Summary of Chapter: Functionals in Many–Particle Physics

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1 Introduction

The chapter develops a functional formulation for interacting many–particle systems. Instead of working directly with the many–body wavefunction, one describes physical quantities as functionals of a key observable (or set of observables). Examples include:

- The electron density $n(\mathbf{r})$ in Density Functional Theory (DFT).
- The one–particle Green's function G and the associated self–energy Σ.
- The screened Coulomb interaction W and its related functional.

This approach underpins many practical methods (such as the GW approximation, Dynamical Mean–Field Theory (DMFT), and conserving approximations) and provides a variational basis that automatically incorporates conservation laws.

2 Functionals of G in the Density Functional Theory and the Hartree–Fock Approximations

This section reformulates Density Functional Theory (DFT) in a way that connects the density-based approach with a Green's function formulation. It introduces the Kohn–Sham auxiliary system and the finite-temperature Mermin generalization. A key idea is to express the grand potential not only as a functional of the electron density $n(\mathbf{r})$ but also in terms of the one–particle Green's function G_{KS}. This approach clarifies the variational basis of DFT and provides a foundation for systematic many-body approximations.

2.1 Variational Principle and Density Functionals

The starting point is the variational principle. In its general form, the total energy is written as

$$E[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle,$$

and if the trial wavefunction is sufficiently flexible, the condition

$$\frac{\delta E[\Psi]}{\delta \Psi} = 0$$

leads to the many–body Schrödinger equation. In DFT, one recasts the energy as a functional of the electron density:

$$E[n] \quad \text{with} \quad \frac{\delta E[n]}{\delta n(\mathbf{r})} = 0,$$

so that the ground-state energy is $E_0 = E[n_0]$ for the true density $n_0(\mathbf{r})$.

2.2 The Kohn–Sham Auxiliary System and Green's Function Formulation

To make the variational problem tractable, Kohn and Sham introduced an auxiliary system of non-interacting particles that reproduces the interacting density. In the Green's function formulation, this is expressed via the Kohn–Sham Green's function G_{KS}, which satisfies a Dyson-like equation:

$$G_{\mathrm{KS}} = G_0 + G_0\, v_{\mathrm{Hxc}}\, G_{\mathrm{KS}}, \tag{1}$$

or, equivalently,

$$G_{\mathrm{KS}}^{-1} = G_0^{-1} - v_{\mathrm{Hxc}}, \tag{2}$$

where:

- G_0 is the Green's function of a non-interacting reference system.
- $v_{\mathrm{Hxc}}(r) = v_{\mathrm{H}}(r) + v_{\mathrm{xc}}(r)$ is the effective potential combining the classical Hartree potential v_{H} with the exchange–correlation potential v_{xc}.

The electron density is recovered from G_{KS} via

$$n(x) = -i\, G_{\mathrm{KS}}(x, t; x, t^{+}).$$

2.3 The Mermin Functional and the Grand Potential

At finite temperature, the Mermin functional extends DFT by defining the grand potential as

$$\Omega = E - TS - \mu N.$$

Within the Kohn–Sham framework, the grand potential is written as

$$\Omega_M^{\mathrm{KS}} = \Omega_{xc}[n] + E_H[n] - \int dr\, v_{\mathrm{Hxc}}(r) n(r) + \Omega_{ip}[v_{\mathrm{eff}}], \tag{3}$$

with the effective potential defined by

$$v_{\mathrm{eff}}(r) = v_{\mathrm{ext}}(r) + v_{\mathrm{H}}(r) + v_{\mathrm{xc}}(r). \tag{4}$$

Here:

- $E_H[n]$ is the Hartree energy, given by

  $$E_H[n] = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}'\, \frac{n(\mathbf{r})\, n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$

  representing the classical Coulomb repulsion between electrons.
- $\Omega_{xc}[n]$ is the exchange–correlation grand potential functional that incorporates many-body quantum effects (exchange and correlation) beyond the classical Hartree term.

3 Avoiding Double Counting in the Kohn–Sham Grand Potential

In the Kohn–Sham formulation, the finite-temperature grand potential is given by

$$\Omega_M^{\text{KS}} = \Omega_{xc}[n] + E_H[n] - \int dr\, v_{Hxc}(r)\, n(r) + \Omega_{ip}[v_{eff}],$$

where:

- $E_H[n]$ is the Hartree energy,

$$E_H[n] = \frac{1}{2} \int dr \int dr' \, \frac{n(r)\, n(r')}{|r - r'|},$$

- $v_{Hxc}(r) = v_H(r) + v_{xc}(r)$ is the effective potential due to electron–electron interactions,
- $v_{eff}(r) = v_{ext}(r) + v_{Hxc}(r)$ is the total effective potential experienced by the electrons, and
- $\Omega_{ip}[v_{eff}]$ is the grand potential of independent (non-interacting) particles in the potential $v_{eff}(r)$.

At first glance, it may seem that the Hartree term appears twice:

- Directly in $E_H[n]$, which represents the classical Coulomb repulsion between electrons.
- Implicitly within $v_{Hxc}(r)$ and thus in the effective potential $v_{eff}(r)$ used in $\Omega_{ip}[v_{eff}]$.

How double counting is avoided:

1. **Independent-Particle Contribution:** The term $\Omega_{ip}[v_{eff}]$ is computed for non-interacting electrons moving in the effective potential $v_{eff}(r) = v_{ext}(r) + v_{Hxc}(r)$. In this calculation, the energy contribution from the Hartree potential $v_H(r)$ is already included.
2. **Subtraction Term:** To compensate for this, the term

$$-\int dr\, v_{Hxc}(r)\, n(r)$$

   is subtracted. This subtraction removes the part of the electron–electron interaction that would otherwise be counted twice.
3. **Addition of the Explicit Hartree Energy:** Finally, the Hartree energy $E_H[n]$ is added separately. This ensures that the classical Coulomb repulsion is properly accounted for without overcounting.

Thus, the combination of the independent-particle term $\Omega_{ip}[v_{eff}]$ and the subtraction $-\int dr\, v_{Hxc}(r) n(r)$ acts as a *double counting correction.* The net effect is that each contribution (the Hartree energy, exchange–correlation energy, and kinetic energy) is counted only once.

3.1 Connection Between Density and Green's Function Formulations

In order to exploit the analogy between the density $n(\mathbf{r})$ and the Green's function G, we can re-express terms in the Mermin functional in terms of the Kohn–Sham Green's function G_{KS}.

For example, the term

$$\int dr\, v_{\text{Hxc}}(r)n(r)$$

can be rewritten as a trace over the Green's function:

$$\int dr\, v_{\text{Hxc}}(r)n(r) = \text{Tr}(v_{\text{Hxc}}\, G_{\text{KS}}). \tag{5}$$

This equivalence (Equation (8.5)) provides a bridge between the density-based description and the Green's function formalism.

Furthermore, by using the Dyson equation (2), one can express the interacting grand potential in a compact form. The full expression (Equation (8.6)) is written as:

$$\Omega_M^{\text{KS}} = \Omega_{xc}[n] + E_H[n] - \text{Tr}(v_{\text{Hxc}}\, G_{\text{KS}}) - \text{Tr}\ln\Big(1 - G_0\, v_{\text{Hxc}}\Big) + \Omega_0, \tag{6}$$

where:

- $\text{Tr}(v_{\text{Hxc}}\, G_{\text{KS}})$ represents the linear coupling of the effective potential with the Green's function.
- $\text{Tr}\ln\Big(1 - G_0\, v_{\text{Hxc}}\Big)$ arises from rewriting the determinant of the interacting propagator. Specifically, since

  $$G_{\text{KS}}^{-1} = G_0^{-1} - v_{\text{Hxc}},$$

  one can write

  $$-G_{\text{KS}}^{-1} = -G_0^{-1}\Big[1 - G_0\, v_{\text{Hxc}}\Big].$$

  Taking the logarithm and using $\ln(AB) = \ln A + \ln B$ yields the logarithmic term. Its expansion as

  $$\text{Tr}\ln\Big(1 - G_0\, v_{\text{Hxc}}\Big) = -\sum_{n=1}^{\infty} \frac{1}{n}\,\text{Tr}\Big[(G_0\, v_{\text{Hxc}})^n\Big]$$

  shows that it sums an infinite series of corrections due to repeated insertions of v_{Hxc} into the free propagator.

3.2 Summary of Section 8.1

1. Variational Principle: The total energy $E[\Psi]$ is expressed as a functional of the many-body wavefunction and recast in terms of the electron density $n(\mathbf{r})$ via DFT:

$$E[n] \quad \text{with} \quad \frac{\delta E[n]}{\delta n(\mathbf{r})} = 0.$$

2. Kohn–Sham Auxiliary System: An auxiliary non-interacting system is introduced such that its density matches that of the interacting system. In the Green's function formulation, the Kohn–Sham Green's function G_{KS} satisfies:

$$G_{\text{KS}} = G_0 + G_0\, v_{\text{Hxc}}\, G_{\text{KS}},$$

or

$$G_{\mathrm{KS}}^{-1} = G_0^{-1} - v_{\mathrm{Hxc}},$$

where $v_{\mathrm{Hxc}}(r) = v_{\mathrm{H}}(r) + v_{\mathrm{xc}}(r)$.

3. Mermin Functional and the Grand Potential: At finite temperature, the grand potential is expressed as

$$\Omega_M^{\mathrm{KS}} = \Omega_{xc}[n] + E_H[n] - \int dr\, v_{\mathrm{Hxc}}(r) n(r) + \Omega_{ip}[v_{\mathrm{eff}}],$$

with $v_{\mathrm{eff}}(r) = v_{\mathrm{ext}}(r) + v_{\mathrm{H}}(r) + v_{\mathrm{xc}}(r)$. Here, $E_H[n]$ is the classical Hartree energy, and $\Omega_{xc}[n]$ is the exchange–correlation grand potential functional.

4. Connecting Density and Green's Function Formulations: The density integral can be recast as

$$\int dr\, v_{\mathrm{Hxc}}(r) n(r) = \mathrm{Tr}(v_{\mathrm{Hxc}}\, G_{\mathrm{KS}}).$$

Using the Dyson equation, one derives the full expression:

$$\Omega_M^{\mathrm{KS}} = \Omega_{xc}[n] + E_H[n] - \mathrm{Tr}(v_{\mathrm{Hxc}}\, G_{\mathrm{KS}}) - \mathrm{Tr}\ln\Big(1 - G_0\, v_{\mathrm{Hxc}}\Big) + \Omega_0.$$

The logarithmic term, $\mathrm{Tr}\ln(1 - G_0 v_{\mathrm{Hxc}})$, sums an infinite series of higher-order corrections due to repeated interactions with the effective potential, ensuring that all many-body effects are properly incorporated.

Equations (8.5) and (8.6) (or their equivalent forms above) build a bridge between the density-based DFT and the Green's function many-body formalism. They establish:

- How the classical Hartree energy $E_H[n]$ and the exchange–correlation functional $\Omega_{xc}[n]$ contribute to the grand potential.
- The role of the effective potential v_{Hxc} and its coupling to the Green's function via $\mathrm{Tr}(v_{\mathrm{Hxc}}\, G_{\mathrm{KS}})$.
- The necessity of the logarithmic term, $\mathrm{Tr}\ln(1 - G_0 v_{\mathrm{Hxc}})$, to account for an infinite series of interaction corrections.

Section 8.1 lays the foundation for the subsequent development of Green's function functionals. By expressing the Kohn–Sham DFT in terms of G_{KS} and incorporating the Mermin extension, we establish a variational formulation that connects density-based and Green's function approaches. Equations (8.5) and (8.6) are central to this formulation, as they:

1. Convert spatial integrals over the density and effective potential into trace operations involving G_{KS}.
2. Introduce the $\mathrm{Tr}\ln(1 - G_0 v_{\mathrm{Hxc}})$ term, which compactly sums an infinite series of many-body corrections.

This framework not only clarifies the internal consistency of DFT but also provides a natural path to advanced methods such as GW and DMFT.

4 Functionals of the Green's Function G and Self–Energy Σ

Section 8.2 develops a variational formulation of many–body theory in which the grand potential is expressed as a functional of the interacting one–particle Green's function G and its associated self–energy Σ. The goal is to provide a framework that unifies density-functional methods with many-body perturbation theory.

4.1 The Luttinger–Ward Functional

A central object in this formulation is the **Luttinger–Ward functional**, denoted $\Phi[G]$. It is defined as the sum over all *skeleton diagrams* constructed with the full interacting Green's function G. Although the explicit diagrammatic series is not given here, the key properties are:

- $\Phi[G]$ is a universal functional, independent of the external potential.
- It contains all the many-body interaction effects in the system.

A crucial relation is that the self–energy Σ is obtained as the functional derivative of $\Phi[G]$ with respect to G:

$$\Sigma = \frac{\delta\Phi[G]}{\delta G}. \tag{7}$$

This relation is a key element in the variational formulation and ensures that, when the grand potential is minimized, the Dyson equation is recovered.

4.2 Expression for the Grand Potential

The grand potential Ω of the interacting system can be expressed as:

$$\Omega = \Phi[G] - \mathrm{Tr}(\Sigma\, G) - \mathrm{Tr}\ln\Big(1 - G_0\,\Sigma\Big) + \Omega_0, \tag{8}$$

where:

- G_0 is the non-interacting Green's function.
- Ω_0 is the grand potential of the non-interacting system.
- The term $\mathrm{Tr}(\Sigma\, G)$ represents the first-order (linear) contribution from the interaction.
- The logarithmic term, $\mathrm{Tr}\ln(1-G_0\,\Sigma)$, arises from rewriting the determinant of the interacting inverse Green's function. Specifically, using the Dyson equation

  $$G^{-1} = G_0^{-1} - \Sigma,$$

  one can factorize the operator as:

  $$-G^{-1} = -G_0^{-1}\Big[1 - G_0\,\Sigma\Big].$$

  Taking the logarithm and using the property $\ln(AB) = \ln A + \ln B$ yields the Tr ln term. This term, when expanded as a series,

  $$\mathrm{Tr}\ln\Big(1 - G_0\,\Sigma\Big) = -\sum_{n=1}^{\infty}\frac{1}{n}\,\mathrm{Tr}\Big[(G_0\,\Sigma)^n\Big],$$

  sums an infinite series of higher-order corrections due to repeated insertions of the interaction.

4.3 Physical Interpretation and Variational Principle

This formulation has several important features:

1. **Unified Description:** The grand potential is expressed solely in terms of the one–particle Green's function G and the self–energy Σ. This bridges density functional approaches and many-body perturbation theory.
2. **Variational Character:** The physical Green's function is determined by the condition that Ω is stationary with respect to variations in G. The relation
$$\Sigma = \frac{\delta\Phi[G]}{\delta G}$$
ensures that the Dyson equation
$$G^{-1} = G_0^{-1} - \Sigma$$
is satisfied at the stationary point.
3. **Role of the Logarithmic Term:** The $\mathrm{Tr}\ln(1 - G_0\,\Sigma)$ term sums over all higher-order corrections. It captures the many-body effects beyond the linear order and is essential for avoiding double counting.

4.4 Summary

- The many-body problem is reformulated as a variational problem in terms of G and Σ.
- The Luttinger–Ward functional $\Phi[G]$ encapsulates all many-body interaction effects via a sum over skeleton diagrams.
- The self–energy is given by
$$\Sigma = \frac{\delta\Phi[G]}{\delta G},$$
which ensures that the Dyson equation is recovered.
- The grand potential is expressed as
$$\Omega = \Phi[G] - \mathrm{Tr}(\Sigma\,G) - \mathrm{Tr}\ln\Big(1 - G_0\,\Sigma\Big) + \Omega_0.$$
The $\mathrm{Tr}\ln$ term arises naturally from the determinant of the interacting inverse propagator and sums an infinite series of interaction corrections.
- This formulation provides a solid foundation for systematic approximations (e.g., GW, DMFT) and a unified framework that links density-based and Green's function-based approaches.

5 From Bare to Dressed Quantities: Incorporating W

In Section 8.3 the formalism is extended to account for screening effects by introducing the screened interaction W as a variable. In the original Luttinger–Ward (LW) formulation the grand potential is expressed as a functional of the one–particle Green's function G (and, implicitly, the self–energy Σ) using the bare Coulomb interaction v_c. However, the bare interaction is strongly renormalized by the electronic response. To capture this, we extend the functional formalism so that the physical, *dressed* quantities appear.

1. Dressed Quantities versus Bare Quantities

In the original formulation, the Dyson equation for the one–particle Green's function is written as

$$G^{-1} = G_0^{-1} - \Sigma,$$

where G_0 is the non-interacting Green's function and Σ is the self–energy. Here, the Coulomb interaction enters via perturbative diagrams constructed with the bare interaction v_c. In this context, screening is implicit and appears only after summing many diagrams.

In contrast, the *dressed* formulation replaces the bare Coulomb interaction v_c with the screened interaction W. The screening is captured by the irreducible polarizability P through the Dyson equation for the interaction:

$$W = v_c + v_c\, P\, W,$$

which can be rearranged as

$$W = \frac{v_c}{1 - v_c\, P}.$$

Here, P quantifies the collective response of the electrons to external perturbations. Thus, while the self–energy Σ accounts for how individual electrons are renormalized by interactions, the polarizability P (and hence W) describes how the Coulomb interaction itself is modified (or "dressed") by screening.

2. Extending the Luttinger–Ward Functional: Incorporating W

In the original LW functional, the grand potential is given as a functional of G (or Σ) only:

$$\Omega_{\mathrm{LW}}[G] = \Phi[G] - \mathrm{Tr}(\Sigma\, G) - \mathrm{Tr}\ln\Big(1 - G_0\, \Sigma\Big) + \Omega_0,$$

with the self–energy obtained via

$$\Sigma = \frac{\delta\Phi[G]}{\delta G}.$$

This formulation uses the bare Coulomb interaction implicitly (through G_0 and the diagrammatic expansion for $\Phi[G]$).

However, one can extend the formalism to include the screened interaction W as an independent variable. In this extended approach, the grand potential becomes a functional $\Psi[G, W]$ that depends on both the dressed Green's function and the screened interaction. Although the full extended functional is more complex, its central idea is that:

$$\Psi[G, W] = \Phi\Big[G, \tilde{v}[G, W]\Big] - \frac{1}{2}\,\mathrm{Tr}'\Big[P\, W - \ln\big(1 + P\, W\big)\Big],$$

where:

- $\tilde{v}[G, W]$ is an effective bare interaction related to W (often via $\tilde{v} = W/(1 + P\, W)$),
- P is the irreducible polarizability, and
- The prime on the trace indicates that certain degrees of freedom (such as spin) are treated separately.

This extended functional explicitly incorporates screening. It allows one to compute the self–energy Σ using the dressed W (for example, in the GW approximation, $\Sigma \approx i\, G\, W$), which provides a more physically realistic description of interactions.

3. Self–Energy vs. Polarizability

It is essential to understand the distinct roles of the self–energy and the polarizability:

- **Self–Energy Σ:** A one–particle quantity that corrects the propagation of an electron. It enters the Dyson equation for G and modifies quasiparticle energies and lifetimes.
- **Polarizability P:** A two–particle quantity that measures the system's response to external perturbations (i.e., how the electron density rearranges). P is central to determining the screening of the Coulomb interaction, and it enters the Dyson equation for W.

Thus, while Σ reflects how a single electron is "dressed" by interactions, P (and consequently W) captures the collective response of the electron gas.

6 From Bare to Dressed Building Blocks in MBPT

6.1 Introduction and Motivation

In many-body perturbation theory, initial expansions typically use bare building blocks: the non-interacting Green's function G_0 and the bare Coulomb interaction v_c. Such expansions often exhibit poor convergence due to strong interactions. Thus, transitioning to dressed quantities significantly improves both convergence and physical clarity.

6.2 From Bare to Dressed Green's Functions

The dressed Green's function G includes all single-particle interaction effects and is defined via the Dyson equation:

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma(1,2),$$

where Σ is the self-energy, representing interaction-induced modifications to single-particle propagation. Diagrammatically, this involves summing infinite classes of self-energy insertions, simplifying perturbation expansions.

6.3 From Bare to Screened Coulomb Interaction

Realistic systems exhibit strong screening effects. The screened Coulomb interaction W incorporates this screening explicitly, defined by:

$$W = v_c + v_c P W,$$

with P being the irreducible polarizability, representing the collective electronic response. Solving explicitly:

$$W = \frac{v_c}{1 - v_c P},$$

clarifies how collective electron density rearrangements reduce the effective electron-electron interaction strength.

6.4 Dressed Quantities and Diagrammatic Reorganization

Employing dressed quantities G and W reorganizes perturbation expansions into simpler and fewer diagrams:

- **Skeleton diagrams**: Diagrams composed entirely of dressed quantities, free of explicit self-energy or polarizability insertions.
- Improved convergence and clearer physical interpretations result from this reorganization.

6.5 Connection to Extended Luttinger–Ward Functional

The shift to dressed quantities naturally leads to an extended LW-type functional, explicitly involving dressed quantities:

$$\Psi[G, W] = \Phi[G, \tilde{v}[G, W]] - \frac{1}{2}\,\mathrm{Tr}'\left[PW - \ln(1 + PW)\right],$$

where the effective interaction is defined as:

$$\tilde{v}[G, W] = \frac{W}{1 + PW}.$$

The stationary condition of this functional recovers Dyson equations for both G and W.

6.6 Advantages of the Dressed Formulation

Moving to dressed quantities offers multiple benefits:

- **Better-controlled approximations**: Inherently include substantial many-body corrections, simplifying higher-order terms.
- **Physical transparency**: Explicit distinction between single-particle and collective phenomena.
- **Unified framework**: Bridges various many-body methods, including GW and DMFT.

7 Generating Functionals, Effective Action, and Conserving Approximations

In many-body theory, generating functionals offer a systematic way to compute expectation values and correlation functions by coupling external source fields to the operators of interest. By performing a Legendre transform of the generating functional, one obtains the *effective action* Γ. The stationarity condition of Γ not only yields the physical observables but also recovers the Dyson equation, which underlies the Ward identities that enforce conservation laws such as particle number conservation.

7.1 Basic Concept and Definition

For a given operator $\hat{O}$, the generating functional is defined as

$$\Omega(u) = -\frac{1}{\beta}\ln \mathrm{Tr}\Big\{e^{-\beta(\hat{H}-\mu\hat{N})}e^{-u\hat{O}}\Big\}. \tag{9}$$

Differentiating with respect to u and then setting $u = 0$ yields the expectation value:

$$\beta\frac{\partial\Omega(u)}{\partial u}\bigg|_{u=0} = \langle\hat{O}\rangle. \tag{10}$$

For operators that depend on space, time, and spin, we generalize this concept by introducing a source function $J(1,1')$ coupled to an operator $\hat{Q}(1,1')$:

$$\Omega[J] = -\frac{1}{\beta}\ln \mathrm{Tr}\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\,T_C\exp\Big[-\int d1\,d1'\,J(1,1')\,\hat{Q}(1,1')\Big]\right\}, \tag{11}$$

where T_C denotes time (or contour) ordering. Then, the expectation value of $\hat{Q}(1,1')$ is given by

$$Q(1,1') = \frac{\delta\Omega[J]}{\delta J(1,1')}\bigg|_{J=0}. \tag{12}$$

For instance, choosing

$$\hat{Q}(1,1') = i\,\hat{\psi}^\dagger(1)\hat{\psi}(1'),$$

one obtains the one-particle Green's function:

$$G(1,1') = \beta\frac{\delta\Omega[J]}{\delta J(1',1)}\bigg|_{J=0}. \tag{13}$$

7.2 Effective Action via Legendre Transform and Auxiliary Systems

The effective action $\Gamma[Q]$ is defined as the Legendre transform of $\Omega[J]$:

$$\Gamma[Q] \equiv \beta\Omega[J_Q] - \int d1\,d1'\,J_Q(1,1')\,Q(1,1'), \tag{14}$$

with the source determined by

$$J_Q(1,1') = -\frac{\delta\Gamma[Q]}{\delta Q(1,1')}. \tag{15}$$

At the physical solution (when $J_Q = 0$), the effective action is stationary:

$$\frac{\delta\Gamma[Q]}{\delta Q(1,1')}\bigg|_{Q=Q_0} = 0, \tag{16}$$

so that Q equals its physical expectation value Q_0 and $\Gamma[Q_0]$ equals the physical grand potential.

It is often useful to split the effective action into a solvable part and corrections:

$$\Gamma[Q] = \Gamma_s[Q] + \Delta\Gamma[Q], \tag{17}$$

and to introduce a coupling constant λ to interpolate between the non-interacting ($\lambda = 0$) and fully interacting ($\lambda = 1$) systems:

$$\Gamma[Q] = \Gamma_s[Q] + \int_0^1 d\lambda\,\frac{d\Gamma_\lambda[Q]}{d\lambda}. \tag{18}$$

7.3 Stationarity, the Dyson Equation, and Conserving Approximations

A central result is that the effective action, when expressed as a functional of the one-particle Green's function G, leads to the Dyson equation upon stationarity. A typical form for the effective action is:

$$\Gamma[G] = \Phi[G] - \mathrm{Tr}(\Sigma\, G) - \mathrm{Tr}\ln\Big(1 - G_0\,\Sigma\Big) + \Omega_0, \tag{19}$$

where:

- $\Phi[G]$ is the Luttinger–Ward functional (expressed as a sum over skeleton diagrams built from G),
- Σ is the self-energy, defined as
$$\Sigma(1,2) = \frac{\delta\Phi[G]}{\delta G(2,1)},$$
- G_0 is the non-interacting Green's function, and
- Ω_0 is the non-interacting grand potential.

Taking the functional derivative of $\Gamma[G]$ with respect to G yields

$$\frac{\delta\Gamma[G]}{\delta G(1,2)} = \frac{\delta\Phi[G]}{\delta G(1,2)} - \Sigma(1,2) - \frac{\delta}{\delta G(1,2)}\,\mathrm{Tr}\ln\Big(1 - G_0\,\Sigma\Big).$$

Since by definition $\Sigma(1,2) = \delta\Phi[G]/\delta G(2,1)$, the first two terms cancel. A careful evaluation of the remaining derivative (using the chain rule and properties of the logarithm) then leads directly to the Dyson equation:

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma(1,2). \tag{20}$$

Thus, the stationarity condition $\delta\Gamma[G]/\delta G = 0$ is equivalent to the Dyson equation.

7.4 Connection to Conservation Laws and Ward Identities

The Dyson equation is not only the equation of motion for G but also a reflection of the underlying symmetries of the system. When the self-energy is derived from a generating functional, i.e.,

$$\Sigma = \frac{\delta\Phi[G]}{\delta G},$$

the resulting theory satisfies the *Ward identities.*

Ward Identities: Ward identities are exact relations between Green's functions and vertex functions that arise due to continuous symmetries (such as gauge invariance or global phase invariance). In the context of an electron system, they relate the one-particle Green's function, the self-energy, and the current vertex. These identities ensure that conservation laws, such as the conservation of charge (and thus particle number), are maintained. For example, the conservation of particle number implies the continuity equation

$$\frac{\partial n(x,t)}{\partial t} + \nabla\cdot j(x,t) = 0,$$

where $n(x,t)$ is the electron density and $j(x,t)$ is the current density. The Ward identities enforce that variations in G and Σ due to external perturbations do not violate this continuity equation.

Thus, if the effective action is constructed such that its stationary condition recovers the Dyson equation, then the associated Ward identities are automatically satisfied. This guarantees that important conservation laws (particle number, momentum, energy) hold as the system evolves.

7.5 Summary

In summary:

1. **Generating Functional:** By introducing a source J coupled to an operator $\hat{Q}$, the generating functional

$$\Omega[J] = -\frac{1}{\beta} \ln \mathrm{Tr} \left\{ e^{-\beta(\hat{H}-\mu\hat{N})} T_C \exp\Big[-\int d1\, d1'\, J(1,1')\, \hat{Q}(1,1') \Big] \right\},$$

   generates expectation values via differentiation.

2. **Effective Action:** The Legendre transform yields the effective action

$$\Gamma[Q] \equiv \beta\Omega[J_Q] - \int d1\, d1'\, J_Q(1,1')\, Q(1,1'),$$

   with the source J_Q given by $-\delta\Gamma[Q]/\delta Q$. At the stationary point, Q equals its physical value.

3. **Dyson Equation:** When Q is chosen as the one-particle Green's function G, the stationarity condition $\delta\Gamma[G]/\delta G = 0$ recovers the Dyson equation:

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma(1,2),$$

   with the self-energy defined as $\Sigma(1,2) = \delta\Phi[G]/\delta G(2,1)$.

4. **Ward Identities and Conservation Laws:** The fact that Σ is derived from $\Phi[G]$ ensures that the Ward identities—exact relations stemming from continuous symmetries—are satisfied. These identities guarantee that conservation laws (e.g., the continuity equation for particle number) are upheld.

This variational framework not only provides a powerful method for computing physical observables but also ensures that approximations built upon it are conserving, preserving essential symmetries of the system.