Density functionals derived from Feynman diagrams.

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Abstract

We construct a stationary density functional for the partition function from a chosen set of one (boson) line irreducible Feynman diagrams. The construction does not proceed by the inversion of a Legendre transform. It is formulated for fermions with Coulomb interactions, in which case a stationary functional of the particle density is constructed, as well as for nucleons interacting with mesons, which involves a stationary functional of several densities. The use of Kohn-Sham orbits is shown to be an unnecessary complication.

1 Introduction.

The advantage of constructing density functionals of finite systems, such as nuclei, atoms and crystals, resides in the fact that they give rise to single particle states which can be calculated with a static (energy independent) potential. This makes computations considerably easier if one needs to go beyond the mean field approximation. For systems which are composed, for example, of electrons with a Coulomb interaction, it is natural to construct a functional of the particle density \( n(\vec{r}) = \langle \psi^\dagger(\vec{r}) \psi(\vec{r}) \rangle \) because this is the density to which the Coulomb field couples. It is for such systems that density functionals were first constructed\[1, 2\]. In nuclei however, there is no reason to single out the particle density \( n(\vec{r}) \). For example, pions couple to the density \( \langle \psi^\dagger(\vec{r}) \tau^a_5 \vec{\alpha} \psi(\vec{r}) \rangle \), scalar and vector mesons couple to densities \( \langle \psi^\dagger(\vec{r}) \gamma_0 \psi(\vec{r}) \rangle \) and \( \langle \psi^\dagger(\vec{r}) \psi(\vec{r}) \rangle \) respectively. In this work, we show how to express the partition function of the finite system in terms of a stationary functional of densities which are determined by the nature of the interactions.

The construction of stationary functionals of the density matrix, appropriate to systems with two-body interactions, was developed in Ref.\[3\], based on an
earlier work [4] which described the theory of a static potential in the presence of two-particle two-hole excitations. In these works, the density functionals are derived from a chosen set of one (interaction) line irreducible Feynman or Goldstone diagrams. More recently, considerable work has been devoted to the construction of stationary density functionals obtained from a Legendre transform (see [5], [6], [7], [8], [9], [10] and references therein).

In this work, we construct a density functional from a chosen subset of one line irreducible Feynman diagrams which are assumed to be dominant. We consider both fermions with Coulomb interactions and nucleons interacting with scalar, vector and \( \pi \) mesons. The formalism is simpler in the former case because it involves only one single-particle density, whereas several densities are involved in the latter. The partition functions of the two systems are defined in Sections 2 and 3. The Feynman diagram rules for the two systems are summarized in Appendices A and B. Section 4 describes the properties of one-line irreducible diagrams. In section 5 the single particle densities are expressed in terms of one-line irreducible diagrams which are calculated in terms of self-consistent potentials. The potentials and single particle densities are related by a simple analytic expression. Section 6 describes iteration procedures to calculate the self-consistent potentials and the single particle densities. In Section 7 the partition function is expressed in terms of one-line irreducible diagrams and in Section 8 it is shown to be a stationary functional of either the potentials or of the single particle densities. In Section 10 the theory is expressed in terms of so-called Kohn-Sham orbits the use of which is shown to be an unnecessary complication.

2 Non-relativistic fermions with Coulomb interactions.

Non-relativistic fermions, such as electrons with Coulomb interactions, can be described by a Hamiltonian of the form:

\[
H = \int d^3r \left( -\frac{\nabla^2}{2M} + U_{\text{ext}}(\vec{r}) - \mu \right) \psi(\vec{r}) + \frac{1}{2} \int d^3r_1 d^3r_2 \psi^\dagger(\vec{r}_1) \psi^\dagger(\vec{r}_2) \frac{e^2}{4\pi |\vec{r}_1 - \vec{r}_2|} \psi(\vec{r}_2) \psi(\vec{r}_1)
\]  

(2.1)

where \( \psi \) is the fermion field, \( M \) the fermion mass, \( e \) its electric charge and \( U_{\text{ext}}(\vec{r}) \) an external potential which could be due, for example, to an applied external field, to a nucleus or to the crystal nuclei. We define:

\[
h_0 = -\frac{\nabla^2}{2M} + U_{\text{ext}}(\vec{r})
\]

(2.2)

The partition function is given by:

\[
Z = \text{Tr} e^{-\beta (H - \mu N)} = e^W = \int D(\psi^\dagger, \psi) e^{-I(\psi^\dagger, \psi)}
\]

(2.3)
where $\psi^\dagger$ and $\psi$ are independent Grassmann variables and where $I(\psi^\dagger, \psi)$ is the euclidean action:

$$I(\psi^\dagger, \psi) = \int d^4x \left[ \psi^\dagger(x) \left( \partial_\tau + h_0 - \mu \right) \psi(x) - \frac{1}{2} \int d^4x_1 d^4x_2 \psi^\dagger(x_1) \psi(x_1) \langle x_1 | K | x_2 \rangle \psi^\dagger(x_2) \psi(x_2) \right]$$

(2.4)

with $x_\mu = x^\mu = (\tau, \vec{r})$ and:

$$-K = \frac{e^2}{-\nabla^2} - \langle x_1 | K | x_2 \rangle = \delta(\tau_1 - \tau_2) \frac{e^2}{4\pi |\vec{r}_1 - \vec{r}_2|}$$

(2.5)

Note that we defined the Coulomb potential to be $-K$ (and not $K$) so that $K$ is a negative definite operator. The reason is to use a common notation for fermions with Coulomb interactions and nucleons interacting with mesons, described in Section 3. We can also express the partition function in terms of an integral over an additional boson field $\omega_0$:

$$I(\psi^\dagger, \psi, \omega_0) = \int d^4x \psi^\dagger(x) \left( h_0 - \mu + i\omega_0 \right) \psi(x) - \frac{1}{2} \int d^4x_1 d^4x_2 \omega_0(x_1) \langle x_1 | K^{-1} | x_2 \rangle \omega_0(x_2)$$

(2.6)

By integrating over the field $\omega_0$ we recover the action (2.4). By integrating over the nucleon fields $\psi^\dagger$ and $\psi$ we obtain the partition function in the form:

$$Z = Tr e^{-\beta(\mathcal{H} - \mu N)} = e^W = \int D(\psi^\dagger, \psi) D(\omega_0) e^{-I(\psi^\dagger, \psi, \omega_0)}$$

(2.7)

In (2.6) the trace is taken over the Hilbert space composed of 0, 1, 2, ... fermions. In equation (2.7) and in the following, $Tr$ is a trace over the euclidean space-time $(\tau, \vec{r})$ and over the spins of the fermions, in other words, over the arguments of the fermion field $\psi$:

$$Tr A = tr \int d^4x \langle x | A | x \rangle = \int_0^\beta d\tau \int d^3r \sum_\sigma \langle \tau \vec{r} \sigma | A | \tau \vec{r} \sigma \rangle$$

(2.8)

and $tr$ denotes a trace over all the discrete indices other than $(\tau, \vec{r})$:

$$tr A = \sum_\sigma \langle \sigma | A | \sigma \rangle$$

(2.9)

The chemical potential of the fermions is $\mu$. In the zero temperature limit $\beta \to \infty$, the energy $E$ of the system composed of $N$ fermions is given by:

$$E - \mu N = -\frac{1}{\beta} W$$

(2.10)

The reader who is not interested in nucleons interacting with mesons can proceed to Section 4.
3 Nucleons interacting with mesons.

We consider a system of nucleons of mass \( M \) interacting with a scalar meson \( \sigma \) of mass \( m_{\sigma} \), an isoscalar vector meson \( \omega_{\mu} \) of mass \( m_{\omega} \) and pions \( \pi_{a} \) of mass \( m_{\pi} \).

The partition function can be expressed as the following path integral over the nucleon and meson fields:

\[
Tre^{-\beta(H-\mu N)} \equiv e^{W} = \int D(\sigma) D(\omega) D(\pi) e^{-I(N^\dagger,N,\sigma,\omega,\pi)} \tag{3.1}
\]

where \( I(N^\dagger,N,\sigma,\pi,\omega) \) is the euclidean action:

\[
I_{J}(N^\dagger,N,\sigma,\pi,\omega) = N^\dagger \left( \partial_{t} + \alpha \cdot \nabla + \beta M - \mu + g\beta \sigma + \frac{g_{A}}{2f_{\pi}} \beta \tau_{a} \gamma_{5} \gamma_{\mu} (\partial_{\mu} \pi_{a}) + \frac{1}{4f_{\pi}^{2}} \beta \varepsilon_{abc} \tau_{c} \pi_{a} \gamma_{\mu} (\partial_{\mu} \pi_{b}) + g_{\omega} \beta \gamma_{\mu} \omega_{\mu} \right) N + \int d^{4}x \left[ \frac{1}{2} \sigma (-\partial^{2} + m_{\sigma}^{2}) \sigma + \frac{1}{2} \pi_{a} (-\partial^{2} + m_{\pi}^{2}) \pi_{a} + \frac{1}{2} \omega_{\mu} \left( -\partial^{2} + m_{\omega}^{2} \right) \delta_{\mu\nu} + \partial_{\mu} \partial_{\nu} \right] \omega_{\nu} \right] \tag{3.2}
\]

The euclidean action (3.2) is expressed in terms of the following euclidean \((g_{\mu\nu} = \delta_{\mu\nu})\) 4-vectors:

\[
x_{\mu} = x^{\mu} = (\tau,\vec{r}) \quad \gamma_{\mu} = \gamma^{\mu} = (i\beta,\vec{\gamma}) \quad \omega_{\mu} = \omega^{\mu} = (\omega_{0},\vec{\omega})
\]

\[
\partial^{2} = \partial_{\tau}^{2} + \nabla^{2} \quad \int d^{4}x = \int^{\beta}_{0} d\tau \int d^{3}r \tag{3.3}
\]

We shall work with the euclidean action obtained by integrating out the nucleon fields, in which case the partition function becomes:

\[
Tre^{-\beta(H-\mu N)} \equiv e^{W} = \int D(\sigma) D(\omega) D(\pi) e^{-I(\sigma,\omega,\pi)} \tag{3.4}
\]

with:

\[
I(\sigma,\pi,\omega) = -Tr \ln \left( \partial_{\tau} + \alpha \cdot \nabla + \beta M - \mu + g\beta \sigma + \frac{g_{A}}{2f_{\pi}} \beta \tau_{a} \gamma_{5} \gamma_{\mu} (\partial_{\mu} \pi_{a}) + \frac{1}{4f_{\pi}^{2}} \beta \varepsilon_{abc} \tau_{c} \pi_{a} \gamma_{\mu} (\partial_{\mu} \pi_{b}) + g_{\omega} \beta \gamma_{\mu} \omega_{\mu} \right) + \int d^{4}x \left[ \frac{1}{2} \sigma (-\partial^{2} + m_{\sigma}^{2}) \sigma + \frac{1}{2} \pi_{a} (-\partial^{2} + m_{\pi}^{2}) \pi_{a} + \frac{1}{2} \omega_{\mu} \left( -\partial^{2} + m_{\omega}^{2} \right) \delta_{\mu\nu} + \partial_{\mu} \partial_{\nu} \right] \omega_{\nu} \right] \tag{3.5}
\]

The trace \( Tr \) is taken over the quantum numbers which define the fermion field \( N(x) \). For example:

\[
Tr \left( \partial_{\tau} + \alpha \cdot \nabla + \beta M - \mu + g\beta \sigma \right) \equiv \int d^{4}x tr \left( x \left| \partial_{\tau} + \alpha \cdot \nabla + \beta M - \mu + g\beta \sigma \right| x \right) \tag{3.6}
\]
and \( tr \) is a trace over the discrete (Dirac, flavor) quantum numbers other than \( x = (\tau, \vec{r}) \).

We stress from the outset that we are not suggesting that (3.5) is the action which should be used to calculate finite nuclei. We are simply introducing the \( \sigma, \omega \) and \( \pi \) mesons to show how to construct a density functional with different types of meson-nucleon interactions.

In order to express the partition function in terms of Feynman diagrams, we adopt a condensed notation. We define the unperturbed fermion hamiltonian:

\[
   h_0 = \frac{\vec{\alpha} \cdot \vec{\nabla}}{i} + \beta M
\]

(3.7)

The following is not restricted to a Dirac unperturbed hamiltonian. It could, for example, be replaced by its non-relativistic reduction

\[
   h_0 = -\nabla^2 \frac{m}{2M},
\]

in which case the couplings would have to be modified accordingly. The hamiltonian \( h_0 \) acts in the Hilbert space of one fermion. We define the following \( \Gamma \) operators which act in the same space:

\[
   \Gamma_a \equiv \left( \Gamma^{(\sigma)}, \Gamma^{(\omega)}_\mu, \Gamma^{(\pi)}_{\mu a} \right) = \left( g_\sigma \beta, g_\omega \beta \gamma_\mu, \frac{g_A}{2f_\pi} \beta \tau_a \gamma_5 \gamma_\mu \right)
\]

(3.8)

as well as the operator:

\[
   \Theta^{(\pi)}_{a(\mu b)} = \frac{1}{4f_\pi^2} \beta \varepsilon_{abc} \tau_c \gamma_\mu
\]

(3.9)

The meson fields are denoted by:

\[
   S_a(x) \equiv (\sigma(x), (\partial_\mu \pi_a(x)), \omega_\mu(x))
\]

(3.10)

We will use the condensed notation:

\[
   (\Gamma S) \equiv \Gamma^{(\sigma)} \sigma + \Gamma^{(\omega)} \omega_\mu + \Gamma^{(\pi)}_\mu (\partial_\mu \pi_a)
\]

\[
   = g_\sigma \beta \sigma + \frac{g_A}{2f_\pi} \beta \tau_a \gamma_5 \gamma_\mu (\partial_\mu \pi_a) + g_\omega \beta \gamma_\mu \omega_\mu
\]

\[
   S (\Theta S) \equiv \pi_a \Theta_{a(\mu b)} (\partial_\mu \pi_b) = \frac{1}{4f_\pi^2} \beta \varepsilon_{abc} \tau_c \pi_a \gamma_\mu (\partial_\mu \pi_b)
\]

(3.11)

In the expressions above, \( \gamma_\mu \) and \( \omega_\mu \) are the euclidean 4-vectors defined in (3.3).

Note that the coupling constants are included in \( \Gamma \) and \( \Theta \).

We further define the meson propagators \( K \):

\[
   K = \begin{pmatrix}
   -\sigma^2 + m_\sigma^2 & 0 & 0 \\
   0 & \delta_{ab} - \sigma^2 + m_\omega^2 & 0 \\
   0 & 0 & \frac{-1}{\delta_{\mu\nu} \omega^2 - \frac{1}{m_\pi^2} \partial_\mu \partial_\nu}
   \end{pmatrix}
\]

(3.12)

With this condensed notation we can write:

\[
   \frac{1}{2} SK^{-1} S = \int d^4x \left\{ \frac{1}{2} \sigma \left( -\partial^2 + m_\sigma^2 \right) \sigma + \frac{1}{2} \pi_a \left( -\partial^2 + m_\pi^2 \right) \pi_a \right\}
\]
\[ + \frac{1}{2} \omega_\mu \left( (\partial^2 + m_\omega^2) \delta_{\mu\nu} + \partial_\mu \partial_\nu \right) \omega_\nu \] (3.13)

and the euclidean actions (3.2) and (3.5) acquire the form:

\[ I (N^\dagger, N, S) \equiv N^\dagger (\partial_\tau + h_0 - \mu + (\Gamma S) + S (\Theta S)) N + \frac{1}{2} SK^{-1} S \]

\[ I (S) \equiv - Tr \ln (\partial_\tau + h_0 - \mu + (\Gamma S) + S (\Theta S)) + \frac{1}{2} SK^{-1} S \] (3.14)

The partition function is given by:

\[ Z = Tr e^{-\beta (H - \mu N)} \equiv e^W = \int D (N^\dagger, N) D (S) e^{-N^\dagger (\partial_\tau + h_0 - \mu + (\Gamma S) + S (\Theta S)) N + \frac{1}{2} SK^{-1} S} \]

\[ = \int D (S) e^{Tr \ln (\partial_\tau + h_0 - \mu + (\Gamma S) + S (\Theta S)) - \frac{1}{2} SK^{-1} S} \] (3.15)

The inclusion of separate chemical potentials for neutrons and protons would cause no difficulty. In the zero temperature limit \( \beta \to \infty \), the energy \( E \) of the system composed of \( A \) nucleons is equal to:

\[ E - \mu A = - \frac{1}{\beta} W \] (3.16)

4 One (boson) line irreducible diagrams.

In this section we define the one (boson) line irreducible diagrams which are used to construct the density functionals. The rules for calculating Feynman diagrams are summarized in Appendices A and B. Consider a general unlabeled connected diagram, such as:

![Diagram](4.1)

We can recognize so-called articulation lines which are dashed lines (boson propagators or interaction lines) such that the diagram separates into two disconnected parts when the dashed line is cut. In the diagram (4.1) the four articulation lines are highlighted by dots. The diagram (4.1) has \( n_a = 4 \) articulation lines. When the articulation lines are cut, the disconnected pieces consist of:
• **cycles**, which are closed loops (formed by oriented fermion propagators) the vertices of which are connected *only* to articulation lines. The diagram (4.1) has \( n_c = 3 \) cycles.

• **one (boson) line irreducible parts**, which are irreducible in the sense that they cannot be separated into two disconnected parts by cutting a dashed line. The diagram (4.1) has \( n_I = 2 \) irreducible parts.

Every diagram which has \( n_a \) articulation lines, \( n_c \) cycles and \( n_I \) irreducible parts is such that:

\[
 n_I + n_c - n_a = 1 \quad (4.2)
\]

This topological property results from the fact that, whenever a boson propagator is added to a diagram, it is either an articulation line or not. If it is, it either adds a cycle or an irreducible part. If it is not, it leaves \( n_I, n_c \) and \( n_a \) unchanged.

The topological property (4.2) does not hold for diagrams with open ended meson dashed lines, which contain in fact a source factor \( j \) at their end point. The latter should be counted as an irreducible part and for such diagrams the topological relation should read:

\[
 n_I + n_j + n_c - n_a = 1 \quad (4.3)
\]

where \( n_j \) is the number of open ends (or the number of source points) of the diagram.

In the following we shall refer to one (boson) line irreducible diagrams simply as one-line irreducible diagrams.

## 5 The particle densities expressed in terms of one-line irreducible diagrams.

In Appendices A.2 and B.2 the particle densities are expressed in terms of connected diagrams \( \Gamma_c \). In the case of fermions with Coulomb interactions, the particle density is given by (A.22):

\[
n(x) = -tr \langle x|g|x \rangle + \int d^4 x_1 d^4 x_2 \frac{\delta \Gamma_c}{\delta \langle x_1 |g|x_2 \rangle} \langle x_1 |g|x \rangle \langle x|g|x_2 \rangle \quad (5.1)
\]

For nucleons interacting with mesons, the various densities are given by (B.33):

\[
\rho_n (x) = -tr \langle x|g|x \rangle \Gamma_a + \int d^4 x_1 d^4 x_2 \frac{\delta \Gamma_c}{\delta \langle x_1 |g|x_2 \rangle} \langle x_1 |g|x \rangle \Gamma_a \langle x|g|x_2 \rangle \quad (5.2)
\]

In (5.1) and (5.2), the connected diagrams are calculated with the unperturbed fermion propagator:

\[
g = \frac{1}{\partial_r + h_0 - \mu} \quad (5.3)
\]
and $\Gamma_a$ are the operators defined in (3.8) and (3.9).  

From here on we use the formalism applicable to nucleons interacting with mesons. It is however simple to recover expressions applicable to fermions with Coulomb interactions. It suffices to set:

$$\Gamma_a = 1 \quad U_a (x) = U (x) \quad \rho_a (x) = n (x) \quad (5.4)$$

In the case of nucleons interacting with mesons, the coupling constants are included in the $\Gamma_a$. As a result, the particle densities $\rho_a (x)$ are multiplied by the coupling constants and they are related to the densities $n_a (x)$ in the usual sense by equations (13.2). In the case of fermions with Coulomb interactions, the coupling constant $e^2$ is included in the interaction (2.5).

We now show that it is also possible to express the particle densities $\rho_a (x)$ in terms of one-line irreducible diagrams $\Phi (U)$ as follows:

$$\rho_a (x) = - \frac{\delta}{\delta U_a (x)} \left( Tr \ln G^{-1} + \Phi (U) \right)$$

$$= - tr \langle x | G | x \rangle \Gamma_a + \int d^4 x_1 d^4 x_2 \frac{\delta \Phi (U)}{\delta (x_1 | G | x_2)} \langle x_1 | G | x \rangle \Gamma_a \langle x_1 | G | x_2 \rangle \quad (5.5)$$

In the expression (5.5), $G$ is the "dressed" fermion propagator:

$$G = \frac{1}{\partial_\tau + h_0 - \mu + U_a \Gamma_a} \quad (5.6)$$

and $U_a (x)$ is a local potential which satisfies the equation:

$$U_a (x) = \int d^4 y \langle x | K_{ab} | y \rangle \frac{\delta}{\delta U_b (y)} \left( Tr \ln G^{-1} + \Phi (U) \right) \quad (5.7)$$

For nucleons interacting with mesons, the boson propagators $K_{ab}$ are defined in (3.12). For fermions with Coulomb interactions, $K_{ab} \equiv K$, where $K$ is (minus) the Coulomb potential (2.5). The oriented lines of the one-line irreducible diagrams $\Phi (U)$ are the dressed propagators $G$. When $h_0$ is time independent, as assumed in this work, the potentials $U_a (x)$ and the densities $\rho_a (x)$ are also time independent because $\langle x | K_{ab} | y \rangle$ depends only on $x_\mu - y_\mu$.

In this formulation, an approximation to the potential $U_a (x)$ and the particle density $\rho_a (x)$ are obtained by choosing a subset $\Phi (U)$ of one-line irreducible diagrams. Any finite or infinite subset can be chosen. For example, $\Phi (U)$ could be limited to the following one-line irreducible diagrams:

$$\Phi (U) = \Phi_1 + \Phi_2 + \Phi_3 + \Phi_4 \quad (5.8)$$

---

1 No confusion should arise from the use of $\Gamma$ to denote connected diagrams $\Gamma_c$ and the operators (3.8).
When the set \(5.8\) of one-line irreducible diagrams is chosen, the density \(5.5\) is:

\[
\rho_a(x) = (x,a) + \langle x,a \rangle + \langle x,a \rangle + (x,a) + \langle x,a \rangle + \langle x,a \rangle + \langle x,a \rangle
\]

The representation of the density in terms of diagrams with a slash labeled \((x,a)\) is explained in Appendices A.2 and B.2.

The potential \(5.7\) can be written as follows:

\[
U_a(x) = \int d^4y \langle x|K_{ab}|y \rangle \left[ tr \langle y|G|y \rangle \Gamma_b - \int d^4x_1d^4x_2 tr \frac{\delta \Phi(U)}{\delta \langle x_1|G|x_2 \rangle} \langle x_1|G|y \rangle \Gamma_b \langle y|G|x_2 \rangle \right]
\]

so that the diagram representation of the potential \(U_a(x)\) is:

\[
U_a(x) = (x,a) + (x,a) + (x,a) + \langle x,a \rangle + (x,a) + \langle x,a \rangle + \langle x,a \rangle
\]

In the diagrams \(5.9\) and \(5.11\) the oriented lines are the dressed fermion propagators \(5.6\).

The dressed propagator \(G\) can be expressed in terms of the unperturbed propagator \(g\) by the series:

\[
G = g - gU\Gamma g + gU\Gamma gU - ...
\]

Therefore each oriented fermion propagator \(G\) in the diagrams \(5.9\) and \(5.11\) generates an infinite set of diagrams composed of oriented lines \(g\) with any number of \(U\) insertions. Furthermore, iterations of equation \(5.10\) will generate, for each one of these insertions, an infinite set of diagrams connected by an articulation line. It is easy to check that the diagrams \(5.11\) generate diagrams with a tree structure and that they yield a particle density \(5.2\) and a potential \(5.7\) in which the contribution of each diagram \(\Gamma c\) is included once and only once.
In many cases, the ground state densities may vanish because of self-consistent symmetries, discussed in Ref. 3, such as spherical symmetry, time-reversal symmetry, isospin or flavor symmetry for example. Self-consistent symmetries depend on the system which is being calculated, whether, for example, it is in a rotating frame, whether it is exposed to an external field, whether the number of nucleons is even or odd, whether there is an excess of neutrons or protons, and so forth. In this work we do not assume such symmetries.

Note that the potentials $U_a(x)$ and the densities $\rho_a(x)$ are related the simple analytic expressions:

$$U_a(x) = -\int d^4 y \langle x| K_{ab} | y \rangle \rho_b(y) \quad \rho_a(x) = -\int d^4 y \langle x| K_{ab}^{-1} | y \rangle U_b(y)$$

This is in sharp contrast with the potentials which are expressed in terms of Kohn-Sham orbits (see Section 10).

In Section 7 we express the partition function in terms of one-line irreducible diagrams and in Section 8 we show that it is a stationary functional of both the particle densities $\rho$ and the potentials $U$.

6 Iteration procedure to calculate the particle densities and potentials.

The time-independent single particle hamiltonian $h_0 + U_a \Gamma_a$ can be diagonalized:

$$(h_0 + U_a \Gamma_a) |\lambda\rangle = e_\lambda |\lambda\rangle$$

The eigenstates $|\lambda\rangle$ are fermion orbits and we distinguish particle orbits $|p\rangle$ with energies $e_p > \mu$ and hole orbits $|h\rangle$ with energies $e_h < \mu$. The eigenvalue problem (6.1) involves the local and static potentials $U_a(x)$. This makes the computation of the fermion orbits $|\lambda\rangle$ considerably simpler and faster than, for example, the determination of the poles and residues of the single particle Green’s function, which involves a non-local and energy dependent mass operator. This is the main interest of constructing density functionals.

In the zero temperature limit, the dressed propagator (5.6) can be expressed in terms of the particle and hole orbits as in (C.4) and (C.5):

$$\langle x_1 |G| x_2 \rangle \equiv \langle \tau_1 \vec{r}_1 |G| \tau_2 \vec{r}_2 \rangle$$

$$= \theta (\tau_1 - \tau_2) \sum_p e^{-(e_p - \mu)(\tau_1 - \tau_2)} \langle \vec{r}_1 | p \rangle \langle p | \vec{r}_2 \rangle - \theta (\tau_2 - \tau_1) \sum_h e^{-(e_h - \mu)(\tau_1 - \tau_2)} \langle \vec{r}_1 | h \rangle \langle h | \vec{r}_2 \rangle$$

$$\langle \tau \vec{r}_1 |G| \tau \vec{r}_2 \rangle = - \sum_h \langle \vec{r}_1 | h \rangle \langle h | \vec{r}_2 \rangle$$

In this representation, the first term of (6.2) (but not the second) acquires the form of a density of an uncorrelated Slater determinant:

$$- tr \langle x |G| x \rangle \Gamma_a = \sum_h \langle h| \vec{r} \rangle \Gamma_a \langle \vec{r}| h \rangle$$

(6.3)
The equations (5.7) or (5.10) can be solved by iteration. We begin by choosing a set \( \Phi (U) \) of one-line irreducible diagrams. Then:

1. We make an initial guess at the potentials \( U_a(x) \). Alternatively, we can make an initial guess at the particle densities \( \rho_a(x) \) and deduce the initial potentials from (5.13).

2. With the potentials \( U_a(x) \) we calculate the fermion orbits (6.1) by diagonalizing \( h_0 + U_a \Gamma_a \). This yields the dressed fermion propagator \( G \) defined in (6.2).

3. We express the set \( \Phi (U) \) of one-line irreducible diagrams in terms of the fermion propagator \( G \) and we recalculate the potentials \( U_a(x) \) using the equations (5.7) or (5.10).

4. We return to step 2 and we continue the process until convergence is achieved.

The densities \( \rho_a(x) \) can then be deduced from (5.13). The equation (5.2) can be used to replace the iteration procedure above by one which yields successive approximations to the densities.

The fact that it is equally easy to calculate either the densities or the potentials is due to the simple equation (5.13) which relates the two. This is why we call the eigenstates (6.1) \( h_0 + U_a \Gamma_a \) the optimal orbits for constructing stationary density functionals. In Section 10 we show that the use of Kohn-Sham orbits is more complicated.

7 The partition function expressed in terms of one-line irreducible diagrams.

In this section we express the partition function in terms of one-line irreducible diagrams. The partition function acquires the form of a stationary functional, namely (7.13), of either the potentials \( U_a(x) \) or the particle densities \( \rho_a(x) \).

In Appendices A and B the partition function \( Z = e^W \) is expressed as a sum of connected diagrams \( \Gamma_c \), calculated with unperturbed fermion propagators \( g \), defined in (5.3):

\[
W = Tr \ln g^{-1} + \Gamma_c
\]

(7.4)

If we wish to express the partition function in terms of one-line irreducible diagrams \( \Phi (U) \), calculated with the dressed propagators \( G \) defined in (5.6), we need to correct for the fact that the one-line irreducible diagrams \( \Phi (U) \) overcount the diagrams \( \Gamma_c \). Indeed, each diagram \( \Gamma_c \), which can be decomposed into \( n_I(\Gamma_c) \) one-line irreducible parts, is included \( n_I(\Gamma_c) \) times in the corresponding one-line irreducible diagram \( \Phi (U) \). Consider, for example, the one-line irreducible
The connected diagram:

\[ \Phi(U) = \begin{array}{c}
\end{array} \]  

which is calculated with dressed propagators \( G \). The connected diagram:

\[ \Gamma_c = \begin{array}{c}
\end{array} \]  

which is calculated with bare propagators \( g \) and which contains \( n_I = 2 \) one-line irreducible parts, is included twice in the diagram \( \Phi(U) \). Indeed either of the two irreducible parts of the diagram \( (7.6) \) can be considered as dressing the propagator of the other. More generally, a set \( \Phi(U) \) of one-line irreducible diagrams, calculated dressed propagators \( G \), generates a set of connected diagrams \( \Gamma_c \) composed of \( n_I \) (\( \Gamma_c \)) irreducible parts and it overcounts them \( n_I \) (\( \Gamma_c \)) times. Its contribution is therefore equal to:

\[ \Phi(U) = \sum_{\Gamma_c} n_I (\Gamma_c) \Gamma_c \]  

(7.7)

There are two other ways to generate connected diagrams. The connected diagrams \( \Gamma_c \) generated by the one-line irreducible diagrams \( \Phi(U) \) can also be generated by the following set of diagrams, consisting of a fermion closed loop interacting once, twice,... with the potential \( U_a \Gamma_a \):

\[ \begin{array}{c}
\end{array} + \begin{array}{c}
\end{array} + \begin{array}{c}
\end{array} + ... \]  

(7.8)

In these diagrams the boson lines appended to the closed oriented fermion line are interactions with the potential \( U_a \Gamma_a \). The contribution of the diagrams \( (7.8) \) is:

\[ tr \int d^4x \left\langle x \left| g\Gamma_a U_a - \frac{1}{2} g\Gamma_a U_a g\Gamma_b U_b + \frac{1}{3} g\Gamma_a U_a g\Gamma_b U_b g\Gamma_c U_c - ... \right| x \right\rangle \]

\[ = Tr \ln (1 + g\Gamma_a U_a) = Tr \ln gG^{-1} \]  

(7.9)

where we used the fact that \( gG^{-1} = 1 + g\Gamma_a U_a \). However, not only does the expression \( (7.9) \) include all the diagrams generated by the one-line irreducible
diagrams $\Phi (U)$, but it overcounts them. Indeed, each diagram $\Gamma_c$, which can be decomposed into $n_c(\Gamma_c)$ fermion loops, occurs $n_c(\Gamma_c)$ times in the contribution (7.9), which is therefore equal to:

$$Tr \ln gG^{-1} = \sum_{\Gamma_c} n_c(\Gamma_c) \Gamma_c$$  (7.10)

A third way to include the diagrams generated by the set $\Phi (U)$ is to calculate the expression:

$$= \frac{1}{2} \int d^4x \int d^4y \rho_a(x) \langle x | K_{ab}^{-1} | y \rangle \rho_b(y) = \frac{1}{2} \int d^4x \int d^4y U_a(x) \langle x | K_{ab}^{-1} | y \rangle U_b(y)$$  (7.11)

where $\rho_a(x)$ is the density (5.5). Not only does the expression (7.11) include all the diagrams generated by the one-line irreducible diagrams $\Phi (U)$, but each diagram $\Gamma_c$ which contains $n_a(\Gamma_c)$ articulation lines, is included $n_a(\Gamma_c)$ times in the contribution (7.11), so that:

$$\frac{1}{2} \int d^4x \int d^4y U_a(x) \langle x | K_{ab}^{-1} | y \rangle U_b(y) = \sum_{\Gamma_c} n_a(\Gamma_c) \Gamma_c$$  (7.12)

We can combine the results (7.7), (7.10) and (7.12) to write:

$$\Phi (U) + Tr \ln gG^{-1} - \frac{1}{2} \int d^4x \int d^4y U_a(x) \langle x | K_{ab}^{-1} | y \rangle U_b(y)$$

$$= \sum_{\Gamma_c} [n_f(\Gamma_c) + n_e(\Gamma_c) - n_a(\Gamma_c)] \Gamma_c = \sum_{\Gamma_c} \Gamma_c$$  (7.13)

where we used the topological relation (4.2). The expression (7.13) therefore sums the diagrams $\Gamma_c$ generated by the set $\Phi (U)$ of one-line irreducible diagrams correctly (meaning that each one is counted once).

The partition function $Z = e^W$ can therefore be expressed in terms of one-line irreducible diagrams as follows:

$$\ln Z = W = tr \ln g^{-1} + \Phi (U) + Tr \ln gG^{-1} - \frac{1}{2} UK^{-1}U$$  (7.14)

which reduces to:

$$W = Tr \ln G^{-1} + \Phi (U) - \frac{1}{2} UK^{-1}U$$  (7.15)

In the zero temperature limit, the energy $E$ of the system composed of $N$ particles is related to $W$ by the equation:

$$W = -\beta (E - \mu N)$$  (7.16)
8 Stationary properties of the density functional.

Consider a variation \( U_a \rightarrow U_a + \delta U_a \) of the potential \( U_a \). The corresponding variation of \( W \) is:

\[
\delta W = \int d^4x \left[ \delta U_a(x) \frac{\delta}{\delta U_a(x)} \left[ \text{Tr} \ln G^{-1} + \Phi(U) \right] - \delta U_a(x) \int d^4y \langle x | K_a^{-1} | y \rangle U_b(y) \right] 
\]

The equation \( \frac{\delta W}{\delta U_a(x)} = 0 \) therefore leads to the equation (5.7). In other words, the equation (5.7) which determines the potential \( U_a(x) \) is equivalent to the equation which states that the functional (7.15) should be stationary with respect to variations of the potential \( U_a(x) \).

Since \( U = -K \rho \), the generating functional (7.15) may equally well be regarded a functional of the densities \( \rho_a \). And since \( \frac{\delta W}{\delta \rho_a} = \frac{\delta W}{\delta U_a} \delta U_a \delta \rho_a = -K \frac{\delta W}{\delta \rho_a} \), the functional (7.15) is also a stationary functional of the particle densities \( \rho_a \).

If all one-line irreducible diagrams \( \Phi \) are neglected, the scheme above reduces to the Hartree approximation. If all one-line irreducible diagrams are included (a goal never achieved) the scheme yields an exact energy and exact particle densities. An approximation is defined in terms of a selected subset of one-line irreducible diagrams. In all cases, the fermion orbits are eigenstates of a single-particle hamiltonian involving a local potential.

9 One-line irreducible diagrams identified in the path integral.

The expression (7.15) has been derived from an analysis of the topology of connected diagrams. It can also be derived by an algebraic manipulation of the path integral (3.15) of the partition function. Indeed, let us make the following change of the integration variable:

\[
S_a(x) \rightarrow S'_a(x) = S_a(x) + U_a(x) 
\]

where \( U_a(x) \) is an as yet unspecified local field. The partition function (3.15) becomes, after dropping the primes:

\[
e^W = \int D(S) e^{\text{Tr} \ln(\partial_x + h_0 - \mu + \Gamma S + \Gamma U + S(\Phi S) + U(\Phi U) + U(\Phi S) + S(\Phi U)) - \int d^4x \left( \frac{1}{2} SK^{-1} S + \frac{1}{2} UK^{-1} U \right)} 
\]

Let us define:

\[
G^{-1} = \partial_x + h_0 - \mu + \Gamma U + U(\Phi U) 
\]

so that:

\[
\text{Tr} \ln(\partial_x + h_0 - \mu + \Gamma S + \Gamma U + S(\Phi S) + U(\Phi U) + U(\Phi S) + S(\Phi U)) \\
= \text{Tr} \ln G^{-1} + \text{tr} \ln \left( 1 + G S + G U(\Phi S) + G S(\Phi S) \right) 
\]

14
The partition function becomes:

$$e^W = e^{-Tr \ln G - \frac{1}{2} UK^{-1}U} \int D(S) e^{Tr \ln(1 + GTS + GU(\Phi S) + GS(\Phi S)) - \int d^4x \left( \frac{1}{2} SK^{-1}S + SK^{-1}U \right)}$$

(9.5)

so that:

$$W = Tr \ln G^{-1} - \frac{1}{2} UK^{-1}U$$

(9.6)

$$+ \ln \int D(S) e^{Tr \ln(1 + GTS + GU(\Phi S) + GS(\Phi S)) - \int d^4x \left( \frac{1}{2} SK^{-1}S + SK^{-1}U \right)}$$

(9.7)

If we compare this to the expression (7.15), we obtain a path integral representation of one-line irreducible diagrams:

$$\Phi (U) = \ln \int D(S) e^{Tr \ln(1 + GTS + GU(\Phi S) + GS(\Phi S)) - \int d^4x \left( \frac{1}{2} SK^{-1}S + SK^{-1}U \right)}$$

(9.8)

To check that the path integral generates only one-line irreducible diagrams, we expand $Tr \ln (1 + GTS + GU(\Phi S) + GS(\Phi S))$ in powers of $(\Gamma S + U(\Phi S) + S(\Phi S))$ and we derive the corresponding Feynman diagrams as done in Appendices A and B. However, the difference with the diagram expansion of the expression (3.15) is due to the occurrence of the term $SK^{-1}U$ in (9.8), which generates diagrams with open ended interaction lines which are attached to fermion propagators at one end and to the potential $U$ at the other. These diagrams are one-line reducible. The reader can check for himself that, when the potential $U$ is chosen to be $U = -K\rho$, these diagrams cancel the one-line reducible diagrams (without open ended interaction lines) so that the expression (9.8) generates only one-line irreducible diagrams.

10 The use of Kohn-Sham orbits.

We now compare the theory expressed in Sections 5 and 7 to the construction of stationary density functionals using Legendre transforms. For simplicity, we limit the discussion to systems of fermions with Coulomb interactions, which involve only one single-particle density $n(x)$ and for which we can set:

$$\Gamma_a = 1 \quad U_a (x) = U (x) \quad \rho_a (x) = n (x)$$

(10.9)

Let us add to $h_0$ a source term $J(x)$ coupled to the particle density $n(x)$. A stationary density functional is then obtained from the Legendre transform:

$$\Gamma (n) = W + Jn$$

(10.10)

The Lagrange multiplier $J(x)$ acts as a local potential. The equation $\frac{\delta \Gamma}{\delta n} = J$ states that, for a given $J$, the density is given by $n = -\frac{\delta W}{\delta J}$ and the equation $\frac{\delta \Gamma}{\delta J} = 0$ states that $J = 0$, in which case the density $n$ is the equilibrium or ground
state density. The inversion of the equation \( n = -\frac{\delta W}{\delta J} \) consists in finding the local potential \( J(x) \) which yields a given density \( n(x) \), thereby making \( \Gamma(n) \) a stationary functional of the density. A frequently used way to invert the equation \( n = -\frac{\delta W}{\delta J} \) consists in separating the source term \( J \) into two parts:

\[
J = J_0 + J_{\text{int}}
\]

(10.11)

where \( J_0 \) is chosen such that the exact density \( n(x) \) is given by the uncorrelated Slater determinant, the orbits of which are eigenstates of the hamiltonian \( h_0 + J_0 \) and which are called Kohn-Sham orbits (see [5], [6], [7], [8], [9], [10] and references therein). The "interacting" part \( J_{\text{int}} \) is then calculated in terms of the density \( n \) and the potential \( J_0 \) by considering, for example, an expansion in powers of the coupling constant, expressed by connected Feynman or Goldstone diagrams, calculated with fermion propagators \( G = \frac{1}{\partial_\tau + h_0 - \mu + J_0} \) which can be constructed from the Kohn-Sham orbits. The interacting part \( J_{\text{int}} \) can then be expressed in terms of one-line irreducible diagrams with, in addition, extra diagrams involving for example the inverse density-density correlation function \( C.7 \). Finally, when \( J_{\text{int}} \) is determined, \( J_0 \) is determined by the equation \( J_0 = -J_{\text{int}} \) which states that, in the ground state, \( J = 0 \).

In section 5 we expressed the density directly in terms of one-line irreducible diagrams, which are calculated with a self-consistent potential \( U(x) \), determined by the equation \( 5.7 \). The potential \( U(x) \) is then simply and analytically related to the density \( n(x) \) by the equation \( 5.13 \). We now show that if we split the self-consistent potential \( U(x) \) into two terms:

\[
U(x) = U_0(x) + U_{\text{int}}(x)
\]

(10.12)

so that the dressed fermion propagator becomes:

\[
G^{-1} = G_0^{-1} + U_{\text{int}} \quad G = G_0 - G_0 U_{\text{int}} G
\]

(10.13)

with:

\[
G_0 = \frac{1}{\partial_\tau + h_0 - \mu + U_0}
\]

(10.14)

and if we choose the potential \( U_0(x) \) such that the density \( n(x) \) is equal to:

\[
n(x) = -tr \langle x|G_0|x\rangle
\]

(10.15)

then \( U_0 \) becomes identical to the source term \( J_0 \) used in the Legendre transform method.

There is no real need to separate the potential into the two terms \( 10.12 \). In fact we shall see that it makes the theory and the calculations somewhat more complicated. We do so however, to compare the present theory to the frequently used Kohn-Sham orbits in the Legendre transform method.

We can express equation \( 10.13 \) in terms of the eigenstates of \( h_0 + U_0 \):

\[
(h_0 + U_0)|\lambda\rangle = \epsilon_\lambda |\lambda\rangle
\]

(10.16)
and "particle" and "hole" orbits \(|p\rangle\) and \(|h\rangle\) are the eigenstates \(|\lambda\rangle\) belonging to eigenvalues respectively \(e_p > \mu\) and \(e_h < \mu\). Since \(G_0\) can be expressed in the form (C.4) and (C.5), the density (10.15) can be written in the form:

\[ n(x) = -\text{tr} \langle x | G_0 | x \rangle = \sum_h \langle h | \vec{r} \rangle \langle \vec{r} | h \rangle \]

(10.17)

The equations (10.15) and (10.17) state the density of the correlated system is equal to the density of a Slater determinant composed of the eigenstates of \(h_0 + U_0\). That is why the eigenstates (10.16) are usually called Kohn-Sham orbits.

### 10.1 Equations for the potentials \(U_0\) and \(U_{int}\).

The equation (5.5) which expresses the density \(n(x)\) in terms of one-line irreducible diagrams can be written in the form:

\[ n(x) = -\text{tr} \langle x | G_0 | x \rangle - \text{tr} \langle x | G_0 U_{int} G | x \rangle - \frac{\delta \Phi(U)}{\delta U(x)} \]

(10.18)

where (10.13) was used. With the choice (10.15) of \(U_0\) this equation reduces to:

\[ \text{tr} \langle x | G_0 U_{int} G | x \rangle = \frac{\delta \Phi(U)}{\delta U(x)} \bigg|_{U=U_0+U_{int}} \]

(10.19)

This is an integral equation for \(U_{int}\) which can be solved by iteration, given the potential \(U_0\). Once \(U_{int}\) is thus determined, \(U_0\) can be obtained from the equation (5.13), which reads:

\[ U_0(x) + U_{int}(x) = - \int d^4x' \langle x | K | x' \rangle n(x') \]

(10.20)

Since \(K\) is (minus) the Coulomb potential (2.5), we obtain:

\[ U_0(\vec{r}) = \int d^3r' \frac{e^2}{4\pi |\vec{r} - \vec{r}'|} n(\vec{r}') - U_{int}(\vec{r}) \]

(10.21)

When \(U = U_0 + U_{int}\) the functional (7.15) becomes:

\[ W(U) = Tr \ln G_0^{-1} + Tr \ln (1 + G_0 U_{int}) + \Phi(U_0 + U_{int}) - \frac{1}{2} (U_0 + U_{int}) K^{-1} (U_0 + U_{int}) \]

(10.22)

Once \(U_0\) and \(U_{int}\) have been determined, we can use (10.20) to simplify \(W(U)\) to:

\[ W = Tr \ln G_0^{-1} - \frac{1}{2} nKn + Tr \ln (1 + G_0 U_{int}) + \Phi(U_0 + U_{int}) \]

(10.23)
10.2 First order approximation.

Let us first consider the case where the one-line irreducible diagrams $\Phi(U)$ are limited to the first order diagram $\Phi_1$:

\[
\Phi_1(U) = \text{\includegraphics[width=1cm]{first-order-diagram.png}}
\]  

(10.24)

We consider an expansion in powers of $e^2$, considering $G_0$, defined in (10.14), to be of zero order. This makes $\Phi_1$ proportional at least to $e^2$. Let $e^2 U_1$ be the first order approximation to $U_{int}$:

\[
U_{int}(x) = e^2 U_1(x)
\]  

(10.25)

Then, to first order, the equation (10.19) can be approximated by:

\[
\text{tr} \langle x | G_0 e^2 U_1 G_0 | x \rangle = \delta \Phi_1(U) \delta U(x)
\]  

(10.26)

We can use (C.6) to reduce this equation to:

\[
- \int d^4 x' \langle \vec{r} | D^{-1} | \vec{r}' \rangle e^2 U_1(\vec{r}') = \frac{\delta \Phi_1(U)}{\delta U_0(x)}
\]  

(10.27)

so that:

\[
e^2 U_1(\vec{r}) = - \int d^3 r' \langle \vec{r} | D^{-1} | \vec{r}' \rangle \frac{\delta \Phi_1(U)}{\delta U_0(x)}
\]  

(10.28)

The equation (10.21) then yields the potential $U_0(\vec{r})$ which generates the Kohn-Sham orbits:

\[
U_0(\vec{r}) = \int d^3 r' \frac{e^2}{4\pi |\vec{r} - \vec{r}'|} n(\vec{r}') + \int d^3 r' \langle \vec{r} | D^{-1} | \vec{r}' \rangle \frac{\delta \Phi_1(U)}{\delta U_0(x)}
\]  

(10.29)

The diagrams in (10.29) are time-independent Goldstone diagrams in which the upgoing lines are particle Kohn-Sham orbits and the downgoing line hole orbits. The double line is the inverse density-density correlation function (C.7). The
first term is the Hartree potential and the second term is the local potential which is generated by the Fock term.

To order $e^2$, the functional (10.23) reduces to:

$$ W_1(U) = Tr \ln G_0^{-1} - \frac{1}{2} nK + Tr G_0 e^2 U_1 + \Phi_1(U_0) \quad (10.30) $$

We can use (10.20) to get:

$$ W_1(U_0) = Tr \ln G_0^{-1} - \frac{1}{2} nK + Tr G_0 (-K n - U_0) + \Phi_1(U_0) \quad (10.31) $$

However:

$$ - Tr G_0 K n = n K \quad - Tr G_0 U_0 = n U_0 \quad (10.32) $$

so that:

$$ W_1(U_0) = Tr \ln G_0^{-1} + n U_0 + \frac{1}{2} n K + \Phi_1(U_0) \quad (10.33) $$

The first order potential (10.29) and functional (10.33) are identical to the first order potential $J_0(x)$ and to the functional $\Gamma_0 + \Gamma_1$ obtained using a Legendre transform as given, for example, by Valiev and Fernando [8].

### 10.3 Second order approximation.

Let consider the second order approximation. We limit the one-line irreducible diagrams to the first and second order diagrams:

$$ \Phi_1 + \Phi_2 = $$

$$ + \quad + \quad + $$

The first order diagram $\Phi_1$ is at least of order $e^2$ and the second order diagrams at least of order $e^4$. The second order approximation to $U_{int}$ can be written in the form:

$$ U_{int} = e^2 U_1 + e^4 U_2 \quad (10.35) $$

By substituting $G = G_0 - G_0 U_{int} G$ in the left hand side of equation (10.19) it becomes:

$$ tr \langle x | G_0 U_{int} G_0 | x \rangle = tr \langle x | G_0 U_{int} G_0 U_{int} G | x \rangle + \frac{\delta \Phi(U)}{\delta U(x)} \bigg|_{U = U_0 + U_{int}} \quad (10.36) $$
To order $e^2$, the equation (10.36) reads:

$$tr \langle x | G_0 e^2 U_1 G_0 | x \rangle = \frac{\delta \Phi_1 (U_0)}{\delta U_0 (x)}$$  \hspace{1cm} (10.37)$$

which is the result (10.26) obtained in first order theory, as expected.

Let us now expand the functional $W (U)$ up to second order. From (10.23), and to order $e^4$, we obtain:

$$W_2 (U) = Tr \ln G_0^{-1} - \frac{1}{2} nKn + Tr G_0 \left( e^2 U_1 + e^4 U_2 \right) - \frac{1}{2} Tr G_0 \left( e^2 U_1 \right) G_0 \left( e^2 U_1 \right) + \Phi_1 \left( U_0 + e^2 U_1 \right) + \Phi_2 \left( U_0 \right)$$  \hspace{1cm} (10.38)$$

For the third term on the right hand side, use (10.20) to write:

$$e^2 U_1 + e^4 U_2 = - \int d^4 x' \langle x | K | x' \rangle n (x')$$  \hspace{1cm} (10.39)$$

so that:

$$W_2 (U) = Tr \ln G_0^{-1} - \frac{1}{2} nKn - \frac{1}{2} Tr G_0 e^2 U_1 G_0 e^2 U_1 + \Phi_1 \left( U_0 + e^2 U_1 \right) + \Phi_2 \left( U_0 \right)$$  \hspace{1cm} (10.40)$$

We see that $W_2 (U)$ depends only on $U_1$. The third term of (10.38) is:

$$- \frac{1}{2} Tr G_0 e^2 U_1 G_0 e^2 U_1 = - \frac{1}{2} tr \int d^4 x \langle x | G_0 e^2 U_1 G_0 | x \rangle e^2 U_1 (x)$$  \hspace{1cm} (10.41)$$

We can use (10.37) to obtain:

$$- \frac{1}{2} Tr G_0 e^2 U_1 G_0 e^2 U_1 = - \frac{1}{2} \int d^4 x \frac{\delta \Phi_1 (U_0)}{\delta U_0 (x)} e^2 U_1 (x)$$  \hspace{1cm} (10.42)$$

The before last term is, to order $e^4$:

$$\Phi_1 \left( U_0 + e^2 U_1 \right) = \Phi_1 \left( U_0 \right) + \int d^4 x \frac{\delta \Phi_1 (U_0)}{\delta U_1 (x)} e^2 U_1 (x)$$  \hspace{1cm} (10.43)$$

Finally $W_2$ becomes:

$$W_2 = Tr \ln G_0^{-1} + \frac{1}{2} nKn + \Phi_1 \left( U_0 \right) + \Phi_2 \left( U_0 \right) + \frac{1}{2} \int d^4 x \frac{\delta \Phi_1 (U_0)}{\delta U_1 (x)} e^2 U_1 (x)$$  \hspace{1cm} (10.44)$$

Since $U_1$ is given by (10.28), the last term is:

$$\frac{1}{2} \int d^4 x \frac{\delta \Phi_1 (U_0)}{\delta U_1 (x)} e^2 U_1 (x)$$  \hspace{1cm} (10.45)$$

The functional $W_2$ is exactly the same as the second order functional obtained using a Legendre transform as given, for example, by Valiev and Fernando.[8]
Comparison to the use of optimal orbits and conclusion.

The potential (10.29) and the density functional (10.45) are expressed in terms of Kohn-Sham orbits (10.16) which are eigenstates of $h_0 + U_0$. Let us compare them to the potential and density functional which are obtained with the optimal orbits (6.1) which are eigenstates of $h_0 + U$. For a given set of one-line irreducible diagrams, the potential $U(x)$ is given by (5.7) as illustrated in (5.11). When the set of irreducible diagrams is limited to the first order diagram (10.24), the potential $U$ is given by:

\[
U(r) = \begin{array}{c}
\text{Feynman diagrams} \\
\text{Goldstone diagrams}
\end{array}
\]

(11.47)

and density $n$ is given by the diagrams illustrated in (5.9), namely:

\[
\begin{aligned}
n(r) &= \begin{array}{c}
\text{Feynman diagrams} \\
\text{Goldstone diagrams}
\end{array} \\
\end{aligned}
\]

(11.48)

The first lines of the diagrams (11.47) are Feynman diagrams whereas the second lines are the corresponding Goldstone diagrams.

The first order potential (11.47), expressed in terms of optimal orbits, is simpler than the first order potential (10.29) expressed in terms of Kohn-Sham orbits, because it does not involve the inverse density-density correlation function (C.6) represented by the double line. But the density (10.17) expressed in terms of Kohn-Sham orbits is simpler than the density (11.48) expressed in terms of the optimal orbits. However, when the potential is expressed in terms of optimal orbits, the density is related to the potential by the analytic expression (5.7), which, in the present case of fermions with Coulomb interactions, is
simply:

\[ n(\vec{r}) = -\frac{1}{e^2} \nabla^2 U(\vec{r}) \]  

(11.49)

Therefore no extra work is required to calculate the density \( n(\vec{r}) \) once the potential \( U(\vec{r}) \) has been calculated. Furthermore, the second order functional \[ (10.45), \] expressed in terms of Kohn-Sham orbits, has the extra contribution \[ (10.46) \] which does not occur in the second order functional expressed in terms of optimal orbits. When optimal orbits are used, the simple relation \[ (5.7) \] between the potential \( U \) and the density \( n \) avoids having to invert the equation \( n(x) = -\frac{\delta W}{\delta J(x)} \) in the Legendre transform method. Furthermore, any (finite or infinite) subset of one-line irreducible diagrams can be chosen. The use of Kohn-Sham orbits appears to be an unnecessary complication.

A. Diagram rules for fermions with Coulomb interactions.

We summarize the Feynman rules in order to fix the diagram notation. A more detailed derivation can be found in textbooks \cite{3,11}.

A.1 Expansion of the partition function in terms of Feynman diagrams.

We add a source term \( j \) for the boson field \( \omega_0 \) so that the euclidean action \[ (2.7) \] becomes:

\[
I_j(\omega_0) = -Tr \ln (\partial_\tau + h_0 - \mu + i\omega_0) \\
- \frac{1}{2} \int d^4x_1 d^4x_2 \omega_0(x_1) \langle x_1 | K^{-1} | x_2 \rangle \omega_0(x_2) - \int d^4x \ j(x) \omega_0(x) 
\]  

(A.1)

and we write the partition function \[ (2.6) \] in the form:

\[
e^W(j) = \int D(\omega_0) e^{-I_j(\omega_0)}
\]

We define an unperturbed partition function in obvious short hand notation:

\[
e^{W_0(j)} = e^{Tr \ln (\partial_\tau + h_0 - \mu)} \int D(\omega_0) \ e^{\frac{1}{2} \omega_0 K^{-1} \omega_0 + j\omega_0}
\]  

(A.2)

so that:

\[
W_0(j) = Tr \ln (\partial_\tau + h_0 - \mu) - \frac{1}{2} jKj = Tr \ln g^{-1} - \frac{1}{2} jKj
\]  

(A.3)

where \( g \) is the unperturbed fermion propagator:

\[
g = \frac{1}{\partial_\tau + h_0 - \mu}
\]  

(A.4)
It is the quantity:

\[ e^{-W_0(j)} e^{W(j)} = \frac{\int D(\omega_0) e^{\frac{1}{2} \omega_0 K^{-1} \omega_0 + j \omega_0} e^{Tr \ln(1 + gi \omega_0)}}{\int D(\omega_0) e^{\frac{1}{2} \omega_0 K^{-1} \omega_0 + j \omega_0}} \equiv \langle e^{Tr \ln(1 + gi \omega_0)} \rangle \quad (A.5) \]

which we expand in terms of Feynman diagrams. In the expression \( \langle \rangle \) signifies an integration over the boson field \( \omega_0 \) according to the expression above.

The expansion of \( Tr \ln (1 + gi \omega_0) \) reads:

\[ Tr \ln (1 + gi \omega_0) = Tr gi \omega_0 - \frac{1}{2} Tr g^2 i \omega_0 + ... \]

\[ = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n} \int d^4x_1...d^4x_n \ tr \langle x_1 | g | x_2 \rangle i\omega_0 \langle x_2 | g | x_3 \rangle i\omega_0 \langle x_3 | ... | x_n | g | x_1 \rangle i\omega_0 \langle x_1 \rangle \quad (A.6) \]

The traces \( Tr \) and \( tr \) are defined in (2.8) and (2.9). The term of order \( n \) gives rise to a closed loop formed by \( n \) fermion propagators \( \langle x | g | x' \rangle \) represented by oriented lines the end points of which are vertices:

An oriented line which reaches a point labelled \( x \) and which stems from a point labelled \( x' \) contributes to a diagram the factor:

\[ \langle x | g | x' \rangle = x \rightarrow x' \quad (A.8) \]

When the expansion (A.6) is inserted into the expression (A.5) and the exponential \( e^{Tr \ln(1 + gi \omega_0)} \) is expanded in turn, one is left with expectation values of products of boson fields:

\[ \langle i\omega_0 \langle x_1 \rangle i\omega_0 \langle x_2 \rangle i\omega_0 \langle x_3 \rangle ... \rangle = \frac{\int D(\omega_0) e^{\frac{1}{2} \omega_0 K^{-1} \omega_0 + j \omega_0} \langle i\omega_0 \langle x_1 \rangle i\omega_0 \langle x_2 \rangle i\omega_0 \langle x_3 \rangle ... \rangle}{\int D(\omega_0) e^{\frac{1}{2} \omega_0 K^{-1} \omega_0 + j \omega_0}} \]
The expectation value of a single field is:

\[
\langle i\omega_0(x) \rangle = i\frac{\delta W_0(j)}{\delta j(x)} = -i \int d^4x' \langle x|K|x'\rangle j(x')
\]

(A.9)

The expectation value (contraction) of a product of two fields is:

\[
\langle i\omega_0(x) i\omega_0(x') \rangle = \langle i\omega_0(x) \rangle \langle i\omega_0(x') \rangle + \langle i\omega_0(x) i\omega_0(x') \rangle_C
\]

(A.10)

and the connected part is the boson propagator:

\[
\langle i\omega_0(x) i\omega_0(x') \rangle_C = -\delta^2 W_0(j) \delta j(x) \delta j(x') \langle x|K|x'\rangle
\]

(A.11)

Note that the dashed interaction line yields a factor \(K\) which is equal to minus the instantaneous Coulomb potential, defined in (2.5). Expectation values of products of three or more fields can be expressed in terms (A.9) and (A.11), using Wick’s theorem.

Then \(e^{-W_0(j)} e^{W(j)}\) is equal to the sum of all distinct unlabeled diagrams formed by closed loops of oriented fermion lines and of dashed interaction lines. The contribution of a diagram is obtained by the following rules:

- Assign a label \(x = (\tau, \vec{r})\) to each vertex.
- Each oriented fermion line contributes a fermion propagator (A.8). The fermion propagators are written in the order in which they appear as one follows the closed loop. For each closed loop we take a trace \(tr\) of the product of the fermion propagators forming the closed loop.
- Each dashed interaction line joining two vertices contributes one of the factors (A.9) or (A.11), depending on whether it joins one or two vertices.
- A diagram containing \(n_v\) vertices and \(n_l\) closed loops is multiplied by the factor \((-1)^{n_v+n_l}\). (Note that in the absence of the source \(j\), the number of vertices is always even.)
- Integrate over the labels \(x = (\tau, \vec{r})\) of the vertices and divide by the symmetry factor, which is equal to the number of permutations of the labels which lead to an identical unlabeled diagram.

The contributions of disconnected diagrams factor and their symmetry factors are such that the sum of all diagrams is equal to the exponential of the
sum $\Gamma_c$ of connected diagrams. It follows that the partition function can be expressed in terms of connected diagrams $\Gamma_c$ as follows:

$$W (j) = W_0 (j) + \Gamma_c$$  \hspace{1cm} (A.12)

where $W_0 (j)$ is given by (A.3). In the absence of the sources $j$, the partition function is given by:

$$\ln \left( Tr e^{-\beta (H - \mu N)} \right) = W = Tr \ln g^{-1} + \Gamma_c$$  \hspace{1cm} (A.13)

where $g$ is the fermion propagator (A.4). An approximation to the partition can be defined by a choice of a subset of connected diagrams $\Gamma_c$.

**A.2 Diagram expansion of the particle density.**

Let us add a local source term $U (x)$ to $h_0$. From (2.3 and (2.4) we see that, upon a variation $U (x) \rightarrow U (x) + \delta U (x)$, we have $\delta \ln Z = \delta W = - \int d^4 x \, \langle \psi^\dagger (x) \delta U (x) \psi (x) \rangle$ so that the particle density is given by:

$$n (x) \equiv \langle \psi^\dagger (x) \psi (x) \rangle = - \frac{\delta W}{\delta U (x)} \bigg|_{U=0}$$  \hspace{1cm} (A.14)

When $h_0$ is time independent, as assumed in this work, the particle density is also time independent:

$$\langle \psi^\dagger (x) \psi (x) \rangle = \langle \psi^\dagger (\vec{r}) \psi (\vec{r}) \rangle \quad n (x) = n (\vec{r})$$  \hspace{1cm} (A.15)

However, for any time independent functional $F$, we have $\int d^4 x \, \delta U (x) \frac{\delta F}{\delta U (x)} = \beta \int d^3 r \, \delta U (\vec{r}) \frac{\delta F}{\delta U (\vec{r})}$. In order to avoid cumbersome $\beta$ factors, we shall always use functional derivatives $\frac{\delta}{\delta U (\vec{r})}$.

In the presence of the source, the fermion propagator (A.4) becomes:

$$g = \frac{1}{\partial_x + h_0 - \mu + U}$$  \hspace{1cm} (A.16)

From the expression (A.13) of the partition function, we see that the diagram expansion of the particle density (A.14) is given by:

$$n (x) \equiv \langle \psi^\dagger (x) \psi (x) \rangle = - \frac{\delta}{\delta U (x)} \left( Tr \ln g^{-1} + \Gamma_c \right) \bigg|_{U=0}$$  \hspace{1cm} (A.17)

In (A.16), $U$ is the following operator acting in the Hilbert space of a single fermion:

$$U = \int d^4 x \, |x\rangle U (x) \langle x|$$  \hspace{1cm} (A.18)

It follows that:

$$\frac{\delta}{\delta U (x)} (x_1 |g| x_2) = - \langle x_1 |g| x \rangle \langle x |g| x_2 \rangle$$
\[
\frac{\delta}{\delta U(x)} \ln g^{-1} = Tr \ g \ |x\rangle \langle x| = tr \ \langle x| g |x\rangle
\]  \hspace{0.5cm} \text{(A.19)}

The first term of (A.17) is the unperturbed particle density:

\[
n_0(x) = -tr \ \langle x| g |x\rangle = \sum_h \langle h| \bar{r} \rangle \langle \bar{r}| h \rangle
\]  \hspace{0.5cm} \text{(A.20)}

where we used (C.5). For the second term of (A.17) we note that the potential \( U \) occurs only in the propagators \( g \) of the diagrams \( \Gamma_c \) so that:

\[
\frac{\delta \Gamma_c}{\delta U(x)} = \int d^4 x_1 d^4 x_2 \frac{\delta \Gamma_c}{\delta \langle x_1| g |x_2\rangle} \frac{\delta \langle x_1| g |x_2\rangle}{\delta U(x)} = -\int d^4 x_1 d^4 x_2 \frac{\delta \Gamma_c}{\delta \langle x_1| g |x_2\rangle} \langle x_1| g |x\rangle \langle x| g |x_2\rangle
\]  \hspace{0.5cm} \text{(A.21)}

The second term is the sum of distinct diagrams obtained from the unlabeled connected diagrams \( \Gamma_c \) by inserting a slash, labelled \( x \), onto its oriented fermion lines. The particle density can therefore be expressed in terms of the connected diagrams thus:

\[
n(x) = -tr \ \langle x| g |x\rangle + \int d^4 x_1 d^4 x_2 \frac{\delta \Gamma_c}{\delta \langle x_1| g |x_2\rangle} \langle x_1| g |x\rangle \langle x| g |x_2\rangle
\]  \hspace{0.5cm} \text{(A.22)}

For example, if the only retained connected diagrams are:

\[
\Gamma_c = \hspace{0.5cm} \text{(A.23)}
\]

the particle density becomes:

\[
n(x) = x \hspace{0.5cm} \text{(A.24)}
\]

The diagrams (A.24) have a slash, labelled \( x \) which does not modify the sign of the diagram.
B Diagram rules for nucleons interacting with mesons.

B.1 Expansion of the partition function in terms of Feynman diagrams.

For a system of nucleons interacting with several mesons, we add to $h_0$ the following source terms for the boson fields:

$$jS = \int d^4x \left[ j_\sigma (x) \sigma (x) + j_\pi (x) \pi_a (x) + j_\mu (x) (\partial_\mu \pi_a)_x + j_\omega (x) \omega_\mu (x) \right]$$

The euclidean action (3.14) becomes:

$$I_j (S) \equiv - Tr \ln (\beta (\partial_\tau + h_0 - \mu + (\Gamma S) + S (\Theta S)) + \frac{1}{2} SK^{-1} S - jS$$

and we write the partition function (3.15) in the form:

$$e^W (j) = \int D (S) e^{- I_j (S)}$$ (B.3)

The unperturbed partition function is obtained by setting to zero the coupling constants so that $(\Gamma S) = S (\Theta S) = 0$. In obvious short hand notation:

$$e^{W_0 (j)} = e^{Tr \ln (\partial_\tau + h_0 - \mu)} \int D (S) e^{- \frac{1}{2} SK^{-1} S + jS} = e^{Tr \ln (\partial_\tau + h_0 - \mu) + \frac{1}{2} jKj}$$

so that:

$$W_0 (j) = Tr \ln (\partial_\tau + h_0 - \mu) + \frac{1}{2} jKj = Tr \ln g^{-1} + \frac{1}{2} jKj$$

where $g$ is the unperturbed fermion propagator:

$$g = \frac{1}{\partial_\tau + h_0 - \mu}$$

In more explicit form, the expression (B.5) reads:

$$W_0 (j) = Tr \ln g^{-1}$$

$$+ \frac{1}{2} J_\sigma \frac{1}{\partial^2 + m^2_\sigma} J_\sigma + \frac{1}{2} J_{\pi a} \frac{1}{\partial^2 + m^2_\pi} J_{\pi a} + \frac{1}{2} J_\omega \frac{1}{\partial^2 + m^2_\omega} \left( \delta_{\mu \nu} + \frac{1}{m^2} \partial_\mu \partial_\nu \right) j_{\omega \nu}$$

The traces $Tr$ and $tr$ are defined in equation (3.6).

It is the quantity:

$$e^{-W_0 (j)} e^W (j) = \frac{\int D (S) e^{Tr \ln (1 + g(\Gamma S) + gS(\Theta S))} e^{- \frac{1}{2} SK^{-1} S + jS}}{\int D (S) e^{- \frac{1}{2} SK^{-1} S + jS}} \equiv \langle e^{Tr \ln (1 + g(\Gamma S) + gS(\Theta S))} \rangle$$

(B.8)
which we express in terms of Feynman diagrams. In the expression \[\langle \rangle\] signifies an integration over the boson fields \(S\) according to the expression above.

The expansion of \(\text{Tr} \ln (1 + g (\Gamma S) + gS (\Phi S))\) in powers of \((\Gamma S) + S (\Phi S)\) reads:

\[
\text{Tr} \ln (1 + g (\Gamma S) + gS (\Phi S)) = \text{Tr} g [(\Gamma S) + S (\Phi S)] - \frac{1}{2} \text{Tr} g [(\Gamma S) + S (\Phi S)] g [(\Gamma S) + S (\Phi S)] + ... 
\]

\[
= \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n} \int d^4x_1 d^4x_2 ... d^4x_n \text{tr} \{\langle x_1 | g | x_2 \rangle [(\Gamma S_{x_2}) + S_{x_2} (\Phi S_{x_2})] \langle x_2 | g | x_3 \rangle [(\Gamma S_{x_3}) + S_{x_3} (\Phi S_{x_3})] ... \langle x_n | g | x_1 \rangle [(\Gamma S_{x_1}) + S_{x_1} (\Phi S_{x_1})] \} \quad (B.9)
\]

The term of order \(n\) is a trace \(\text{tr}\) of a product of terms the explicit form of which is:

\[
\langle x_1 | g | x_2 \rangle [(\Gamma S_{x_2}) + S_{x_2} (\Phi S_{x_2})] = \langle x_1 \left| \frac{1}{\partial_\tau + h_0 - \mu} \right| x_2 \rangle \left[ \Gamma^{(\sigma)} \sigma (x_2) + \Gamma^{(\omega)} \omega_\mu (x_2) + \Gamma^{(\pi)} a_{(\mu b)} (\partial_\mu \pi_b) x_2 + \pi_a (x_2) \Phi^{(\pi)} a_{(\mu b)} (\partial_\mu \pi_b) x_2 \right] \quad (B.10)
\]

The product can be represented by a diagram of the form: 

\[\text{Diagram}\]
in which the oriented (fermion propagator) lines form a closed loop. Each oriented fermion propagator contributes one of the following factors:

\[
\begin{align*}
\Gamma^{(\sigma)} &= \langle x_1 | g | x_2 \rangle g_{\sigma \beta} \\
\Gamma^{(\omega)} &= \langle x_1 | g | x_2 \rangle g_{\omega \beta} \gamma_{\mu} \\
\Gamma^{(\pi)} &= \langle x_1 | g | x_2 \rangle \frac{g A}{2 f_{\pi}} \beta_{\gamma_5} \gamma_{\mu} \\
\Phi_{\alpha(\mu b)} &= \langle x_1 | g | x_2 \rangle \frac{1}{4 f_{\pi}^2} \varepsilon_{abc} \beta_{\gamma_5} \gamma_{\mu}
\end{align*}
\]

Note that the order of the non-commuting operators \( g \) and \( (\Gamma S) \) or \( S(\Phi S) \) is determined by the direction of the arrow on the fermion propagator. The point at which a meson (dashed) line joins a fermion (oriented) line is called a vertex. The proper labelling of the vertices is important. Note also that the black dot denotes the absence of a derivative of the pion field.

When the expansion (B.9) is inserted into the expression (B.8) and the exponential \( e^{Tr\ln(1+g(\Gamma S)+gS(\Phi S))} \) is expanded in turn, we are left with expectation
values of products of boson fields which can be evaluated using Wick’s theorem. The expectation values of single fields are:

\[ \langle S_i(x) \rangle = \int d^4y \langle x | K_{ij} | y \rangle j_j(y) = \langle x | K_{ij} | j_j \rangle \]  

(B.13)

In more explicit form:

\[ \langle \sigma(x) \rangle = \frac{\partial W_0}{\partial \sigma(x)} = \int d^4y \langle x | \frac{1}{(-\partial^2 + m_\sigma^2)} | y \rangle j_\sigma(y) = \langle x | K^{(\sigma)} | j_\sigma \rangle \]

\[ \langle \pi_a(x) \rangle = \frac{\partial W_0}{\partial \pi_a(x)} = \int d^4y \langle x | \frac{1}{(-\partial^2 + m_\pi^2)} | y \rangle j_{\pi a}(y) = \langle x | K^{(\pi)} | j_{\pi a} \rangle \]

\[ \langle \partial_\mu \pi_a(x) \rangle = \int d^4y \langle x | \partial_\mu \frac{1}{(-\partial^2 + m_\pi^2)} | y \rangle j_{\pi a}(y) = \langle x | \partial_\mu K^{(\pi)} | j_{\pi a} \rangle \]

\[ \langle \omega_{\mu \nu}(x) \rangle = \frac{\partial W_0}{\partial j_{\omega \mu \nu}} = \int d^4y \langle x | \frac{1}{(-\partial^2 + m_\pi^2)} \left( \delta_{\mu \nu} - \frac{1}{m_\omega} \partial_\mu \partial_\nu \right) | y \rangle j_{\omega \mu}(y) = \langle x | K^{(\omega)} | j_{\omega \mu} \rangle \]

The expectation values of products of two fields are:

\[ \langle S_a(x) S_b(y) \rangle = e^{-W_0(x)} \frac{\delta^2}{\delta j_a(x) \delta j_b(y)} e^{W_0(y)} = \langle S_i(x) \rangle \langle S_j(y) \rangle + \langle S_i(x) S_j(y) \rangle_c \]  

(B.15)

where the connected part is the boson propagator:

\[ \langle S_a(x) S_b(y) \rangle_c = \frac{\delta^2 W_0(j)}{\delta j_a(x) \delta j_b(y)} = \langle x | K_{ab} | y \rangle \]  

(B.16)

where \( K_{ab} \) is the meson propagator \( (3.12) \). We can use \( (B.7) \) to deduce the following explicit forms of the boson propagators:

\[ \langle \sigma(x) \sigma(y) \rangle_c = \frac{1}{(-\partial^2 + m_\sigma^2)} \langle x | y \rangle = \langle x | K^{(\sigma)} | y \rangle \]
\begin{align*}
\langle \omega_\mu (x) \omega_\nu (y) \rangle_c &= \left( \frac{1}{-\partial^2 + m^2_\omega} \right) \left( \delta_{\mu\nu} - \frac{1}{m^2_\omega} \partial_\mu \partial_\nu \right) y = \left. x \right| K_\mu^{(\omega)} \left. y \right| \\
&= x_{\mu} - \omega_{\nu}
\end{align*}

and:
\begin{align*}
\langle \pi_a (x) \pi_b (y) \rangle_c &= \delta_{ab} \left( \frac{1}{-\partial^2 + m^2_\pi} \right) y = \delta_{ab} \left. x \right| K^{(\pi)} \left. y \right| \\
&= x_{\int a} - \pi_{b} - y
\end{align*}

\begin{align*}
\langle (\partial_\mu \pi_a (x)) \pi_b (y) \rangle_c &= \delta_{ab} \left( \frac{1}{-\partial^2 + m^2_\pi} \partial_\nu \right) y = \delta_{ab} \left. x \right| \partial_\mu K^{(\pi)} \left. y \right| \\
&= x_{\int a} - \pi_{b} - y
\end{align*}

\begin{align*}
\langle (\partial_\mu \pi_a (x)) (\partial_\nu \pi_b (y)) \rangle_c &= -\delta_{ab} \left( \frac{1}{-\partial^2 + m^2_\pi} \partial_\nu \right) y = -\delta_{ab} \left. x \right| \partial_\mu K^{(\pi)} \partial_\nu \left. y \right| \\
&= x_{\int a} - \pi_{b} - y
\end{align*}

Expectation values of products of three or more fields can be expressed in terms of (B.14) and (B.17), using Wick’s theorem.

Then \( e^{-W_0(j)} e^{W(j)} \) is equal to the sum of all distinct unlabeled diagrams formed by closed loops of oriented fermion propagators joined to dashed boson propagator lines at points called vertices. The contribution of a diagram is obtained by the following rules:

- Assign a label \( \sigma, \omega \) or \( \pi \) to each dashed boson line. Then assign distinct
labels to the vertices. An example of a labeled diagram is:

![Diagram](image)

(B.18)

- Each oriented fermion line, which reaches a point labeled $x_1$ and which stems from a point labeled $x_2$, to which a meson dashed line (or two meson lines) is attached, contributes one of the factors (B.12).

- Each meson dashed line contributes one of the factors (B.17) or (B.14), depending on whether it joins one or two vertices. For example, the two pion lines in the labeled diagram (B.18), joining the vertices bearing the labels $x_2, x_8$ and $x_5$, contribute the following factor (remember that the black dot indicates the absence of a derivative of the pion field):

$$(-) \delta_{a_2, b_8} \left( x_2 \left| \frac{1}{-\partial^2 + m_\pi^2} \right. \partial_{\mu_8} \left| x_8 \right. \right) (-) \delta_{a_5, b_2} \left( x_2 \left| \partial_{\mu_2} \frac{1}{-\partial^2 + m_\pi^2} \partial_{\mu_5} \right. \left| x_5 \right. \right)$$

(B.19)

- The factors are written in the order in which they appear as one follows each closed fermion loop and for each loop we take a trace $tr$ of the product of fermion propagators forming the loop.

- A diagram containing $n_v$ vertices and $n_l$ closed loops is multiplied by the factor $(-)^{n_v + n_l}$. (Note that in the absence of the source terms $j_a$, the number of vertices is always even.)

- Integrate over the space-time labels $x = (\tau, \vec{r})$ of the vertices and divide by the symmetry factor, which is equal to the number of permutations of the labels which lead to an identical unlabeled diagram.
The contributions of disconnected diagrams factor and their symmetry factors are such that the sum of all diagrams is equal to the exponential of the sum $\Gamma_c$ of connected diagrams. It follows that the partition function can be expressed in terms of connected diagrams $\Gamma_c$ as follows:

$$W(j) = W_0(j) + \Gamma_c$$  \hspace{1cm} (B.20)

where $W_0(j)$ is given by (B.7). In the absence of the sources $j$, the partition function is given by:

$$\ln \left( Tr e^{-\beta(H-\mu N)} \right) = W = Tr \ln g^{-1} + \Gamma_c$$  \hspace{1cm} (B.21)

where $g$ is the fermion propagator (B.6). An approximation to the partition can be defined by a choice of a subset of connected diagrams.

### B.2 Diagram expansion of the particle densities.

Let us add the following local source terms to $h_0$:

$$\Gamma_a U_a(x) \equiv \Gamma^{(\sigma)} U_{\sigma}(x) + \Gamma^{(\mu)} U_{\mu}(x) + \Gamma_{\mu a} U_{\mu a}(x) + \Phi_{a(\mu b)} U_{a(\mu b)}(x)$$  \hspace{1cm} (B.22)

From (3.15) we see that upon a variation $U_a(x) \rightarrow U_a(x) + \delta U_a(x)$, we have:

$$\delta \ln Z = \delta W = - \int d^4x \left\langle N^\dagger(x) \Gamma_a \delta U_a(x) N(x) \right\rangle$$  \hspace{1cm} (B.23)

so that:

$$\rho_a(x) \equiv \left\langle N^\dagger(x) \Gamma_a N(x) \right\rangle = - \frac{\delta W}{\delta U_a(x)}$$  \hspace{1cm} (B.24)

The operators $\Gamma_a$ are defined in (3.8). They include the coupling constants. Therefore the particle densities $n(x)$, in the usual sense of the word, are related to the densities $\rho(x)$ as follows:

$$n_{\sigma}(x) \equiv \left\langle \bar{N}(x) N(x) \right\rangle = \frac{1}{g_\sigma} \rho_{\sigma}(x)$$

$$n(x) = \left\langle N^\dagger(x) N(x) \right\rangle = \frac{1}{ig_\omega} \rho_{\mu=0}(x)$$

$$n_i(x) = \left\langle N^\dagger(x) \alpha_i N(x) \right\rangle = \frac{1}{g_\omega} \rho_{\mu=i}(x)$$

$$n_{\mu a}(x) = \left\langle N^\dagger(x) \beta_{\tau a} \gamma_\tau \gamma_\mu N(x) \right\rangle = \frac{2f_\pi}{g_A} \rho_{\mu a}(x)$$

$$n_{a(\mu b)}(x) = \left\langle \bar{N}(x) \varepsilon_{abc} \gamma_\tau \gamma_\mu N(x) \right\rangle = 4f_\pi^2 \rho_{a(\mu b)}(x)$$  \hspace{1cm} (B.25)

(In the case of fermions with Coulomb interactions, only one density occurs with $\Gamma_a = 1$ so that $n(x) = \rho(x)$.)
In the presence of the source term, the fermion propagator (B.6) becomes:

\[
g = \frac{1}{\partial_x + h_0 - \mu + \Gamma_a U_a}
\]

(B.26)

From the expression (B.21) of the partition function, we see that the particle densities (B.24) can be expressed in terms of connected diagrams as follows:

\[
\rho_a(x) \equiv \langle N^+ (x) \Gamma_a N(x) \rangle = -\frac{\delta}{\delta U_a (x)} (Tr \ln g^{-1} + \Gamma_c) \bigg|_{U=0}
\]

(B.27)

In (B.26), \( \Gamma_a U_a \) is the following operator acting in the Hilbert space of a single fermion:

\[
\Gamma_a U_a = \int d^4x \mid x \rangle \Gamma_a U_a \langle x \mid
\]

(B.28)

It follows that:

\[
\frac{\delta}{\delta U_a (x)} \langle x_1 | g | x_2 \rangle = -\langle x_1 | g | x \rangle \Gamma_a \langle x | g | x_2 \rangle
\]

\[
\frac{\delta}{\delta U_a (x)} Tr \ln g^{-1} = Tr g \langle x \rangle \Gamma_a \langle x \rangle = tr \langle x | g | x \rangle \Gamma_a
\]

(B.29)

The first term of (B.27) is the unperturbed particle density:

\[
\rho_a^{(0)} (x) = -tr \langle x | g | x \rangle \Gamma_a
\]

(B.30)

We can use (C.5) to get:

\[
\rho_a^{(0)} (x) = \sum_h \langle h | \bar{r} \rangle \Gamma_a \langle \bar{r} | h \rangle = \rho^{(0)} (\bar{r})
\]

(B.31)

For the second term of (B.27) we note that the potential \( U_a \) occurs only in the propagators \( g \) of the connected diagrams \( \Gamma_c \) so that:

\[
\frac{\delta \Gamma_c}{\delta U_a (x)} = \int d^4x_1 d^4x_2 \frac{\delta \Gamma_c}{\delta \langle x_1 | g | x_2 \rangle} \frac{\delta \langle x_1 | g | x_2 \rangle}{\delta U_a (x)} = -\int d^4x_1 d^4x_2 \frac{\delta \Gamma_c}{\delta \langle x_1 | g | x_2 \rangle} \langle x_1 | g | x \rangle \Gamma_a \langle x | g | x_2 \rangle
\]

(B.32)

The particle density can therefore be expressed in terms of the connected diagrams thus:

\[
\rho_a (x) = -tr \langle x | g | x \rangle \Gamma_a + \int d^4x_1 d^4x_2 \frac{\delta \Gamma_c}{\delta \langle x_1 | g | x_2 \rangle} \langle x_1 | g | x \rangle \Gamma_a \langle x | g | x_2 \rangle
\]

(B.33)

The second term is the sum of distinct diagrams obtained from the unlabeled connected diagrams \( \Gamma_c \) by inserting a slash onto its oriented fermion lines, exactly as in (A.24), except that the slash now bears the label \((x,a)\). An oriented
fermion line, stemming from a vertex labelled \( x_2 \), reaching a vertex labelled \( x_1 \), and bearing a slash labelled \((x, a)\) contributes a factor equal to:

\[
(x, a) = \langle x_1 | g | x \rangle \Gamma_a \langle x | g | x_2 \rangle
\]

(B.34)

The slash does not modify the sign of the diagram.

C  Particle and hole orbits and density-density correlation functions.

When \( h_0 \) is time-independent, the unperturbed fermion propagator \( g^{-1} = (\partial_\tau + h_0 - \mu) \) is diagonal in the \( |\omega \lambda\rangle \) representation, where the states \( |\lambda\rangle \) are eigenstates of \( h_0 \):

\[
h_0 |\lambda\rangle = e_\lambda |\lambda\rangle
\]

(C.1)

and where \( |\omega\rangle \) are the (euclidean) time plane wave states:

\[
\langle \tau | \omega \rangle = \frac{1}{\sqrt{\beta}} e^{i\omega \tau} \quad \partial_\tau |\omega\rangle = i\omega |\omega\rangle
\]

(C.2)

so that:

\[
g^{-1} |\omega \lambda\rangle = (\partial_\tau + h_0 - \mu) |\omega \lambda\rangle = (i\omega + e_\lambda - \mu) |\omega \lambda\rangle
\]

(C.3)

In the zero temperature limit \( \beta \to \infty \), the matrix elements of \( g \) are equal to:

\[
\langle x_1 | g | x_2 \rangle \equiv \langle \tau_1 \vec{r}_1 | g | \tau_2 \vec{r}_2 \rangle = \sum_{\omega \lambda} \langle \tau_1 \vec{r}_1 | \omega \lambda \rangle \left( \frac{1}{i\omega + e_\lambda - \mu} \langle \omega \lambda | \tau_2 \vec{r}_2 \rangle \right)
\]

\[
= \theta (\tau_1 - \tau_2) \sum_p e^{-\left(e_p - \mu\right)(\tau_1 - \tau_2)} \langle \vec{r}_1 | p \rangle \langle p | \vec{r}_2 \rangle - \theta (\tau_2 - \tau_1) \sum_h e^{-\left(e_h - \mu\right)(\tau_1 - \tau_2)} \langle \vec{r}_1 | h \rangle \langle h | \vec{r}_2 \rangle
\]

(C.4)

where the "particle" and "hole" orbits \(|p\rangle\) and \(|h\rangle\) are the eigenstates \(|\lambda\rangle\) belonging to energies respectively \(e_p > \mu\) and \(e_h < \mu\). The equal time propagator is:

\[
\langle \tau \vec{r}_1 | g | \tau \vec{r}_2 \rangle = -\sum_h \langle \vec{r}_1 | h \rangle \langle h | \vec{r}_2 \rangle
\]

(C.5)

We shall encounter the so-called density-density correlation function:

\[
\langle \vec{r}_1 | D | \vec{r}_2 \rangle \equiv -\text{tr} \int d\tau \langle \tau_1 \vec{r}_1 | g | \tau \vec{r} \rangle \langle \tau \vec{r} | g | \tau_1 \vec{r}_2 \rangle = -\text{tr} \int d\tau_1 \langle \tau_1 \vec{r}_1 | g | \tau \vec{r} \rangle \langle \tau \vec{r} | g | \tau_1 \vec{r}_2 \rangle
\]

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\[
\sum_{ph} \frac{1}{e_p - e_h} \left( \langle p | \vec{r}_2 \rangle \langle \vec{r}_2 | h \rangle \langle h | \vec{r}_1 \rangle \langle \vec{r}_1 | p \rangle + \langle h | \vec{r}_2 \rangle \langle \vec{r}_2 | p \rangle \langle p | \vec{r}_1 \rangle \langle \vec{r}_1 | h \rangle \right)
\]

The diagram (C.6) is a time-independent Goldstone diagram in which upgoing propagators are particle orbits and downgoing propagators hole orbits. The inverse correlation function will be represented in diagrams by a double line:

\[
\langle \vec{r}_1 D^{-1} | \vec{r}_2 \rangle
\]

(C.7)

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