Variational Perturbation Theory for Density Functional Theory

Towards a systematic improvement
of the Hartree-Fock-Bogoliubov approximation

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Research discussion
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Contents

Ultimate goal

Develop a systematic and constructive strategy to obtain a Density Functional Theory from first principle including beyond mean field and pairing effects

Framework:
effective action formalism

Fermionic field operators

Considering a spin-saturated many-body system of A fermions (mass $2m = 1$ and spin projection $\sigma = \pm 1/2$) associated to a (time-independent) local two-body interaction. The many-body Hamiltonian is decomposed as $\widehat{H} = \widehat{T} + \widehat{V}$

$$\widehat{T}(t) = -\sum_{\sigma} \int d\boldsymbol{r}\, \psi^{\dagger}_{\sigma}(\boldsymbol{r}t)\nabla^2\psi_{\sigma}(\boldsymbol{r}t)$$

$$\widehat{V}(t) = \frac{1}{2}\sum_{\sigma_1\sigma_2} \iint d\boldsymbol{r_1} d\boldsymbol{r_2}\, \psi^{\dagger}_{\sigma_1}(\boldsymbol{r_1}t)\psi^{\dagger}_{\sigma_2}(\boldsymbol{r_2}t) v_{\sigma_1\sigma_2}(\boldsymbol{r_1},\boldsymbol{r_2})\psi_{\sigma_2}(\boldsymbol{r_2}t)\psi_{\sigma_1}(\boldsymbol{r_1}t)$$

$$\psi_{\sigma}(\boldsymbol{r}t) = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\varphi_{\boldsymbol{k}\sigma}(\boldsymbol{r})c_{\boldsymbol{k}\sigma}(t) \qquad \psi^{\dagger}_{\sigma}(\boldsymbol{r}t) = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\varphi^{*}_{\boldsymbol{k}\sigma}(\boldsymbol{r})c^{\dagger}_{\boldsymbol{k}\sigma}(t)$$

[Fetter & Walecka book's]

Path integral formulation

Solving the **many-body Schrödinger equation** $i\partial_t |\phi\rangle = \widehat{H} |\phi\rangle$ in the **Feynman path integral formalism** requires

- the action $\mathcal{S}[\psi^\dagger, \psi] \equiv \mathcal{S}_1[\psi^\dagger, \psi] + \mathcal{S}_2[\psi^\dagger, \psi]$

$$\mathcal{S}[\psi^\dagger, \psi] = \int_0^\infty dt \sum_\sigma \int d\boldsymbol{r}\, \psi_\sigma^\dagger(\boldsymbol{r}t) \underbrace{[i\partial_t + \nabla^2 + \mu_\sigma]}_{\sim \textit{ free propagator}} \psi_\sigma(\boldsymbol{r}t) + \int_0^\infty dt\, \widehat{V}(t)$$

- the partition function $\mathcal{Z} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \exp\Big(i\mathcal{S}[\psi^\dagger, \psi]\Big)$ as a path integral
  - ✓ analogy with statistical mechanics [Negele & Orland book's]
  - ✗ path integral undoable in practice (except for Gaussian, etc.)
    → approximation e.g. **Variational Perturbation Theory**
    [Feynman & Kleinert, Phys. Rev. A **34**, (1986)]

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- Introduce some well chosen auxiliary classical fields $(\rho, \kappa, \kappa^*, \cdots)$ associated to an action $\mathcal{S}_a$ such that

$$\mathcal{S} = \underbrace{(\mathcal{S}_1 - \mathcal{S}_a)}_{\equiv \mathcal{S}_0} + \underbrace{(\mathcal{S}_2 + \mathcal{S}_a)}_{\equiv \mathcal{S}_i}$$

  - normal density related to $\langle\psi^\dagger\psi\rangle \to \mathcal{S}_a[\rho] \sim \int \rho\,\psi^\dagger\psi$
  - anormal density related to $\langle\psi\psi\rangle$ and $\langle\psi^\dagger\psi^\dagger\rangle \to \mathcal{S}_a[\kappa,\kappa^*] \sim \frac{1}{2}\int [\kappa\,\psi^\dagger\psi^\dagger + \kappa^*\psi\psi]$

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- Treat the action $\mathcal{S}_i$ in perturbation according to the reference Gaussian action $\mathcal{S}_0$
- Apply the variational principle to extremize the perturbative action according to the auxiliary fields

[Kleinert, EJTP **8**, (2011)]

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After some technical manipulations using Grassmann variables, the action $\mathcal{S}_0$ can be written as a convenient Gaussian matrix expression

$$\begin{aligned}\mathcal{S}_0 &= (\mathcal{S}_1 - \mathcal{S}_a[\rho] - \mathcal{S}_a[\kappa, \kappa^*]) \\ &= \frac{1}{2}\int \xi^\dagger_\sigma(\boldsymbol{r_1}t_1) \underbrace{\begin{bmatrix} g^{-1} + \rho & \kappa \\ \kappa^* & \widetilde{g}^{-1} - \rho \end{bmatrix}}_{\equiv \mathbb{A}_{\sigma\sigma'}(\boldsymbol{r_1}t_1, \boldsymbol{r_2}t_2)} \xi_{\sigma'}(\boldsymbol{r_2}t_2)\end{aligned}$$

$g^{-1}_{\sigma\sigma'}(\boldsymbol{r_1}t_1, \boldsymbol{r_2}t_2) = \delta(\boldsymbol{r_1} - \boldsymbol{r_2})\delta(t_1 - t_2)[i\partial_t + \nabla^2 + \mu_\sigma]\delta_{\sigma\sigma'}$ free Green's function

$\xi^\dagger_\sigma(\boldsymbol{r}t) = (\psi^\dagger_\sigma(\boldsymbol{r}t), \psi_\sigma(\boldsymbol{r}t))$ doublet Nambu spinor fields

[Gor'kov, Sov. Phys. JETP **7** (1958)]

Generating partition function

- The one-body reference states (generated by the action $\mathcal{S}_0$) are encoded in the generating partition function

$$\mathcal{Z}_0 = \int \mathcal{D}\xi^\dagger \mathcal{D}\xi \, \exp\Big(i\mathcal{S}_0[\xi^\dagger, \xi, \rho, \kappa, \kappa^*]\Big) = \int \mathcal{D}\xi^\dagger \mathcal{D}\xi \, \exp\left(\frac{i}{2}\int \xi^\dagger \mathbb{A}\, \xi\right)$$

- The one-body Green's function denote $\mathbb{G} = i\mathbb{A}^{-1}$
  $\rightarrow$ functional matrix equation

$$\int dt \sum_\sigma \int d\boldsymbol{r} \, \mathbb{A}_{\sigma_1\sigma}(\boldsymbol{r}_1 t_1, \boldsymbol{r} t)\mathbb{G}_{\sigma\sigma_2}(\boldsymbol{r} t, \boldsymbol{r}_2 t_2) = i\mathbb{I}\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(t_1 - t_2)\delta_{\sigma_1\sigma_2}$$

- Integrating out the $\xi, \xi^\dagger$ d.o.f. define the effective action $\Omega_0[\rho, \kappa, \kappa^*]$

$$\mathcal{Z}_0 \equiv \exp(i\Omega_0) \qquad \rightarrow \qquad \Omega_0 = -\frac{i}{2}\,\mathrm{tr}\ln\left(-\mathbb{G}^{-1}\right)$$

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✓ **By construction, the generating partition function $\mathcal{Z}_0$ contains everything we want to known about the system** [cf. analogy with statistical mechanics]

$$\langle \mathcal{O} \rangle_{\rho,\kappa,\kappa^*} \equiv \frac{1}{\mathcal{Z}_0} \int \mathcal{D}\xi^\dagger \mathcal{D}\xi \, \mathcal{O}[\xi^\dagger, \xi] \, \exp\Big(i\mathcal{S}_0[\xi^\dagger, \xi, \rho, \kappa, \kappa^*] \Big)$$

✓ The physical mean value $\langle \mathcal{O} \rangle$ should be **independent of the auxiliary classical fields**, or equivalently, using the principle of least action

$$\frac{\delta \langle \mathcal{O} \rangle}{\delta \rho} = \frac{\delta \langle \mathcal{O} \rangle}{\delta \kappa} = \frac{\delta \langle \mathcal{O} \rangle}{\delta \kappa^*} = 0$$

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- The partition function of the system can be expanded using the decomposition $\mathcal{S} = \mathcal{S}_0 + \mathcal{S}_i \rightarrow \exp(i\mathcal{S}) = \exp(i\mathcal{S}_0)\exp(i\mathcal{S}_i)$

$$\mathcal{Z} = \int \mathcal{D}\xi^\dagger \mathcal{D}\xi \exp(i\mathcal{S}) \quad \Leftrightarrow \quad \mathcal{Z} = \mathcal{Z}_0 \sum_{n=0}^{\infty} \frac{i^n}{n!} \langle \mathcal{S}_i^n \rangle_{\rho,\kappa,\kappa^*}$$

- **Truncating the infinite sum** at a given order N define the effective classical action Ω_N in perturbation

$$\mathcal{Z}_N = \mathcal{Z}_0 \sum_{n=0}^{N} \frac{i^n}{n!} \langle \mathcal{S}_i^n \rangle_{\rho,\kappa,\kappa^*} \equiv \exp(i\Omega_N[\rho,\kappa,\kappa^*])$$

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How to obtain the ground state energy of the system?

- The grand canonical potential at order N in perturbation $E_N - \mu A$ can be identified as proportional to the effective classical action at **zero-temperture**

  [cf. analogy with statistical mechanics]

$$E_N - \mu A = \lim_{\beta\to\infty} \frac{\Omega_N}{\beta} \qquad \beta = \int_0^\beta dt \sim \frac{1}{k_B T}$$

- The physical value is given by the principle of least action

$$\frac{\delta\Omega_N}{\delta\rho} = \frac{\delta\Omega_N}{\delta\kappa} = \frac{\delta\Omega_N}{\delta\kappa^*} = 0$$

  The functional derivative of the zero-order effective action are related to the one-body Green's functions

$$\Omega_0 = -\frac{i}{2}\,\mathrm{tr}\ln \underbrace{\begin{bmatrix} -G_\rho & -G_\kappa \\ -G_\kappa^\dagger & -\widetilde{G}_\rho \end{bmatrix}^{-1}}_{\equiv -\mathbb{G}^{-1}} \quad \rightarrow \quad \frac{\delta\Omega_0}{\delta\rho} = G_\rho \qquad \frac{\delta\Omega_0}{\delta\kappa} = G_\kappa$$

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- The Wick contractions in Hartree, Fock, and Bogoliubov channel of the k-point correlation functions in terms of the **two-point correlation functions** directly related to the normal and anormal densities

$$\langle \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1 \rangle = \langle \psi_1^\dagger \psi_1 \rangle \langle \psi_2^\dagger \psi_2 \rangle - \langle \psi_1^\dagger \psi_2 \rangle \langle \psi_2^\dagger \psi_1 \rangle + \langle \psi_1^\dagger \psi_2^\dagger \rangle \langle \psi_2 \psi_1 \rangle$$

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- The variational principle leads naturally to two types of equations
  - the two-point correlation functions in terms of the one-body Green's functions
    $\longrightarrow$ **many-body diagrams of the theory**
  - the auxiliary classical fields in terms of the one-body Green's functions
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Critical discussion

✓ Adventages

- Systematic improvement of the Hartree-Fock-Bogoliubov Theory from first principles based on the **two-point correlation functions** as building blocs.
- Generalizable to include more relevant classical fields associated to collective d.o.f. of interest allowing for **spontaneous symmetry breaking** in the ground state.
- The theory is explicit in terms of the densities (Wick contractions) contrary to the highly non-explicit inversion method due to the use of Legendre transform [Drut, Furnstahl, and Platter (2010)]
- Contrary to similar approaches relying on Hubbard-Stratanovich transform, the variational principle fix the auxiliary classical fields and do not induce quantum fluctuations of the collective fields.

✗ Drawbacks

- Schematic and requires developments to obtain a clear Density Functional Theory.
- No guidance to solve the **functional matrix equation** $\mathbb{G} = i\mathbb{A}^{-1}$ and get the expression of the one-body Green's function in terms of the auxiliary classical fields.

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- No guidance to solve the **functional matrix equation** $\mathbb{G} = i\mathbb{A}^{-1}$ and get the expression of the one-body Green's function in terms of the auxiliary classical fields.

Critical discussion

✓ Advantages

- Systematic improvement of the Hartree-Fock-Bogoliubov Theory from first principles based on the **two-point correlation functions** as building blocs.
- Generalizable to include more relevant classical fields associated to collective d.o.f. of interest allowing for **spontaneous symmetry breaking** in the ground state.
- The theory is explicit in terms of the densities (Wick contractions) contrary to the highly non-explicit inversion method due to the use of Legendre transform [Drut, Furnstahl, and Platter (2010)]
- Contrary to similar approaches relying on Hubbard-Stratanovich transform, the variational principle fix the auxiliary classical fields and do not induce quantum fluctuations of the collective fields.

✗ Drawbacks

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Approximation: gradient expansion

Wigner-Weyl transform

- Center-of-mass and relative coordinate change of variables $f(\boldsymbol{r_1}, \boldsymbol{r_2}) = f(\boldsymbol{R}, \boldsymbol{r})$

$$\boldsymbol{R} \equiv \frac{\boldsymbol{r_1} + \boldsymbol{r_2}}{2} \qquad \boldsymbol{r} \equiv \boldsymbol{r_1} - \boldsymbol{r_2}$$

- Wigner-Weyl transform (map quantum phase space and Hilbert space operators)

$$f(\boldsymbol{R}, \boldsymbol{k}) = \int d\boldsymbol{r} e^{+i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{R}, \boldsymbol{r})$$

- Fourier transform in the frequency domain

$$f(t = t_1 - t_2) = \int \frac{d\omega}{2\pi} e^{-i\omega t} f(\omega)$$

Master functional equation

Spacial coordinates (Hilbert space)

$$\int dt \sum_{\sigma} \int d\boldsymbol{r}\, \mathbb{A}_{\sigma_1\sigma}(\boldsymbol{r_1} t_1, \boldsymbol{r} t)\mathbb{G}_{\sigma\sigma_2}(\boldsymbol{r} t, \boldsymbol{r_2} t_2) = i\mathbb{I}\delta(\boldsymbol{r_1} - \boldsymbol{r_2})\delta(t_1 - t_2)\delta_{\sigma_1\sigma_2}$$

$$\Updownarrow \quad \mathbb{G} = i\mathbb{A}^{-1}$$

Wigner coordinates (phase space)

$$\sum_{\sigma} \lim_{\boldsymbol{R'}\to\boldsymbol{R}} \lim_{\boldsymbol{k'}\to\boldsymbol{k}} \underbrace{\exp\left(-\frac{i}{2}[\nabla_{\boldsymbol{R}} \cdot \nabla_{\boldsymbol{k'}} - \nabla_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{R'}}]\right)}_{\equiv \exp(\Lambda)} \mathbb{A}_{\sigma_1\sigma}(\boldsymbol{R}, \boldsymbol{k}, \omega)\mathbb{G}_{\sigma\sigma_2}(\boldsymbol{R'}, \boldsymbol{k'}, \omega) = i\mathbb{I}\delta_{\sigma_1\sigma_2}$$

[Baraff & Borowitz, Phys. Rev. **121** (1961)]

Gradient expansion of the one-body Green's functions

Expansion of the locating operator

$$\exp(\Lambda) = \sum_{q=0}^{\infty} \frac{\Lambda^q}{q!}$$

Expansion of the Green's functions

$$\mathbb{G} = \sum_{m=0}^{\infty} \mathbb{G}^{(m)}$$

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The knowledge of the propagator $\mathbb{A}$ allow a systematic gradient expansion of the one-body Green's functions [Ullrich & Gross, Aust. J. Phys. **49** (1996)]

$$\mathbb{G} = \mathbb{G}^{(0)}[\mathbb{A}] + \mathbb{G}^{(1)}[\mathbb{A}, \nabla_{\boldsymbol{R}}\mathbb{A}, \nabla_{\boldsymbol{k}}\mathbb{A}] + \mathbb{G}^{(2)}[\nabla_{\boldsymbol{R}} \cdot \nabla_{\boldsymbol{k}}\mathbb{A}, \cdots] + \cdots$$

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Application:
Hatree-Fock approximation

Illustration with a simple model

Considering a spin-saturated many-body even-even ($A_\uparrow = A_\downarrow = A/2$) system of fermions (mass $2m = 1$ and spin projection $\sigma = \pm 1/2$) associated to a (time-independent) local two-body interaction.

For simplicity, the two-body interaction is spin-independent and central ($v_{\sigma_1\sigma_2}(\boldsymbol{r_1}, \boldsymbol{r_2}) = v(r)$ with $r = |\boldsymbol{r_1} - \boldsymbol{r_2}|$)

- Everything is **diagonal in spin**, i.e. $\mathbb{G}_{\sigma\sigma'} \equiv \mathbb{G}\delta_{\sigma\sigma'}$, $\mu_\uparrow = \mu_\downarrow \equiv \mu$, etc.
- Focus on **normal state**, i.e. $\kappa = \kappa^* = 0$ and $(\mathbb{A}, \mathbb{G}) \to (A, G)$
- **Spherical symmetry** assumed
- **No off-shell effects** at Hatree-Fock level, i.e. $\rho(t_1, t_2) \propto \delta(t_1 - t_2)$

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Generating partition function

- **reference action** $\mathcal{S}_0 = \iint \psi^\dagger_\sigma(\boldsymbol{r_1} t_1) A_{\sigma\sigma'}(\boldsymbol{R}, \boldsymbol{r}, t) \psi_{\sigma'}(\boldsymbol{r_2} t_2)$
- **propagator** $A_{\sigma\sigma'}(\boldsymbol{R}, \boldsymbol{r}, t) = \underbrace{\delta(t)\delta(\boldsymbol{r})[i\partial_t + \nabla^2 + \mu_\sigma]}_{\equiv g^{-1}(\boldsymbol{R}, \boldsymbol{r}, t)} \delta_{\sigma\sigma'} - \underbrace{\rho(\boldsymbol{R}, \boldsymbol{r})\delta(t)\delta_{\sigma\sigma'}}_{auxiliary\ field}$
- **one-body Green's function** $G = iA^{-1}$ (functional equation for operator)
- effective action $\mathcal{Z}_0 = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \exp(i\mathcal{S}_0) \equiv \exp(i\Omega_0) \to \Omega_0 = -i \operatorname{tr} \ln\left(-G^{-1}\right)$

$$\langle \mathcal{O} \rangle_\rho \equiv \frac{1}{\mathcal{Z}_0} \int \mathcal{D}\psi^\dagger \mathcal{D}\psi\, \mathcal{O}[\psi^\dagger, \psi] \exp\Big(i\mathcal{S}_0[\psi^\dagger, \psi, \rho]\Big)$$

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Hartree-Fock effective action

$$\Omega_1 - \Omega_0 = \langle \mathcal{S}_i \rangle = \langle \mathcal{S}_2 \rangle + \langle \mathcal{S}_a \rangle$$
$$= \frac{1}{2} \sum_{\sigma\sigma'} \iint v(r) \underbrace{\langle \psi^\dagger_\sigma(\boldsymbol{r_1} t_1) \psi^\dagger_{\sigma'}(\boldsymbol{r_2} t_2) \psi_{\sigma'}(\boldsymbol{r_2} t_2) \psi_\sigma(\boldsymbol{r_1} t_1) \rangle}_{\langle \psi^\dagger_1 \psi_1 \rangle \langle \psi^\dagger_2 \psi_2 \rangle - \langle \psi^\dagger_1 \psi_2 \rangle \langle \psi^\dagger_2 \psi_1 \rangle} \delta(t)$$
$$+ \sum_{\sigma\sigma'} \iint \rho(\boldsymbol{R}, \boldsymbol{r}) \langle \psi^\dagger_\sigma(\boldsymbol{r_1} t_1) \psi_{\sigma'}(\boldsymbol{r_2} t_2) \rangle \delta(t) \delta_{\sigma\sigma'}$$

First extremization → many-body diagrams

$$\frac{\delta \Omega_1}{\delta \rho} = 0 \quad \rightarrow \quad \langle \psi^\dagger_\sigma(\boldsymbol{r_1} t_1) \psi_{\sigma'}(\boldsymbol{r_2} t_2) \rangle = \frac{\delta \Omega_0}{\delta \rho} = -G_{\sigma\sigma'}(\boldsymbol{R}, \boldsymbol{r}, t)$$

Hartree-Fock effective action

$$
\begin{aligned}
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Hartree-Fock self-energy

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$$= \sum_{\sigma\sigma'} \iint v(r)\delta(t)[\underbrace{G_{\sigma\sigma}(\mathbf{R},0,0)G_{\sigma'\sigma'}(\mathbf{R},0,0)}_{\text{direct (Hartree)}} - \underbrace{G_{\sigma\sigma'}(\mathbf{R},\mathbf{r},t)G_{\sigma'\sigma}(\mathbf{R},-\mathbf{r},-t)}_{\text{exchange (Fock)}}]$$

$$- \sum_{\sigma\sigma'} \iint \rho(\mathbf{R},\mathbf{r})G_{\sigma\sigma'}(\mathbf{R},\mathbf{r},t)$$

Second extremization → self-consistent equation (self-energy)

$$\frac{\delta\Omega_1}{\delta\rho} = 0 \quad \rightarrow \quad \rho(\mathbf{R},\mathbf{k}) = \underbrace{\int d\mathbf{R}' \int \frac{d\mathbf{k}'}{(2\pi)^3}}_{\text{phase space}} \int \frac{d\omega'}{2\pi} \underbrace{K_v(\mathbf{R},\mathbf{k}|\mathbf{R}',\mathbf{k}')}_{\text{direct + exchange}} G(\mathbf{R}',\mathbf{k}',\omega')$$

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One-body density matrix

- the propagator defined in terms of the auxiliary field: $A = g^{-1} - \rho$
- the one-body Green's function given by the gradient expansion of $G = iA^{-1}$
  $\rightarrow G[\rho, \nabla_{\boldsymbol{R}} \cdot \nabla_{\boldsymbol{k}}\rho, \nabla_{\boldsymbol{R}} \cdot \nabla_{\boldsymbol{R}}\rho, \nabla_{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}}\rho, \cdots]$
- the auxiliary field given by the solution of the self-consistent equation $\rho = K_v G$

$$n(\boldsymbol{R}, \boldsymbol{k}) = \int \frac{d\omega}{2\pi} G(\boldsymbol{R}, \boldsymbol{k}, \omega) \quad \rightarrow \quad n(\boldsymbol{R}, \boldsymbol{r})$$

$$\lim_{\beta\to\infty} \frac{\Omega_1 - \Omega_0}{\beta} = \underbrace{2v_0 \int d\boldsymbol{R}\, n(\boldsymbol{R}, 0)(\boldsymbol{R}, 0)}_{direct\ (Hartree)} - \underbrace{\int d\boldsymbol{R} \int d\boldsymbol{r}\, v(r) n(\boldsymbol{R}, \boldsymbol{r}) n(\boldsymbol{R}, -\boldsymbol{r})}_{exchange\ (Fock)}$$

$$\equiv \frac{1}{2} \mathrm{tr}(n_1 V_{12}(1 - P_{12}) n_2) \qquad \checkmark \text{ Hartree-Fock result}$$

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Density Matrix Expansion

The idea of the density matrix expansion (DME) is to factorize the non-local part of the one-body density matrix using an **expansion around a momentum scale**, typically the local Fermi-momentum $k_F(\boldsymbol{R})$

[Negele & Vautherin] [Gebremariam, Duguet, Bogner, Furnstahl, Schunck, Navarro Pérez, ...]

$$n(\boldsymbol{R}, \boldsymbol{r}) \simeq n(\boldsymbol{R})\Pi_0(rk_F) + \frac{\tau(\boldsymbol{R})}{k_F^2}\Pi_1(rk_F) + \frac{\nabla^2 n(\boldsymbol{R})}{k_F^2}\Pi_2(rk_F) + \cdots$$

$$n(\boldsymbol{R}) = n(\boldsymbol{R}, \boldsymbol{r})|_{r=0} = n(\boldsymbol{r_1}, \boldsymbol{r_2})|_{\boldsymbol{r_1}=\boldsymbol{r_1}} \qquad \textit{local density}$$

$$\tau(\boldsymbol{R}) = \nabla_{\boldsymbol{r_1}} \cdot \nabla_{\boldsymbol{r_2}} n(\boldsymbol{r_1}, \boldsymbol{r_2})|_{\boldsymbol{r_1}=\boldsymbol{r_1}} \qquad \textit{local kinetic density}$$

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Link with the Density Matrix Expansion

At second order in the gradient expansion of the one-body Green's function, the one-body density matrix reads ✗ technical

$$n(\boldsymbol{R},\boldsymbol{k}) = \int \frac{d\omega}{2\pi} G(\boldsymbol{R},\boldsymbol{k},\omega) = \underbrace{\theta(\mu - \rho(\boldsymbol{R},\boldsymbol{k}) - k^2)}_{infinite\ \ matter}$$

$$+ \underbrace{f_1(\rho)\delta'(\rho(\boldsymbol{R},\boldsymbol{k}) + k^2 - \mu) + f_2(\rho)\delta''(\rho(\boldsymbol{R},\boldsymbol{k}) + k^2 - \mu)}_{gradient\ \ corrections}$$

$f_1(\rho)$ and $f_2(\rho)$ are functions of the auxiliary fields ρ and its gradients
Local Fermi momentum $k_F(\boldsymbol{R})$ defined by $\mu - \rho(\boldsymbol{R}, k_F(\boldsymbol{R})) - k_F(\boldsymbol{R})^2 = 0$

Taking the inverse Wigner transform $(\boldsymbol{R},\boldsymbol{k}) \to (\boldsymbol{R},\boldsymbol{r})$ ✗ technical

$$n(\boldsymbol{R},\boldsymbol{r}) = \frac{k_F^3}{6\pi^2}\frac{3j_1(rk_F)}{rk_F} + \left[\frac{\tau(\boldsymbol{R})}{k_F^2} - \frac{3}{5}\frac{k_F^3}{6\pi^2} - \frac{\nabla^2 n(\boldsymbol{R})}{4k_F^2}\right]\mathcal{B}_\theta^\tau(rk_F)$$
$$+ \left[n(\boldsymbol{R}) - \frac{k_F^3}{6\pi^2}\right]\mathcal{B}_\theta^0(rk_F) + \frac{k_F^3}{6\pi^2}\left[\frac{\nabla^2 m^\star(\boldsymbol{R})}{k_F^2 m^\star(\boldsymbol{R})} - \frac{(\nabla m^\star(\boldsymbol{R}))^2}{2k_F^2 m^\star(\boldsymbol{R})}\right]\mathcal{B}_\theta^\star(rk_F)$$

- ✓ non-local contribution factorized (very similar but not identical to the DME)
- ✓ local Fermi-momentum $k_F \equiv k_F(\boldsymbol{R})$ and local [kinetic] density $n(\boldsymbol{R})$ $[\tau(\boldsymbol{R})]$
- ✓ angle $\widehat{\boldsymbol{R}} \cdot \widehat{\boldsymbol{r}} = \cos\theta$ (averaged in the DME at Hartree-Fock level)
- ✓ effective mass correction appears naturally (not present in the DME)

[cf. Landau theory of Fermi liquid]

$$\text{self-energy} \quad \sim \quad \frac{k^2}{2m} + \rho(\boldsymbol{R},\boldsymbol{k}) = \frac{k^2}{2m^\star(\boldsymbol{R},k_F)} + \mathcal{O}(k-k_F)^3$$

Towards Density Functional Theory

- Use the gradient expansion of the one-body density matrix, and integrate out the non-locality in the energy expression

$$\lim_{\beta\to\infty}\frac{\Omega_1}{\beta} = \lim_{\beta\to\infty}\frac{\Omega_0}{\beta} + \frac{1}{2}\mathrm{tr}(n_1 V_{12} n_2)$$
$$= \sum_\sigma \int d\boldsymbol{R}\left\{\frac{\tau(\boldsymbol{R})}{2m^\star(\boldsymbol{R},k_F)} + n(\boldsymbol{R})\Gamma[n(\boldsymbol{R})]\right\}$$

- Leads to the self-consistent Kohn-Sham equations

$$\left\{-\nabla\frac{1}{2m^\star(\boldsymbol{R},k_F)}\cdot\nabla + U[n(\boldsymbol{R}),\tau(\boldsymbol{R})]\right\}\phi_i(\boldsymbol{R}) = \epsilon_i\phi_i(\boldsymbol{R})$$

$$U[n,\tau] = \tau\frac{\delta}{\delta n}\frac{1}{2m^\star} + \frac{\delta}{\delta n}(n\Gamma[n]) \qquad n(\boldsymbol{R}) = \sum|\phi_i(\boldsymbol{R})|^2 \qquad \tau(\boldsymbol{R}) = \sum|\nabla\phi_i(\boldsymbol{R})|^2$$

[Lipparini book's] [Boulet & Lacroix, J. Phys. G **46**, (2019)]

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$$= \sum_\sigma \int d\boldsymbol{R}\left\{\frac{\tau(\boldsymbol{R})}{2m^\star(\boldsymbol{R}, k_F)} + n(\boldsymbol{R})\Gamma[n(\boldsymbol{R})]\right\}$$

- Leads to the self-consistent Kohn-Sham equations

$$\left\{-\nabla\frac{1}{2m^\star(\boldsymbol{R}, k_F)}\cdot\nabla + U[n(\boldsymbol{R}), \tau(\boldsymbol{R})]\right\}\phi_i(\boldsymbol{R}) = \epsilon_i\phi_i(\boldsymbol{R})$$

$$U[n,\tau] = \tau\frac{\delta}{\delta n}\frac{1}{2m^\star} + \frac{\delta}{\delta n}(n\Gamma[n]) \qquad n(\boldsymbol{R}) = \sum|\phi_i(\boldsymbol{R})|^2 \qquad \tau(\boldsymbol{R}) = \sum|\nabla\phi_i(\boldsymbol{R})|^2$$

[Lipparini book's] [Boulet & Lacroix, J. Phys. G **46**, (2019)]

Perspectives

Summary and critical discussion

- **Extension of the Variational Perturbation Theory**
  - include auxiliary fields related to the collective d.o.f. of interest
  - perform perturbative approach of the effective action according to the reference partition function
  - apply the variational principle and Wick contractions to get physical observable
- **Gradient expansion of the one-body Green's functions**
  - ✓ direct connection with the density matrix expansion
- Neutron drops with a semi-realistic Hamiltonian compared to other perturbative treatments and to *ab-initio* results

Provide a systematic and constructive approach for Density Functional Theory beyond mean field including pairing from first principle but:

- ✗ Very technical even for simple model
- ✗ Explosion of the number of many-body diagrams

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