Functionals in Many-Particle Physics

March 24, 2025

Introduction: Functional Formulation

Key Idea

Instead of working with the full many–body wavefunction, we describe physical quantities as functionals of a key observable.

- Examples:
  - Electron density $n(\mathbf{r})$ in DFT.
  - One–particle Green's function G and self–energy Σ.
  - Screened Coulomb interaction W and related functionals.
- Provides a variational basis that automatically incorporates conservation laws.
- Underpins practical methods like the GW approximation, DMFT, and conserving approximations.

Comparison of Different Calculation Methods

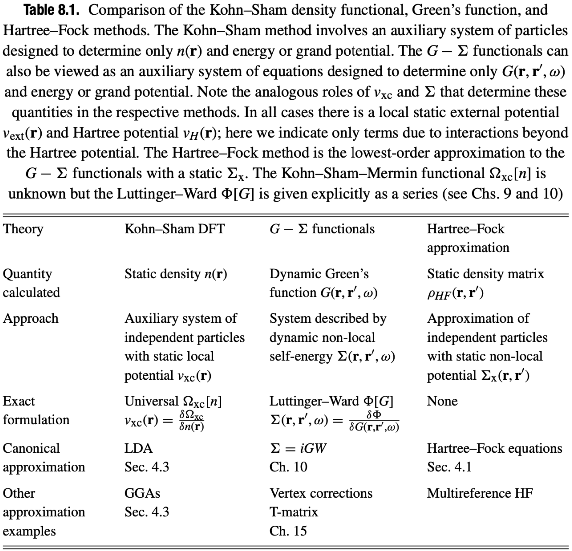

Table 8.1. Comparison of the Kohn–Sham density functional, Green's function, and Hartree–Fock methods. The Kohn–Sham method involves an auxiliary system of particles designed to determine only $n(\mathbf{r})$ and energy or grand potential. The $G - \Sigma$ functionals can also be viewed as an auxiliary system of equations designed to determine only $G(\mathbf{r}, \mathbf{r}', \omega)$ and energy or grand potential. Note the analogous roles of v_{xc} and Σ that determine these quantities in the respective methods. In all cases there is a local static external potential $v_{\mathrm{ext}}(\mathbf{r})$ and Hartree potential $v_H(\mathbf{r})$; here we indicate only terms due to interactions beyond the Hartree potential. The Hartree–Fock method is the lowest-order approximation to the $G - \Sigma$ functionals with a static Σ_{x}. The Kohn–Sham–Mermin functional $\Omega_{\mathrm{xc}}[n]$ is unknown but the Luttinger–Ward $\Phi[G]$ is given explicitly as a series (see Chs. 9 and 10)

Theory	Kohn–Sham DFT	$G - \Sigma$ functionals	Hartree–Fock approximation
Quantity calculated	Static density $n(\mathbf{r})$	Dynamic Green's function $G(\mathbf{r}, \mathbf{r}', \omega)$	Static density matrix $\rho_{HF}(\mathbf{r}, \mathbf{r}')$
Approach	Auxiliary system of independent particles with static local potential $v_{\mathrm{xc}}(\mathbf{r})$	System described by dynamic non-local self-energy $\Sigma(\mathbf{r}, \mathbf{r}', \omega)$	Approximation of independent particles with static non-local potential $\Sigma_{\mathrm{x}}(\mathbf{r}, \mathbf{r}')$
Exact formulation	Universal $\Omega_{\mathrm{xc}}[n]$ $v_{\mathrm{xc}}(\mathbf{r}) = \frac{\delta \Omega_{\mathrm{xc}}}{\delta n(\mathbf{r})}$	Luttinger–Ward $\Phi[G]$ $\Sigma(\mathbf{r}, \mathbf{r}', \omega) = \frac{\delta \Phi}{\delta G(\mathbf{r}, \mathbf{r}', \omega)}$	None
Canonical approximation	LDA Sec. 4.3	$\Sigma = iGW$ Ch. 10	Hartree–Fock equations Sec. 4.1
Other approximation examples	GGAs Sec. 4.3	Vertex corrections T-matrix Ch. 15	Multireference HF

Variational Principle and Density Functionals

Variational Principle

$$E[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle \quad \text{with} \quad \frac{\delta E[\Psi]}{\delta \Psi} = 0.$$

In DFT the energy is recast 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 $n_0(\mathbf{r})$.

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

- Kohn and Sham introduced an auxiliary system of non-interacting particles that reproduces the interacting density.
- In the Green's function formulation, the Kohn–Sham Green's function G_{KS} obeys:

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

  or equivalently,

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

  where:
  - G_0 is the Green's function of a non-interacting reference system.
  - $v_{\mathrm{Hxc}}(r) = v_{\mathrm{H}}(r) + v_{\mathrm{xc}}(r)$ combines the Hartree and exchange–correlation potentials.
- The electron density is recovered from G_{KS} via:

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

The Mermin Functional and the Grand Potential

- At finite temperature, the grand potential is defined by:

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

- In the Kohn–Sham framework, the Mermin functional for the grand potential is written as:

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

  with the effective potential:

$$v_{\text{eff}}(r) = v_{\text{ext}}(r) + v_{\text{H}}(r) + v_{\text{xc}}(r).$$

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

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

  - $\Omega_{xc}[n]$ incorporates exchange–correlation effects.

Connecting Density and Green's Function Formulations

- The coupling term between the effective potential and density is rewritten as a trace:

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

- Using the Dyson equation:

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

  one derives the full expression for the grand potential:

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

- The term

$$\mathrm{Tr}\ln\Big(1 - G_0\, v_{\mathrm{Hxc}}\Big)$$

  represents the sum over all repeated interactions:

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

Functionals of G and Σ

- Variational formulation of the grand potential using G and Σ
- The Luttinger–Ward functional $\Phi[G]$
- Expression for the grand potential Ω
- Physical interpretation and variational principle

The Luttinger–Ward Functional

- $\Phi[G]$ is defined as the sum over all *skeleton diagrams* constructed with the full interacting Green's function G.
- It is a universal functional; it does not depend on the external potential.
- It contains all the many-body interaction effects in the system.

A crucial relation:

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

Expression for the Grand Potential

The grand potential is expressed as:

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

where:

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

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

  so that

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

  Taking the logarithm and using $\ln(AB) = \ln A + \ln B$ leads to the trace-log term.

Physical Interpretation and Variational Principle

- **Unified Description:** Ω is expressed entirely in terms of G and Σ, bridging density-functional methods and many-body perturbation theory.
- **Variational Character:** The physical Green's function G is determined by the stationarity condition:

$$\frac{\delta\Omega}{\delta G} = 0.$$

- 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.

- **Logarithmic Term:** $\mathrm{Tr}\ln\left(1 - G_0\,\Sigma\right)$ sums over all higher-order corrections due to repeated interactions, avoiding double counting.

Summary So Far

- We have reformulated the many-body problem as a variational problem in terms of G and Σ.
- The Luttinger–Ward functional $\Phi[G]$ is the sum over all skeleton diagrams and is universal.
- The self-energy is given by:

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

- The grand potential is expressed as:

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

- At the stationary point, the variational condition recovers the Dyson equation:

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

- This unified framework lays the groundwork for systematic approximations like GW and DMFT.

Dressed Quantities versus Bare Quantities

In the original formulation we have the Dyson equation:

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

where:

- G_0 is the non-interacting Green's function.
- Σ is the self–energy.

The bare Coulomb interaction v_c appears in the diagrams that build up Σ. In that

picture, screening is hidden; it only shows up after you sum many diagrams.
In the dressed formulation, we replace v_c with the screened interaction W. Screening is taken into account explicitly via the irreducible polarizability P through:

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

which can be rearranged to:

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

Extending the Functional: Incorporating W

In the original LW formulation, the grand potential is expressed as:

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

with the self–energy given by:

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

This expression uses the bare interaction implicitly.
To account for screening explicitly, we extend the functional so that the grand potential becomes a functional of both G and W:

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

Here:

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

Self–Energy vs. Polarizability

It is important to distinguish two key quantities:

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

Thus, while Σ represents how an individual electron gets "dressed" by interactions, P (and consequently W) captures the collective response of the electrons.

Summary

- We start with the bare formulation where the Dyson equation is:

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

- In the bare picture, screening only appears after summing many diagrams.
- The dressed formulation replaces v_c with the screened interaction W, defined by:

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

- We extend the functional formalism so that the grand potential becomes a functional $\Psi[G, W]$, where the effective interaction is expressed in terms of W and the polarizability P.
- The self–energy Σ describes the dressing of single electrons, while P (and thus W) captures the collective screening effect.

Transition: Linking Screening to Many-Body Perturbation Theory

- So far we introduced dressed quantities by replacing the bare Coulomb interaction v_c with the screened interaction W.
- Next, we connect this idea with many-body perturbation theory (MBPT), where the Green's function is expanded in powers of the interaction via adiabatic switching.
- After writing the Dyson series, the formalism naturally leads back to an expression for the grand potential in a form similar to the Luttinger–Ward (LW) functional.

From Bare to Dressed Building Blocks in MBPT

- MBPT initially expands using bare quantities: the non-interacting Green's function G_0 and the bare Coulomb interaction v_c.
- Such bare expansions can converge poorly because the Coulomb interaction is very strong.
- Transitioning to dressed quantities improves convergence and provides a clearer physical picture.

From Bare to Dressed Green's Functions

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

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

  where Σ is the self–energy.
- Diagrammatically, this amounts to summing over an infinite series of self–energy insertions.

From Bare to Screened Coulomb Interaction

- The bare Coulomb interaction v_c is modified by the electronic response.
- The screened Coulomb interaction W is defined by:

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

or equivalently,

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

where P is the irreducible polarizability.

Dressed Quantities and Diagrammatic Reorganization

- Using dressed quantities G and W reorganizes the perturbation series.
- We form **skeleton diagrams**: diagrams built entirely from dressed quantities without redundant self-energy or polarizability insertions.
- This reorganization leads to simpler diagrams, improved convergence, and better physical insight.

Connection to Extended Luttinger–Ward Functional

- With dressed quantities, the grand potential becomes a functional $\Psi[G, W]$ of both G and W.
- It takes the form:

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

where the effective interaction is given by:

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

- The stationary condition of $\Psi[G, W]$ recovers the Dyson equations for both G and W.

Advantages of the Dressed Formulation

- **Better-controlled approximations:** Dressed quantities already include many-body corrections.
- **Physical transparency:** Clear separation of single-particle effects (Σ) and collective responses (P and W).
- **Unified framework:** Provides a common language that connects approaches such as GW and DMFT.

Generating Functionals, Effective Action, and Conserving Approximations: Outline

- Basic Concept and Definition of Generating Functionals
- Effective Action via Legendre Transform and Auxiliary Systems
- Stationarity of the Effective Action and Recovery of the Dyson Equation
- Connection to Ward Identities and Conservation Laws
- Summary

Basic Concept and Definition

Generating functionals provide a way to compute expectation values by coupling an external source to an operator.

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

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

Differentiating with respect to u at $u = 0$ gives:

$$\beta \frac{\partial \Omega(u)}{\partial u}\bigg|_{u=0} = \langle \hat{O} \rangle. \tag{2}$$

Time-Ordered Generating Functional

For operators depending on space, time, and spin, we introduce a source function $J(1,1')$ coupled to an operator $\hat{Q}(1,1')$:

$$\Omega[J] = -\frac{1}{\beta} \ln \mathrm{Tr} \left\{ e^{-\beta(\hat{H}-\mu\hat{N})} \, T_C \exp \left[- \int d1 \, d1' \, J(1,1') \, \hat{Q}(1,1') \right] \right\}, \tag{3}$$

where T_C denotes time (or contour) ordering.

The expectation value is then obtained by

$$Q(1,1') = \left. \frac{\delta \Omega[J]}{\delta J(1,1')} \right|_{J=0} . \tag{4}$$

Effective Action via Legendre Transform

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

$$\Gamma[Q] \equiv \beta\,\Omega[J_Q] - \int d1\, d1'\, J_Q(1,1')\, Q(1,1'). \tag{5}$$

The source is given by

$$J_Q(1,1') = -\frac{\delta\Gamma[Q]}{\delta Q(1,1')}. \tag{6}$$

At the stationary point (when $J_Q = 0$), we have

$$\left.\frac{\delta\Gamma[Q]}{\delta Q(1,1')}\right|_{Q=Q_0} = 0, \tag{7}$$

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

Stationarity and the Dyson Equation

A common form for the effective action in terms of the one-particle Green's function G is:

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

where:

- $\Phi[G]$ is the Luttinger–Ward functional.
- $\Sigma(1,2) = \dfrac{\delta\Phi[G]}{\delta G(2,1)}$ is the self-energy.
- G_0 is the non-interacting Green's function.
- Ω_0 is the non-interacting grand potential.

Taking the functional derivative,

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

and noting that $\Sigma(1,2) = \delta\Phi[G]/\delta G(2,1)$, the first two terms cancel. A careful evaluation of the remaining term yields the Dyson equation:

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma(1,2). \tag{9}$$

Connection to Ward Identities and Conservation Laws

The Dyson equation is not only the equation of motion but also underpins conservation laws via the Ward identities.

Ward Identities:

- They are exact relations among Green's functions and vertex functions.
- They follow from continuous symmetries (e.g., gauge invariance or global phase invariance).
- For example, in an electron system, a Ward identity relates the one-particle Green's function, the self-energy, and the current–vertex function.

Conservation Laws:

- *Particle number conservation:* The particle number

  $$N = -i \ \mathrm{Tr} \ G(t, t^{+})$$

  remains constant, ensuring the continuity equation:

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

- When Σ is derived as $\Sigma = \delta\Phi[G]/\delta G$, the Ward identities hold, guaranteeing that any variation in G due to external perturbations will not violate these conservation laws.

Summary

1. Generating functionals allow us to compute expectation values by coupling external sources to operators.
2. The effective action $\Gamma[Q]$ is obtained by a Legendre transform of the generating functional, with

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

   and $J_Q(1,1') = -\delta\Gamma[Q]/\delta Q(1,1')$.
3. The stationary condition $\delta\Gamma[G]/\delta G = 0$ recovers the Dyson equation,

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

   where $\Sigma = \delta\Phi[G]/\delta G$.
4. The Dyson equation is the basis for the Ward identities, which enforce conservation laws (e.g., particle number conservation) by ensuring that variations in G are consistent with the underlying symmetries.