k=3}^{\infty} \frac{(-1)^{k-1}}{k} \int dx_1 \ldots dx_k G_c(x_k,x_1) \ldots G_c(x_{k-1},x_k)(ib(x_1)) \ldots (ib(x_k)) . \quad (185)
\end{align*}
\]

Note that in the final expression of the exponent of the integrand in (23) the terms linear in \( \phi \) (or \( b \)) cancel out as one may verify and we arrive at

\[
\begin{align*}
-I[\varphi_c + \phi] - iJ \circ (\varphi_c + \phi) &= -\frac{1}{2} \varphi_c \circ U \circ \varphi_c - \varphi_c \circ b - \frac{1}{2} b \circ U^{-1} \circ b + \text{Tr} \ln (G_{\phi}^{-1}) \\
&+ \frac{1}{2} \text{Tr} \ln (U) - iJ \circ \varphi_c - iJ \circ \phi \\
&= \frac{1}{2} \text{Tr} \ln (U) - \frac{1}{2} \varphi_c \circ U \circ \varphi_c + \text{Tr} \ln (G_c^{-1}) - iJ \circ \varphi_c \\
&- \frac{1}{2} b \circ D_c^{-1} \circ b + \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots b_k , \quad (186)
\end{align*}
\]
where
\[
\mathcal{D}_c^{-1} = U^{-1} - D_c,
\]
\[
D_c(x, y) = G_c(x, y) G_c(y, x),
\]
and
\[
I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \equiv \frac{(-1)^{k-1}}{k} \int dx_1 \ldots dx_k G_c(x_k, x_1) \ldots G_c(x_{k-1}, x_k) [(ib(x_1)) \ldots (ib(x_k))] .
\]

We therefore have (based on the linked-cluster theorem)
\[
\beta W_\phi[J] = \frac{1}{2} \varphi_c \circ U \circ \varphi_c - \text{Tr} \ln (G_c^{-1}) + iJ \circ \varphi_c
\]
\[
+ \frac{1}{2} \text{Tr} \ln \left( \mathcal{D}_c^{-1} \circ U \right) - \sum_{n=1}^{\infty} \frac{1}{n!} \left( \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \right)^n \rangle_{\text{conn.}},
\]
where the subscript “conn.” is used to indicate connected Feynman diagrams.

Consequently, the effective action, defined by
\[
\Gamma[n] = \beta W_\phi[J] - \frac{1}{2} J \circ U^{-1} \circ J - J \circ n = \beta W_\phi[J] + \frac{1}{2} J \circ U^{-1} \circ J - iJ \circ \varphi
\]
and with \( \varphi = \varphi_c + \langle \phi \rangle \equiv \varphi_c + \tilde{\varphi} \) as well as with \( J = J_c - U \circ n_H \), can now be written as
\[
\Gamma[n] = -\text{Tr} \ln (G_c^{-1}) - J \circ n_H + \frac{1}{2} n_H \circ U \circ n_H + \frac{1}{2} \text{Tr} \ln \left( \mathcal{D}_c^{-1} \circ U \right)
\]
\[
- iJ \circ \tilde{\varphi} - \sum_{n=1}^{\infty} \frac{1}{n!} \left( \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \right)^n \rangle_{\text{conn.}}.
\]
This expression should be contrasted with Eq. (45) where the true particle density is introduced as the natural variable.

From the definition of \( \varphi \) (see Eq. (26) we have
\[
i \varphi(x) = \frac{\int D\phi (i\phi(x)) e^{-I[\phi]-iJ_0\phi}}{\int D\phi e^{-I[\phi]-iJ_0\phi}} = i \varphi_c(x) + \int dy U^{-1}(x, y) \frac{\int Db (ib(y)) e^{-I[\varphi_c+\phi]-iJ_0(\varphi_c+\phi)}}{\int Db e^{-I[\varphi_c+\phi]-iJ_0(\varphi_c+\phi)}} ,
\]
which means that
\[
i \tilde{\varphi} = \frac{\int Db (iU^{-1} \circ b) e^{-\frac{i}{2} b_0 \mathcal{D}_c^{-1} b_0 + \sum_{k=3}^{\infty} \frac{1}{k!} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k}}{\int Db e^{-\frac{i}{2} b_0 \mathcal{D}_c^{-1} b_0 + \sum_{k=3}^{\infty} \frac{1}{k!} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k}} .
\]
On the basis of a simple replica argument, one sees that the above expression may be written as

\[ i\tilde{\varphi}(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \int dy U^{-1}(x,y) \left( \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \right)^n \text{ib}(y) \text{conn.} \]

\[ = \sum_{n=1}^{\infty} \frac{1}{n!} \int dy U^{-1}(x,y) \left( \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \right)^n \text{ib}(y) \text{conn.}, \quad (192) \]

where the \( n = 0 \) term vanishes because \( \int Db e^{-\frac{1}{2} \rho \tilde{b} \rho^{-1} \circ b(x)} = 0 \). Eq. (192) implies that \( i\tilde{\varphi}(x) \) at each point \( x \) is a functional of \( \varphi_c \). Returning to (189), this implies that one may express the effective action \( \Gamma \) in terms of \( i\varphi_c \) although its canonical argument is supposed to be \( n \). The relation between \( n \) and \( i\varphi_c \) is obtained through

\[ n = i\varphi_c + i\tilde{\varphi}[i\varphi_c] - U^{-1} \circ J[i\varphi_c] = n_H + i\tilde{\varphi}[i\varphi_c] \quad (193) \]

with \( i\tilde{\varphi}(x) \) expressed as a functional of \( i\varphi_c \). This implies that given an \( i\varphi_c \), we may obtain \( n \) through (i) the diagrammatic expansion of (192) to produce the corresponding \( i\varphi \), and (ii) equation (179) to find \( -U^{-1} \circ J \). Since in general, we have

\[ \int d\mathbf{x} (i\tilde{\varphi}(\mathbf{x})) \neq 0, \]

one cannot expect the integral of the Hartree electron density to be \( N_e \), the total number of electrons. Instead, we have

\[ N_e = \int d\mathbf{x} n(\mathbf{x}) = \int d\mathbf{x} \left[ n_H(\mathbf{x}) + i\tilde{\varphi}(\mathbf{x}) \right] \quad (194) \]

and \( \int d\mathbf{x} n_H(\mathbf{x}) \) is not necessarily an integer. In particular, when \( \int d\mathbf{x} n_H(\mathbf{x}) \) deviates significantly from \( N_e \) or \( \int d\mathbf{x} |i\tilde{\varphi}(\mathbf{x})| \gg 1 \), forcing \( \int d\mathbf{x} n_H(\mathbf{x}) = N_e \) may lead to the occurrence of a self-consistent solution that differs significantly from the true solution.

Note that \( n_H(\mathbf{x}) = -G_c(x,x) \) and in the absence of the source term \( n_H(\mathbf{x}) = i\varphi_c(\mathbf{x}) \). Furthermore, since \( (U^{-1} \circ J)(x) \propto \nabla^2 \varphi(x) \), \( \int n_H(\mathbf{x}) d\mathbf{x} = \int (i\varphi_c(\mathbf{x})) d\mathbf{x} \). The constraint (194) for the total number of electrons can also be written as

\[ N_e = \int d\mathbf{x} n(\mathbf{x}) = \int d\mathbf{x} \left[ n_H(\mathbf{x}) + i\tilde{\varphi}(\mathbf{x}) \right] = \int d\mathbf{x} \left[ i\varphi_c(\mathbf{x}) + i\tilde{\varphi}(\mathbf{x}) \right]. \quad (195) \]

The Hartree-like Green’s function \( G_c(x,x') \) shown in (180) may be viewed as a functional of \( i\varphi_c(x) \). When expressing \( G_c(x,x') \) using only single particle orbitals, we define
in Eq. (88) \( v(x) \equiv v_{\text{ion}}(x) - \mu + U \cdot (i\varphi_c)_x \). For the evaluation of \( G_c(x, y) \), we solve first
the eigensystem (93). The single-particle wave functions (91) associated with \( \hat{h} \) are to be obtained self-consistently. Basically, one starts with a \textit{guess} for the electronic density \( i\varphi_c(x) \) satisfying \( \int dx (i\varphi_c(x)) \approx N_e \), where \( N_e \) is the number of electrons. One then obtains the single-particle wave functions, and then computes the corresponding Green’s function \( G_c \), obtains \( \int dx (i\tilde{\varphi}(x)) \) and tunes the chemical potential to ensure that
\[-\int dx \ G_c(x, x) = N_e - \int dx (i\tilde{\varphi}(x)) \]. One then takes \(-G_c(x, x)\) in place of \( i\varphi_c(x) \) in the next
round of iteration until convergence is reached.

The procedure of the saddle-point method is now obvious. One starts with an external
potential, and then determines the Hartree electron density via \( n_H(x) = -G_c(x, x), n_H = i\varphi_c - U^{-1} \circ J \) and Eq. (195). This self-consistent procedure will also provide the physical
electron density \( n(x) \). The ground state energy is obtained by using (189) to calculate the
effective action, which is the ground state energy times \( \beta \) in the limit \( T \to 0 \). When one
wishes to obtain the density functional \( \Gamma[n] \) at an electron density other than \( n_T \), one adds
the source term into the potential \( v_{\text{ion}}(x) \) and then solves for the Hartree density, shown in
(181), as outlined above.

\[ \text{B. Remark on the single-particle limit} \]

The single electron limit for the Hartree-method is more complicated than for the method
presented in section IV C. Because \( \int n_H(x) \, dx \) is not necessarily 1 in the single electron limit,
due to Eq. (195), in general one needs to obtain \( n_1 \) self-consistently. The other issue is that
the diagrammatic expansion contained in (189) does not cover all the diagrams for a given
order of \( U \). This means that one can’t use the Hugenholtz diagram argument to eliminate
vertex matrix element even when \( n_1 \leq 1 \). To see this point explicitly, we rewrite (189) as

\[ \Gamma[n] = -\text{Tr} \ln (G_c^{-1}) + (J - J_c) \circ n_H + \frac{1}{2} n_H \circ U \circ n_H + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}_c^{-1} \circ U \right) \]

\[ - \sum_{n=1}^{\infty} \frac{1}{n!} \left[ \sum_{k=3}^{\infty} I^{(k)}[\varphi_c] \circ b_1 \ldots \circ b_k \right]_{\text{conn.}}^n \]  \( J \circ n \).

(196)
Evidently, except for the last term above, the rest of the terms must constitute $\beta W[J]$. Since $J - J_c = -U \delta n_H$, one can also write $\beta W[J]$ as

$$
\beta W[J] = -\text{Tr} \ln \left( G_c^{-1} \right) - n_{H^T} U \delta n_H + \frac{1}{2} n_{H^T} U \delta n_H + \frac{1}{2} \text{Tr} \ln \left( \tilde{D}_c^{-1} U \right)
$$

$$
- \sum_{n=1}^{\infty} \frac{1}{n!} \left( \sum_{k=3}^{\infty} I^{(k)} \varphi_c[b_1 \ldots b_k] \right)_\text{conn}.
$$

Diagrammatic expansion of the last two terms shows that the following diagrams of order $U^2$ are absent, when compared to the regular field theoretic perturbation calculation. This is not a disadvantage of the method. Instead, what our derivation shows is that the missing diagrams eventually will be compensated by the $-n_{H^T} U \delta n_H$ term. However, it is obvious that the saddle-point formalism makes the single-electron limit hard to analyze.

When $n_1 > 0$ but $n_1 \ll 1$ at the low temperature limit, we know that $D_c(x,y) = G_c(x,y)G_c(y,x)$ will be of order $n_1$. This is because

$$
G_c(x,y) = \sum_\alpha \phi_\alpha(x)\phi_\alpha^*(y)e^{-(\varepsilon_\alpha-\mu)(\tau_x-\tau_y)} \times \begin{cases} 
(-n_\alpha) & \text{if } \tau_x \leq \tau_y \\
(1-n_\alpha) & \text{if } \tau_x > \tau_y 
\end{cases},
$$

and whenever $\tau_x \leq \tau_y$, the propagator is of order $n_1$. Since $D_c(x,y) = G_c(x,y)G_c(y,x)$, one of the propagators in the product must be of order $n_1$. In principle, one needs to solve for the occupation number $n_1$ of the lowest energy state using $i\varphi_c(x) - (U^{-1}J)_x = -G_c(x,x)$ and Eq. (195). Nevertheless, the correct one particle limit can be seen if one starts with a chemical potential $\mu$ such that $n_1 \approx 0$. In this case, we have at the $J = 0$ limit $i\varphi_c(x) = n_H(x) \approx 0$ as well as $D_c(x,y) \propto n_1 \approx 0$. This way, the higher order exchange-correlation terms may be viewed as the having smaller contributions and one may control the accuracy by controlling the number of higher order terms included. Of course, one then has $n(x) \approx i\tilde{\varphi}(x)$ and the condition $\int dx \left( i\tilde{\varphi}(x) \right) = 1 - n_1$ must be satisfied.

### C. Obtaining excitations using the Hartree method

In general the excitations are determined by Eqs. (163) and (164). Under the Hartree formalism described in this section, the natural variable used is the Hartree density $n_H$ rather than the true particle density $n_T$. One thus must transform the variable used in Eqs. (163) and (164) from $n_T$ to $n_H$. We describe below how this can be achieved.
At the physical condition \( (J = 0) \), one has

\[
0 = \left. \frac{\delta \Gamma}{\delta n(x)} \right|_{n=n_T} = \int dx_1 dx_2 \frac{\delta \Gamma}{\delta n_H(x_2)} \left. \frac{\delta n_H(x_2)}{\delta \delta n_H(x_1)} \right|_{n=n_T} \frac{\delta \Gamma}{\delta n(x)} \left. \frac{\delta J_c(x_1)}{\delta n(x)} \right|_{n=n_T}.
\]

Note that \( \delta n_H/\delta J_c \) contains no zero mode because \( n_H = \delta W_H/\delta J_c \), where \( W_H[J_c] \equiv -\text{Tr} \ln \left( G_{c}^{-1} \right) \), and \( \delta^2 W_H/\delta J_c \delta J_c \) is known to be strictly negative from a theorem proved by Valiev and Fernando.\(^{20}\) The strict negative-definiteness of \( \delta^2 W/\delta J \delta J \) can also be interpreted as the stability condition

\[
\int dx \, \delta n(x) \, \delta J(x) < 0,
\]

which means raising the local one-particle potential leads to an average decrease of the local particle concentration and vice versa. The strict negative-definiteness means that \( \delta n_H/\delta J_c \) contains no zero modes and is invertible. Also, because \( n = n_H + i \tilde{\varphi}_c \), \( \delta n/\delta J_c = \delta n_H/\delta J_c + \delta(i \tilde{\varphi})/\delta J_c \) exists via diagrammatic expansion of \( i \tilde{\varphi} \) in terms of \( J_c \). The existence of \( \delta n/\delta J_c \) implies that \( \delta J_c/\delta n \) is invertible (i.e., has no zero eigenvalues). Therefore, after multiplying the inverse of \( \delta J_c/\delta n \) and \( \delta n_H/\delta J_c \) on both sides of the above equation, one has

\[
\left. \frac{\delta \Gamma}{\delta n_H(x)} \right|_{n=n_T} = 0,
\]

which then leads to

\[
\Gamma^{(2)}(x,y) = \left. \frac{\delta^2 \Gamma}{\delta n(x) \delta n(y)} \right|_{n=n_T} = \left[ \int dx_1 dx_2 dy_1 dy_2 \frac{\delta J_c(x_1)}{\delta n(x)} \frac{\delta n_H(x_2)}{\delta \delta J_c(x_1)} \frac{\delta^2 \Gamma}{\delta n_H(y_2) \delta n_H(y_2) \delta J_c(y_1) \delta n(y)} \right]_{n=n_T}.
\]

Using Eq. (159), one may write \( \Gamma^{(2)}(x,y,\omega) \) as the analytic continuation of the integral of \( \Gamma^{(2)}(x,y) \) over time. To achieve this goal, one first writes down

\[
\Gamma^{(2)}(x,y,\nu_n) = \int_0^\beta d(\tau_y - \tau_x) \, e^{i \nu_n (\tau_y - \tau_x)} \, \Gamma^{(2)}(x,y)
\]

\[
= \int_0^\beta d(\tau_y - \tau_x) \, e^{i \nu_n (\tau_y - \tau_x)} \, \Gamma^{(2)}(x,y)
\]

\[
\equiv \int dx_1 dx_2 dy_1 dy_2 f^{x_1}_x(-i \nu_n) g^{y_1}_y(-i \nu_n) \tilde{\Gamma}^{(2)}(x_2,y_2,\nu_n) e^{i \nu_n} = \int dx_2 dy_2 h^{x_2}_x(-i \nu_n) \tilde{\Gamma}^{(2)}(x_2,y_2,\nu_n) e^{i \nu_n} ,
\]

(197)
where
\[
\tilde{\Gamma}^{(2)}(x, y, \nu_n) = \int_{0}^{\beta} d(\tau_y - \tau_x) \frac{\delta^2 \Gamma}{\delta n_H(x) \delta n_H(y)}
\]
\[
g^y_{\nu_n}(i\nu_n) \equiv \int_{0}^{\beta} d(\tau_{y_1} - \tau_{y_2}) e^{i\nu_n(\tau_{y_1} - \tau_{y_2})} \frac{\delta n_H(y_2)}{\delta J_c(y_1)} \bigg|_{n=n_T}
\]
\[
f^y_{\nu_n}(i\nu_n) \equiv \int_{0}^{\beta} d(\tau_y - \tau_{y_1}) e^{i\nu_n(\tau_y - \tau_{y_1})} \frac{\delta J_c(y_1)}{\delta n(y)} \bigg|_{n=n_T}
\]
\[
h^y_{\nu_n}(i\nu_n) \equiv \int dy_1 g^y_{\nu_n}(i\nu_n) f^y_{\nu_n}(i\nu_n).
\]

Therefore, Eq. (166) for finding the excitations becomes
\[
\int dz \tilde{\Gamma}^{(2)}(x, z, -\omega) \tilde{\Delta}(z) = 0,
\]
with \(\tilde{\Delta}(z)\) given by
\[
\tilde{\Delta}(z) = \int dy \ h^z_{\omega}(-\omega) \Delta(y).
\]

One therefore obtains the excitation energy via solving Eq. (198). Since \(h^z_{\nu_n}(-\omega)\) is invertible, one may also obtain \(\Delta(z)\) via \(\tilde{\Delta}(z)\) if desired. Within this framework, the first two terms of (189) correspond to the non-interacting part \(\Gamma_0\) of the effective action in section V. The protocol for obtaining the excitation energy is then the same as described in section V with the one exception that the ground state of the Hartree system is not the same as the ground state of the real system.

VII. DISCUSSION AND FUTURE DIRECTIONS

In this paper we focus on the auxiliary field method applied to the development of the density functional. It is natural to inquire into the physical meaning of the auxiliary, bosonic field \(\phi\) introduced in eqs (15-20). In the path integral treatment of relativistic quantum electrodynamics, if one were to integrate out the photon field, one generates the current-current interaction which is quartic in fermionic field. When viewing this process backwards, one sees that the quartic fermionic interaction is disentangled by introducing the photon field. The \(\phi\) field here thus plays a similar role to the photon field as it disentangles the quartic fermionic interaction term. As we will argue below, the \(\phi\) variable is closely related to the “time” component of the photon field, i.e., the electric potential.

To make the connection between the photon field and \(\phi\), let us first seek the nonrelativistic limit of the Lagrangian density, \(L_{EM} = -F^{\mu\nu} F_{\mu\nu}/(16\pi)\), associated with the relativistic
photon field. Note that in the limit when the speed of light approaches infinity (removal of terms involving time derivative of the three-vector potential), the Lagrangian density turns into \((\nabla A_0)^2/8\pi\), which contains no quadratic derivative with respect to time. Therefore, at finite temperature (with \(it \to \tau\)) this implies that the exponent associated with the photon field path integral will behave as

\[
i \int dt \int d\mathbf{x} \mathcal{L}_{EM} \rightarrow \int d\tau \int d\mathbf{x} \frac{(\nabla A_0)^2}{8\pi} = -\int d\tau \int d\mathbf{x} \frac{1}{8\pi} A_0 \nabla^2 A_0.
\] (199)

Setting \(U(x - y) = e^2/|x - y|\) [thus \(U^{-1}(x, y) = -\frac{1}{4\pi e^2} \nabla_x^2 \delta(x - y)\)] and comparing (199) with Eqs. (15-16), we make the identification \((iU \circ \phi)/e = A_0\), because now

\[
-\frac{1}{2} \phi_0 U \circ \phi \rightarrow \frac{1}{2} A_0 \circ (e^2 u^{-1}) \circ A_0 = -\int d\tau \int d\mathbf{x} \frac{1}{8\pi} A_0 \nabla^2 A_0.
\]

In the non-relativistic limit, the electric part and the magnetic part of electromagnetism are decoupled. Starting with a non-relativistic many–electron system, one may ask what is the quantum mechanical analog of the Poisson equation that forms the basis of electrostatics. It turns out that this is easily obtained via computing \(\delta Z[J]/\delta J|_{J=0}\) in two different ways. First, upon taking the derivative of (15) and using Eqs. (16) and (17), one obtains

\[
\frac{\delta Z[J]}{\delta J(x)}|_{J=0} = -\beta Z_{J=0} \langle \psi^\dagger(x) \psi(x) \rangle = -\beta Z_{J=0} \frac{\langle e \psi^\dagger(x) \psi(x) \rangle}{e}.
\]

Second, while taking the derivative of (15), if using Eqs. (19) and (20) one arrives at

\[
\frac{\delta Z[J]}{\delta J(x)}|_{J=0} = -\beta Z_{J=0} \langle i \phi \rangle = -\beta Z_{J=0} e U^{-1} \circ \langle A_0 \rangle = \beta Z_{J=0} \frac{1}{4\pi e} \nabla_x^2 \langle A_0(x) \rangle.
\]

We therefore obtain the thermal quantum-mechanical analog of the Poisson equation

\[
\nabla_x^2 \langle A_0(x) \rangle = -4\pi \langle e \psi^\dagger(x) \psi(x) \rangle,
\]
a result also obtained in reference 23. This connection to classical electrostatics is essential since it provides the quantum-mechanical correspondence of an important ingredient in (bio)molecular interactions that have been extensively studied in the presence of dielectrics.\(^{65–68}\)

The UDF described in this paper is systematically constructed, uniquely determined, and in principle exact. However, in terms of real computations, one can only keep \(\Gamma_i\) terms up to some order in \(\lambda\). A natural question thus arises. How well will the truncated version work? In general, this question can only be answered with numerical results. However, by
providing theoretical arguments and comparisons to other approaches, we wish to convey that this method is likely to produce good results and thus to attract computational efforts towards using the proposed approach.

It is worth pointing out the relation between the expression (46) and the scheme\textsuperscript{21} motivated by the renormalization-group. The vertex functions $I^{(j\leq l)}$ in (46) will contribute to the so-called $l$-local approximation of reference 21. The absence of $I^{(2)}$ manifests the absence of the correction term due to the bi-local contribution, as shown in reference 21. Furthermore, with the bilocal approximation\textsuperscript{21} included, Polonyi and Sailer obtained an approximate energy functional which corresponds exactly to our $\Gamma_0 + \Gamma_1$. To reach an equivalent form of the proposed $l$-local approximation of reference 21, we simply keep terms up to $\Gamma_{l/2}$. Therefore, our formulation provides an explicit means for achieving an $l$-local approximation without resorting to the Hellmann-Feynman theorem.

As shown in (87), the propagator $\tilde{D}_0$ can be expanded as

$$\tilde{D}_0 = U + U \circ D_0 \circ U + U \circ D_0 \circ U \circ D_0 \circ U + \ldots ,$$

when $U$ can be viewed as a small quantity and treated perturbatively. When one is not allowed to treat $U$ as a small parameter (say in the strong coupling regime), or when one needs to treat $U^{-1}$ as a small parameter instead, the conventional perturbative expansion in $e^2$ breaks down completely while our approach is still applicable. In the case when $U^{-1}$ must be treated as small, we expand $\tilde{D}_0$ as

$$\tilde{D}_0 = -D_0^{-1} - U^{-1} \circ D_0^{-1} - D_0^{-1} \circ U^{-1} \circ D_0^{-1} \circ U^{-1} \circ D_0^{-1} - \ldots . \quad (200)$$

And in this case, $U \gg 1$, our effective action expansion does have the Hartree term $\frac{1}{2} n \circ U \circ n$ as the leading order, followed by terms of order $U^0$ and then the expansion of $\tilde{D}_0$ provides series in powers of $U^{-1}$. Note that in this case, the exchange-correlation functional is not led by order $U$ at all, but is led by order $U^0$. This feature is not present in the conventional perturbative approach using $U$ (or $e^2$) as the expansion parameter.

As mentioned earlier, there also exist different functional methods for many electron systems. For example, the exchange correlation functional outlined by Sham\textsuperscript{27} is founded on the perturbative functional approach developed by Luttinger and Ward\textsuperscript{25} or equivalently by Klein.\textsuperscript{52} A succinct review of the Luttinger-Ward/Klein functional and its applications can be found in reference 69. The Luttinger-Ward/Klein functional yields the
grand-potential/ground-state-energy only when the functional argument is equal to the *fully-interacting*, physical, one-particle Green’s function. Instead of allowing the physical, full, one-particle Green’s function, Dahlen *et al.* proposed to find that stationary point of the Luttinger-Ward/Klein functional while restricting the argument to the Hartree-Fock Green’s functions or the Green’s functions of non-interacting systems. However, even if the Luttinger-Ward/Klein functional is computed to all orders, the error in the value of the grand potential (or the ground state energy) due to restriction on the Green’s functions remains unknown.

Furthermore, it should be noted that when the functional argument is equal to the physical one-particle Green’s function, the Luttinger-Ward/Klein functional reaches a stationary point, *not* the minimum. This means that it is possible for the Klein/Luttinger-Ward functional to assume an even lower value than the ground state energy (or the grand potential) when the functional argument deviates from the physical Green’s function. In other words, the Klein/Luttinger-Ward functional only retains its meaning as the ground state energy (or grand potential) when the Green’s function takes the value of the true (physical) Green’s function. Our effective action expression of the energy functional, on the other hand, truly represents energy of the system. Our effective action energy functional, when no truncation on the series is made, reaches its *minimum* when the electron density assumes the true (physical) density, and for any other υ-representable density profile prescribed, it represents the lowest energy possible associated with that prescribed density profile.

The method of Hedin is largely identical to that of Luttinger and Ward. This includes the fact that the energy functional reaches a stationary point, rather than the minimum, when the functional argument is the fully-interacting one-particle Green’s function. However, Hedin aims to replace the $e^2$-based (bare Coulomb) perturbative expansion of the electron self energy by another expansion using a screened interaction $W$. Hedin expresses the electron self energy and the screened interaction as a functional of the electron Green’s function of the interacting system. Interestingly, the first order result, also termed the GW approximation, of Hedin has been shown to produce good results when compared to other density functionals. This suggests that not treating $e^2$ as small might have some advantage. It is worth pointing out that the first order term, $\Gamma_1 = -\frac{1}{2} \text{Tr} \ln(D_0^{-1} \circ U)$, of the UDF described here is equivalent to the celebrated GW approximation.

Like the $W$ propagator of Hedin, the $\tilde{D}_0$ propagator introduced here also corresponds
to that of a screened interaction (see section IVD), thereby avoiding any possible infrared divergence associated with perturbative expansion based on bare Coulomb interactions. However, the screening associated with $D_0$ is from the KS particles and thus keeps the same form no matter how many orders one wishes to include. This is different from that of Hedin’s where the expression of $W$ in terms of the electron Green’s function changes with the order included. The other difference between the proposed approach and reference 31 is that the UDF proposed here depends on $J_0$, a function of three spatial variables (and possibly with one additional time variable), while the method of reference 31 expresses via $W$ the electron self energy as a functional of the Green’s function, a function of six spatial variables (and possibly with two additional time variables).

It is well known that a loopwise expansion may also be viewed as an $\hbar$ expansion, that is, an expansion of quantum-mechanical effects. By first integrating out the fermionic degrees of freedom completely, the proposed method is an expansion of bosonic loops formed by $D_0$ propagators associated with the auxiliary field $b$. The $b$ field describes the potential produced by electron density fluctuations around $n_g$. Since the ground state charge density $n_g$ captures the full quantum information of the ground state thanks to the HK theorem, one anticipates a weaker quantum effect associated with the auxiliary $b$ field than with the fermionic field. This makes the auxiliary $b$ field a suitable candidate for loop (or quantum effect) expansion, the approach pursued in this paper.

Finally, let us remark on the issue of convexity. The full $\Gamma[n]$ is supposed to be convex, thus guaranteeing a unique solution without any local minima when searching for the minimum of $\Gamma[n]$. However, in real computations only a finite number of terms of the effective action can be kept. This approximate/truncated expression may not warrant convexity and thus it is not guaranteed to be free of local minima while numerically searching for the ground state density $n_g$ (or thermal averaged density $n_T$ at finite temperature). In the near future, we plan to implement numerically the methods presented in this paper, and will describe in a separate publication the results obtained as well as the investigation on the issue of convexity.
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