Towards Density Functional Calculations from Nuclear Forces

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Abstract

We propose a method for microscopic calculations of nuclear ground-state properties in the framework of density functional theory (DFT). We discuss how the density functional is equivalent to the effective action for the density, thereby establishing a constructive framework for DFT calculations from nuclear forces. The presented approach starts from non-interacting nucleons in a background potential (a simple approximation for the mean field). The nuclear forces are then gradually turned on, while the background potential is removed. The evolution equation yields the ground-state energy and density of a system of interacting nucleons, including exchange-correlations beyond the RPA approximation. The method can start from non-local low momentum ($V_{\text{low}k}$) or chiral interactions.

1 Introduction

Microscopic approaches to large nuclei are inherently difficult, since nucleons interact strongly and the number of possible configurations increases rapidly with the number of nucleons. As a consequence, for the largest nuclei the computational method of choice has been mean field theory. A promising framework to extend and systematize mean-field calculations is density functional theory (DFT). DFT is the underlying theory in modern nuclear structure approaches to heavy nuclei, see e.g., [1-6].

In this talk, we discuss an approach complementary to parameterizing the nuclear density functional. We present a DFT method to calculate nuclear ground-state properties from microscopic two-nucleon and few-nucleon forces. In a DFT framework, the dynamic degrees of freedom are one-body densities, which simplify a microscopic description for larger systems and are computationally feasible compared to solving for the many-body wave function. In
addition, DFT can start from the softer low momentum \((V_{\text{low}} k)\) or chiral interactions [7-13], which are non-local. This is particularly important as the effective field theory approach offers at present the only consistent and practical counting scheme to construct three-nucleon forces. We start by showing that the effective action formalism provides a microscopic foundation for DFT. We focus especially on how exchange-correlations are included. A direct calculation of the effective action for non-interacting fermions shows possible expansions of the density functional when interactions are included. We then present a functional RG-inspired method to calculate nuclear ground-state properties from microscopic interactions and discuss possible extensions.

2 Effective action formalism and DFT

We consider non-relativistic fermions in a time-independent background potential \(V(x)\) (e.g., the ionic potential for electronic systems; for nuclei, \(V = 0\)) interacting through two-body forces \(U(x, y)\). We note that three-body interactions can be easily included and for simplicity we also suppress isospin indices. The action \(S\) consists of a one-body \(S_1\) and an interacting two-body part \(S_2\) (in Euclidean space-time with spin indices \(\sigma\) and \(\hbar = 1\))

\[
S[\psi^\dagger, \psi] = S_1[\psi^\dagger, \psi] + S_2[\psi^\dagger, \psi] = \sum_{\sigma} \int dx \psi_\sigma^\dagger(x) \left[ \partial_t - \frac{1}{2m} \nabla_\sigma^2 + V_\sigma(x) \right] \psi_\sigma(x) + \frac{1}{2} \sum_{\sigma_1, \sigma_1'} \int dx \, dy \, dt \, \psi_{\sigma_1}^\dagger(x, t) \psi_{\sigma_1'}(x, t) \psi_{\sigma_2}^\dagger(y, t) \psi_{\sigma_2'}(y, t).
\]

(1)

The generating functional \(W[K]\) for connected density correlation functions is given by a path integral over all configurations

\[
e^{W[K]} = \int D[\psi^\dagger] D[\psi] \, e^{-S[\psi^\dagger, \psi] + (\psi^\dagger \psi) \cdot K},
\]

(2)

where we have introduced spin-dependent sources \(K_{\sigma, \sigma'}(x)\) coupled to the possible density operators \(\psi_{\sigma_1}^\dagger(x) \psi_{\sigma_2'}(x)\). The strategy for introducing the source term is (loosely) analogous to the calculation of the magnetization of spins on

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1For simplicity, we introduce the short-hand notation \(\psi^\dagger \cdot \psi \equiv \sum_\sigma \int dx \, \psi_\sigma^\dagger(x) \psi_\sigma(x)\) or \((\psi^\dagger \psi) \cdot M \equiv \sum_{\sigma, \sigma'} \int dx \, \psi_\sigma^\dagger(x) \psi_{\sigma'}(x) M_{\sigma, \sigma'}(x)\). This allows to rewrite the action in compact form \(S_1[\psi^\dagger, \psi] = \psi^\dagger \cdot G^{-1} \cdot \psi\) and \(S_2[\psi^\dagger, \psi] \equiv \frac{1}{2} (\psi^\dagger \psi) \cdot U \cdot (\psi^\dagger \psi)\), where the free propagator \(G\) includes the background potential \(V\).
a lattice. For spin systems, one introduces a magnetic source $H$ coupled to the total spin of the system, $H \sum_i S_i$. The variation of the source $H$ then probes all different configurations and allows one to determine the spin configuration, i.e., the magnetization, which minimizes the free energy. For ground-state properties of many-body system, the source is coupled to the density operator and variations probe different density profiles. Thus, by varying the generating functional $W[K]$ with respect to the source $K$ one obtains the density $\rho_{\sigma,\sigma'}(x)$ in the presence of the source (and the ground-state density for $K = 0$)

$$\rho_{\sigma,\sigma'}(x) \equiv \langle \psi_\sigma^+(x) \psi_{\sigma'}(x) \rangle_K = \frac{\delta W[K]}{\delta K_{\sigma,\sigma'}(x)}. \quad (3)$$

Assuming that Eq. (3) is invertible, it can be used to express the source in terms of the density $K[\rho]$, and one can perform a functional Legendre transformation from $W[K]$ to the effective action $\Gamma[\rho]$ given by

$$\Gamma[\rho] = -W[K] + K \cdot \rho. \quad (4)$$

The effective action has the advantageous property that it is minimal at the physical (zero source) ground-state density $\rho = \rho_{gs}$

$$\left. \frac{\delta \Gamma[\rho]}{\delta \rho} \right|_{\rho=\rho_{gs}} = 0. \quad (5)$$

Moreover, the effective action at the minimum yields the ground-state energy of the system $E_{gs}$. This follows from the spectral representation of the path integral $e^W = \sum_n e^{-\beta E_n}$ and for $K = 0$ one has in the zero temperature limit

$$E_{gs} = E[\rho_{gs}] = \lim_{\beta \to \infty} \frac{1}{\beta} \Gamma[\rho_{gs}]. \quad (6)$$

Summarizing, the effective action is a functional of the density which is minimal at the ground-state density and reproduces the energy. Therefore, the effective action for the density is equivalent to the energy density functional in the sense of Hohenberg-Kohn [14] (more precisely for time-independent sources). This has been pointed out in the literature, see e.g., recently [15-18].

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2 Two more comments are in order. First, a chemical potential corresponds to a constant source, which requires some attention in the calculation of the effective action and leads to a minimum condition $\frac{\delta \Gamma[\rho]}{\delta \rho}|_{\rho=\rho_{gs}} = \mu$ for homogeneous systems, since the source and the chemical potential cannot be distinguished. Second, while the densities are to be expanded in a set of orbitals, $\rho_{gs}(x) = \sum_n c_n |\phi_n(x)|^2$, density fluctuations such as $\rho(x) - \rho_{gs}(x)$ must be expanded in a set of basis functions whose integral vanishes.
of the effective action formalism is that it presents a constructive framework for microscopic calculations of the density functional. For completeness, we further prove the Hohenberg-Kohn universality (i.e., the trivial $V$ dependence) of the density functional. This simply follows by noticing that the one-body potential $V$ enters in the many-body dynamics in the same way as the external source $K$. Therefore, the dependence of the generating functional $W[K]$ on $V$ is linear, $W[K] = W_{V=0}[K - V]$ and the Legendre transformation gives

$$\Gamma[\rho] = -W[K] + K \cdot \rho = -W_{V=0}[K - V] + (K - V + V) \cdot \rho = \Gamma_{V=0}[\rho] + V \cdot \rho,$$

where $\tilde{K} = K - V$ is taken as source for the Legendre transformation.

### 3 Non-interacting fermions

After discussing the microscopic basis of DFT using effective action techniques, we consider the non-interacting case. This provides insight into physical expansions of the effective action and how exchange-correlations will be included. In the non-interacting case, the generating functional is a Gaussian integral over the fermion fields and one has

$$W_{\text{free}}[K] = \text{Tr} \log[G^{-1} - K] = \text{Tr} \log G^{-1} - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} [(G \cdot K)^n].$$

The density in the presence of the source is given by $\delta W_{\text{free}}[K]/\delta K_{\sigma,\sigma'}(x)$,

$$\rho_{\sigma,\sigma'}(x) = -G_{\sigma',\sigma}(x,x) - \sum_{n=0}^{\infty} G_{\sigma',\ldots}(x,\ldots) \cdot K \cdot (G \cdot K)^n \cdot G_{\ldots,\sigma}(\ldots, x),$$

where the source is diagonal in the space-time index $x$ and summed over indices are indicated by $\ldots$. For $K = 0$, we have the familiar expression for the ground-state density, $\rho_{g;\sigma,\sigma'}(x) = -G_{\sigma',\sigma}(x,x)$. A second variation of the generating functional yields the particle-hole propagator $\tilde{G}$ (or density-density correlator). From Eq. (9), we find for vanishing source in the ground state

$$\tilde{G}_{X,Y} \equiv \tilde{G}_{(\sigma_1,\sigma'_1,x),(\sigma_2,\sigma'_2,y)} = \left. \frac{\delta^2 W_{\text{free}}}{\delta K_{\sigma_2,\sigma'_2}(y) \delta K_{\sigma_1,\sigma'_1}(x)} \right|_{K=0} = \langle \psi_{\sigma_1}^\dagger(x) \psi_{\sigma'_1}(x) \psi_{\sigma'_2}(y) \psi_{\sigma_2}^\dagger(y) \rangle = -G_{\sigma'_1,\sigma_2}(x,y) G_{\sigma'_2,\sigma_1}(y,x),$$

where we have introduced a combined index $X = (\sigma_1,\sigma'_1, x)$. It is important to realize that the second functional derivatives of the generating functional and
the effective action are related (as for thermodynamic potentials conjugate by a Legendre transformation). Thus, one has
\[
\left( \frac{\delta^2 \Gamma[\rho]}{\delta \rho_X \delta \rho_Y} \right)^{-1} = \frac{\delta^2 W[K]}{\delta K_X \delta K_Y}.
\] (11)

Eq. (11) relates the dressed particle-hole propagator (for the interacting system) to the curvature of the effective action in the ground state. We will later see that all exchange-correlations are built up in this way.

For the Legendre transformation, we need the inverse expression to Eq. (9), i.e., the source as a function of density. By rewriting Eq. (9) in compact form
\[
\rho_X = \rho_{gs,X} + \tilde{G}_{X\ldots} \cdot K_\ldots + \mathcal{O}(K^2),
\] (12)

it is clear that the source $K$, and thus the generating functional $W[K]$ can be expanded in a power series in $\rho - \rho_{gs}$ around the ground-state density. For the source, one similarly has
\[
K_X = -\tilde{G}_{X\ldots}^{-1} \cdot (\rho - \rho_{gs})_\ldots + \mathcal{O}((\rho - \rho_{gs})^2).
\] (13)

We can now perform the Legendre transformation order-by-order, where the effective action has the same expansion around the ground-state
\[
\Gamma_{\text{free}}[\rho] = \Gamma^{(0)}_{\text{free}} + \sum_{n=2}^{\infty} \int_{X_1,\ldots,X_n} \frac{1}{n!} \Gamma^{(n)}_{\text{free};X_1,\ldots,X_n} (\rho - \rho_{gs})_{X_1} \cdots (\rho - \rho_{gs,\lambda})_{X_n},
\] (14)

with ground-state energy $E_{gs} = \lim_{\beta \to \infty} \Gamma^{(0)}_{\text{free}}/\beta$. Moreover, by keeping the $X$-dependence of the expansion coefficients, no local density approximation has been made. A straightforward calculation of the expansion coefficients yields
\[
\Gamma^{(0)}_{\text{free}} = -\text{Tr} \log \tilde{G}^{-1},
\] (15)
\[
\Gamma^{(2)}_{\text{free};X,Y} = \tilde{G}_{X,Y}^{-1},
\] (16)
\[
\Gamma^{(3)}_{\text{free};X_1,X_2,X_3} = 2 \int_{Y_1,Y_2,Y_3} S^{(3)}_{Y_1,Y_2,Y_3} \tilde{G}_{Y_1,X_1}^{-1} \tilde{G}_{Y_2,X_2}^{-1} \tilde{G}_{Y_3,X_3}^{-1},
\] (17)

where $S^{(3)}$ denotes the totally symmetric 3-propagator ring
\[
S^{(3)}_{X_1,X_2,X_3} = \frac{1}{3!} \left( G_{\sigma_1',\sigma_2'}(x_1, x_2) G_{\sigma_2',\sigma_3'}(x_2, x_3) G_{\sigma_3',\sigma_1'}(x_3, x_1) + \text{permutations} \right).
\] (18)

Higher-order expansion coefficients have a similar structure as $\Gamma^{(3)}$. With the expansion around the ground state, we next present a method that includes the interactions among nucleons in a non-perturbative manner. It is reminiscent of the quasiparticle picture and the adiabatic turning on of the interaction.
4 Evolution equation for the density functional

We are interested in solving for the ground-state properties of the physical system, where the nucleons interact by means of the microscopic interactions, without the presence of a background potential. To this end, we introduce a control parameter $\lambda$, with $0 \leq \lambda \leq 1$, by replacing

$$V \rightarrow (1 - \lambda)V_\lambda \quad U \rightarrow \lambda U,$$

where we allow the background potential $V$ to depend on $\lambda$, as long as the corresponding eigenfunctions are localized and physically reasonable. At $\lambda = 0$, when the two- and higher-body interactions are absent, the system is trivially bound by employing an attractive background potential (a simple guess for the mean field). The nucleons fill up the lowest-lying states to the Fermi energy. (Generally, the initial background potential should be chosen to improve the convergence of the presented algorithm.) For $\lambda = 1$, we have the physical system, where the background potential is switched off. We use the control parameter to evolve a simple shell-model configuration to the fully-interacting system including many configurations. This is depicted in Fig. 1. We note that such an RG-inspired method does not require the coupling strength to be small. The smallness of the interaction in perturbation theory is taken over by the differential change, $\delta \lambda$ serving as a “small parameter”.

Figure 1: A graphical illustration of the initial condition of the evolution equation (left figure) and the final, physical system of nucleons (right figure). The evolution equation interpolates between the two cases.

As the control parameter is gradually increased from $\lambda = 0$ to $\lambda = 1$, the density functional follows an evolution equation given by [19]

$$\partial_\lambda \Gamma_\lambda[\rho] = -\partial_\lambda W_\lambda[K] = \partial_\lambda[(1 - \lambda)V_\lambda]\cdot \rho + \frac{1}{2} \rho \cdot U \cdot \rho + \frac{1}{2} \text{Tr} \left[U \cdot \left( \frac{\delta^2 \Gamma_\lambda[\rho]}{\delta \rho \delta \rho} \right)^{-1} \right],$$

(20)
where the derivation is similar to [17]. Since Eq. (20) is exact, the solution for general density configurations is cumbersome and is not directly related to physical quantities. Therefore, we propose to solve the evolution equation only in the vicinity of the physical point, i.e., expanded around the evolving ground-state density \( \rho_{gs,\lambda} \). Before we discuss further details of the approach, we separate off the background and Hartree contributions to the density functional, since their density dependence is known exactly. Thus, we introduce the kinetic and exchange-correlation part \( \tilde{\Gamma}^{\lambda}[\rho] \) of the density functional through

\[
\Gamma^{\lambda}_{\rho} = (1 - \lambda)V_{\lambda} \cdot \rho + \frac{\lambda}{2} \rho \cdot U \cdot \rho + \tilde{\Gamma}^{\lambda}[\rho],
\]

which leads to a simplified evolution equation for \( \tilde{\Gamma}^{\lambda}[\rho] \)

\[
\partial_{\lambda} \tilde{\Gamma}^{\lambda}[\rho] = \frac{1}{2} \text{Tr} \left[ U \cdot \left( \frac{\delta^2 \tilde{\Gamma}^{\lambda}[\rho]}{\delta \rho \delta \rho} + \lambda U \right)^{-1} \right]. 
\]

As the ground-state density changes under the RG, we expand the effective action around the current ground state \( \rho_{gs,\lambda} \) of the evolving system. This is the underlying theme and efficacy of our RG-inspired approach. As in the non-interacting case, we have

\[
\tilde{\Gamma}^{\lambda}[\rho] = \tilde{\Gamma}^{(0)}^{\lambda} + \sum_{n=1}^{N_{\Gamma}} \int_{X_1,\ldots,X_n} \frac{1}{n!} \tilde{\Gamma}^{(n)}_{\lambda;X_1,\ldots,X_n} \cdot (\rho - \rho_{gs,\lambda})_{X_1} \cdots (\rho - \rho_{gs,\lambda})_{X_n}.
\]

We make the approximation and truncate the expansion for \( \tilde{\Gamma}^{\lambda} \) at a given order \( N_{\Gamma} \) in density fluctuations. Since one expects five- and higher-body correlations to be relatively small, due to the Pauli principle, a truncation at \( N_{\Gamma} = 3 \) or \( N_{\Gamma} = 4 \) seems a reasonable choice. Obviously, the convergence of such an expansion must be checked by including higher-order contributions. (We note that, as for the Fermi liquid RG approach used in [20, 21], the flow equation generates upon integration an infinite set of diagrams in the underlying two-body interaction \( U \).

The truncation of the evolution equation at three-density correlations, \( N_{\Gamma} = 3 \), leads to coupled RG-like equations for the expansion coefficients, i.e., for the kinetic and exchange-correlation (kxc) energy \( E_{\text{kxc}} \), the evolving ground-state density, the dressed particle-hole propagator \( \tilde{G}^{\lambda} = (\tilde{\Gamma}^{(2)}_{\lambda} + \lambda U)^{-1} \) and the three-density correlator \( \tilde{\Gamma}^{(3)}_{\lambda} \). To provide further insight, we focus on
the flow equation for the ground-state energy and density, given by [10]

\[ \beta \partial_\lambda E_{\text{kxc}}[\rho_{\text{gs}},\lambda] \equiv \partial_\lambda \tilde{\Gamma}^{(0)}_\lambda = -(1-\lambda)V_\lambda \cdot \partial_\lambda \rho_{\text{gs}},\lambda - \lambda \rho_{\text{gs}},\lambda \cdot U \cdot \partial_\lambda \rho_{\text{gs}},\lambda + \frac{1}{2} \text{Tr} \left[U \cdot \tilde{G}_\lambda\right], \]  

(24)

Here, the contributions are due to the change in the ground-state density (first and second terms in Eq. (24)) and due to the dressed particle-hole propagator \( \tilde{G}_\lambda \) (last term). The flow equation is shown diagrammatically in Fig. 2. The last term in Eq. (24) explicitly reads \( \text{Tr} \left[U \cdot \tilde{G}_\lambda\right] \equiv \int_{Y_1,Y_2} U_{Y_1,Y_2} \tilde{G}_{\lambda,Y_2,Y_1} \), and thus to lowest order is the Fock contribution to the energy. This establishes that all exchange-correlations are built in through the dressed particle-hole propagator \( \tilde{G}_\lambda \). (Obviously, such a theory with densities as variables is not mean-field theory.) Moreover, we note that one recovers the standard RPA approximation when only \( \tilde{G}_\lambda \) is maintained, i.e., \( N_T = 2 \) for the effective action. The flow equation for the ground-state density is given by

\[ \partial_\lambda \rho_{\text{gs}},\lambda;X = -\partial_\lambda \left[(1-\lambda) V_\lambda \cdot \tilde{G}_{\lambda;X} - \rho_{\text{gs}},\lambda \cdot U \cdot \tilde{G}_{\lambda;X}\right] + \frac{1}{2} \text{Tr} \left[U \cdot \tilde{G}_\lambda \cdot \left(\tilde{\Gamma}^{(3)}_\lambda \cdot \tilde{G}_{\lambda;X}\right) \cdot \tilde{G}_\lambda\right], \]  

(25)

where the expansion coefficients are totally symmetric and the indices not written explicitly are traced over. In the first iteration of the flow equation, \( \tilde{\Gamma}^{(3)} \) is given by the 3-propagator ring with three inverse density-density correlators, which cancel with the three \( G \) in the last term of Eq. (25). The remaining exchange contributions from the 3-propagator ring \( \text{Tr} \left[U \cdot S^{(3)}_{\lambda;X}\right] \) will lead to a quasiparticle-like distribution over the initially unoccupied orbitals.

Figure 2: Graphical representation of the RG-like equation for the ground-state energy \( E_{\text{kxc}} \), the ground-state density \( \rho_{\text{gs}},\lambda \) and the density-density correlator \( \tilde{G}_\lambda \) are denoted by a blob with \( n = 0, 1, 2 \) dots respectively, which label the index structure. \( (1-\lambda)V_\lambda \) is represented by a wiggly line and the two-body interaction \( U \) by a dashed line. Open dots further label open indices, and filled dots represent indices which are traced over.
5 Conclusions and extensions

In summary, the effective action formalism is a constructive framework for the density functional. It allows for calculations of ground-state properties starting from microscopic two- and three-nucleon interactions, which can be non-local such as the soft low momentum (\(V_{\text{low}k}\)) or chiral interactions [7-13]. The main advantage of DFT lies in using densities as degrees of freedom, as compared to many-body wave functions. As a consequence, microscopic DFT approaches should scale well to larger nuclei. There is some insight from electronic systems, where DFT (see e.g., [22]) and the coupled cluster method give overall good results for ground-state properties in larger systems.

We believe that the presented DFT approach may be a step towards the derivation of nuclear structure of heavier systems from nuclear forces. We are currently working on the feasibility of this approach for strongly-interacting one-dimensional models [19]. Systematic, microscopic approaches are particularly important for extrapolations to neutron/proton-rich systems, e.g., due to the constraints on the isospin dependence from nuclear forces or to maintain a complete basis of induced non-central interactions [23].

Extensions of this method are under investigation. A projection on vanishing center-of-mass kinetic energy can be implemented by introducing sources for the center-of-mass motion. The harmonic oscillator frequency of the background potential can be adapted under the evolution to improve the convergence (reflecting the variational character of the single-particle basis). Explicit pairing correlations can be introduced by coupling a source to the off-diagonal densities \(\psi_\sigma(x)\psi_{\sigma'}(x)\) (and the Hermitian conjugate). The additional minimum condition of the effective action is then equivalent to the BCS gap equation.

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