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Functional renormalization group and Kohn–Sham scheme in density functional theory

Haozhao Liang (梁豪兆) [a,b,*], Yifei Niu (牛一斐) [c], Tetsuo Hatsuda (初田 哲男) [d,a]

[a] Nishina Center, RIKEN, Wako 351-0198, Japan
[b] Department of Physics, Graduate School of Science, The University of Tokyo, Tokyo 113-0033, Japan
[c] ELI-NP, "Horia Hulubei" National Institute for Physics and Nuclear Engineering, RO-077125 Bucharest-Magurele, Romania
[d] iTHEMS Program and iTHES Research Group, RIKEN, Wako 351-0198, Japan

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ABSTRACT

Deriving accurate energy density functional is one of the central problems in condensed matter physics, nuclear physics, and quantum chemistry. We propose a novel method to deduce the energy density functional by combining the idea of the functional renormalization group and the Kohn–Sham scheme in density functional theory. The key idea is to solve the renormalization group flow for the effective action decomposed into the mean-field part and the correlation part. Also, we propose a simple practical method to quantify the uncertainty associated with the truncation of the correlation part. By taking the φ^4 theory in zero dimension as a benchmark, we demonstrate that our method shows extremely fast convergence to the exact result even for the highly strong coupling regime.

1. Introduction

The density functional theory (DFT) [1,2] is a successful approach to reduce quantum many-body problem to one-body problem with the local density distribution $\rho(\mathbf{x})$. Due to its high accuracy with relatively low computational cost, DFT has great success in various fields including condensed matter physics, nuclear physics, and quantum chemistry. According to the Hohenberg–Kohn (HK) theorem [1], there exits an energy density functional of $\rho(\mathbf{x})$ as $E_U[\rho] = F_{\text{HK}}[\rho] + \int d^3\mathbf{x}\, U(\mathbf{x})\rho(\mathbf{x})$, where the universal functional $F_{\text{HK}}[\rho]$ is independent of the external potential $U(\mathbf{x})$. The ground-state energy of the system corresponds to a global minimum of $E_U[\rho]$. In DFT, deriving $F_{\text{HK}}[\rho]$ in a systematic and controllable way is the most important issue, see, e.g., the overviews [3–6], as well as recent topical reviews in condensed matter physics [7,8], nuclear physics [9,10], and quantum chemistry [11–13]. Also, the theoretical error estimates or uncertainty quantification is a key issue in modern DFT applications [14–17].

Another successful approach to quantum many-body problem is the functional renormalization group (FRG) [18]: It is based on the one-parameter flow equation which leads to the quantum effective action at the end of the flow, see, e.g., the review [19]. A close connection between the effective action $\Gamma[\rho]$ in FRG and the universal functional $F_{\text{HK}}[\rho]$ in DFT has been established on the basis of the two-particle point-irreducible (2PPI) scheme, which we call 2PPI-FRG, by Polonyi, Sailer, and Schwenk [20,21], so that FRG provides a practical way to construct $F_{\text{HK}}[\rho]$. The 2PPI-FRG was further developed in Refs. [22–24] with the case studies including the zero-dimensional (0-D) φ^4 theory, (0+1)-D anharmonic oscillator, and (1+1)-D Alexandrou–Negele nuclei. See also Ref. [25] for a comparative study. Although the 2PPI-FRG is a systematic formalism, the resultant accuracy in these case studies was found to be not so satisfactory: Up to the next-to-leading order, the ground-state energies of (1+1)-D nuclei missed by about 30% comparing to the Monte Carlo results [24]. Even for the simplest 0-D model [23], the ground-state energy still missed by about 2% with the sixth-order calculation for intermediate coupling strength. Note that the sixth-order calculations are almost infeasible for actual (3+1)-D problems, and even if it is achieved, the 2%-accuracy would not be good enough for practical applications of nuclear binding energies, not to mention the chemical accuracy.

The purpose of this Letter is twofold: First of all, we propose a novel optimization method of FRG in analogy with the Kohn–Sham (KS) scheme in DFT, which we call KS-FRG. The convergence of the energy density functional in KS-FRG is shown to be much faster than the un-optimized scheme. Secondly, we propose a method to estimate the truncation uncertainty in the KS-FRG. By taking the 0-D φ^4 theory as an example, we demonstrate explicitly that these methods work well in practice.

* Corresponding author.
E-mail addresses: haozhao.liang@riken.jp (H.Z. Liang), yifei.niu@eli-np.ro (Y.F. Niu), thatsuda@riken.jp (T. Hatsuda).

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2. Formalism

Let us consider a general non-relativistic system with a two-body interaction $V(\mathbf{x}_1, \mathbf{x}_2)$. The bare action S in the Euclidean space reads

$$S[U,V] = \int \psi^\dagger(x)\,(\partial_\tau + K + U(\mathbf{x}) - \mu)\,\psi(x) + \frac{1}{2}\iint \psi^\dagger(x_1)\psi^\dagger(x_2)V(\mathbf{x}_1,\mathbf{x}_2)\psi(x_2)\psi(x_1)\,, \tag{1}$$

with $x = (\tau, \mathbf{x})$, $\int = \int_0^\beta d\tau \int d^d\mathbf{x}$, d the space dimension, β the inverse temperature, μ the chemical potential, and $K = -\nabla^2/(2M)$. The external potential $U(\mathbf{x})$ vanishes for self-bound systems such as atomic nuclei, while it represents physical harmonic trap for ultracold atoms.

The generating functional of connected Green's functions is defined by

$$e^{W[J]} = \int \mathfrak{D}(\psi^\dagger\psi)\,\exp\{-S[U,V] + \int J(x)\psi^\dagger(x)\psi(x)\}\,, \tag{2}$$

where $J(x)$ is a local external source. The functional derivative of $W[J]$ with respect to J is nothing but the local density

$$\rho(x) = \langle\psi^\dagger(x)\psi(x)\rangle = \frac{\delta W[J]}{\delta J(x)}\,. \tag{3}$$

The 2PPI effective action is then defined as the Legendre transform,

$$\Gamma[\rho; U, V] = -W[J] + \int J(x)\rho(x)\,, \tag{4}$$

and the energy density functional at zero temperature is obtained by

$$E[\rho] = \lim_{\beta\to\infty}\frac{\Gamma[\rho]}{\beta}\,. \tag{5}$$

In the 2PPI-FRG formalism [20,21], a flow parameter $\lambda \in [0,1]$ is introduced to replace V by λV and U by a *given* regulator function U_λ with the boundary condition $U_{\lambda=1} = U$. Then the λ-dependent 2PPI effective action is defined by $\Gamma_\lambda[\rho] \equiv \Gamma[\rho; U_\lambda, \lambda V]$ whose renormalization group flow reads [21],

$$\partial_\lambda\Gamma_\lambda[\rho] = \rho\cdot\partial_\lambda U_\lambda + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}\mathrm{Tr}\left\{V\cdot\left(\Gamma^{(2)}_\lambda[\rho]\right)^{-1}\right\}\,. \tag{6}$$

Here the dots and trace imply $X\cdot Y = \int X(x)Y(x)$, $X\cdot A\cdot Y = \iint X(x)A(x,y)Y(y)$, and $\mathrm{Tr}\{A\cdot B\} = \iint A(x,y)B(y,x)$. The n-point vertex functions are obtained by

$$\Gamma^{(n)}_{\lambda;x_1,\ldots,x_n}[\rho] = \frac{\delta^n\Gamma_\lambda[\rho]}{\delta\rho(x_1)\ldots\delta\rho(x_n)}\,. \tag{7}$$

The ground-state density for a fixed λ denoted by $\bar\rho_\lambda$ is a solution of

$$\left.\frac{\delta\Gamma_\lambda[\rho]}{\delta\rho(x)}\right|_{\rho=\bar\rho_\lambda} = 0\,, \tag{8}$$

so that the effective action $\Gamma_\lambda[\rho]$ can be expanded around $\bar\rho_\lambda$ as

$$\Gamma_\lambda[\rho] = \Gamma^{(0)}_\lambda[\bar\rho_\lambda] + \frac{1}{2}\iint \Gamma^{(2)}_{\lambda;x_1,x_2}[\bar\rho_\lambda](\rho-\bar\rho_\lambda)_{x_1}(\rho-\bar\rho_\lambda)_{x_2} + \cdots \equiv \bar\Gamma^{(0)}_\lambda + \sum_{n=2}^{\infty}\frac{1}{n!}\int\bar\Gamma^{(n)}_\lambda\cdot(\rho-\bar\rho_\lambda)^n\,, \tag{9}$$

where $\bar\Gamma^{(n)}_\lambda \equiv \Gamma^{(n)}_\lambda[\bar\rho_\lambda]$. This power series expansion together with the flow equation (6) leads to an infinite hierarchy of coupled integro-differential equations for $\bar\Gamma^{(n)}_\lambda$ and $\bar\rho_\lambda$. As shown in some case studies, however, such a "naive" expansion converges rather slowly to the exact results [23,24].

Here we propose the KS-FRG which is a novel optimization theory of FRG with faster convergence under the same spirit with the KS scheme in DFT [2]. The basic idea is to introduce an effective action for a hypothetical non-interacting system with a mean-field KS potential $U_{\mathrm{KS},\lambda}(\mathbf{x})$ and to split the total effective action into the mean-field part $\Gamma_{\mathrm{KS},\lambda}$ and the correlation part γ_λ,

$$\Gamma_\lambda[\rho] = \Gamma_{\mathrm{KS},\lambda}[\rho] + \gamma_\lambda[\rho]\,, \tag{10}$$

with $\Gamma_{\mathrm{KS},\lambda}[\rho] \equiv \Gamma[\rho; U_{\mathrm{KS},\lambda}, 0]$. These two terms are determined simultaneously by solving the FRG flow equation together with the KS equation.

Explicit form of the self-consistent equation to obtain $\Gamma_{\mathrm{KS},\lambda}[\rho]$ through $U_{\mathrm{KS},\lambda}$ is

$$\left.\frac{\delta\Gamma_{\mathrm{KS},\lambda}[\rho]}{\delta\rho(x)}\right|_{\rho=\bar\rho_\lambda} = 0\,. \tag{11}$$

This implies that $\bar\rho_\lambda$ is a common stationary point for both $\Gamma_{\mathrm{KS},\lambda}[\rho]$ and $\Gamma_\lambda[\rho]$. Equation (11) is equivalent with the standard KS equation [2,9] written in terms of the single-particle wave functions, since it is nothing more than the one-body problem with $V = 0$. The flow equation for the correlation part is obtained from Eqs. (6)–(11) as

$$\partial_\lambda\gamma_\lambda[\rho] = \rho\cdot\left(\partial_\lambda U_\lambda + \bar\Gamma^{(2)}_{\mathrm{KS},\lambda}\cdot\partial_\lambda\bar\rho_\lambda\right) + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}\mathrm{Tr}\left\{V\cdot\left(\Gamma^{(2)}_{\mathrm{KS},\lambda}[\rho] + \gamma^{(2)}_\lambda[\rho]\right)^{-1}\right\}\,. \tag{12}$$

Here we have used the following chain rule,

$$\partial_\lambda\Gamma_{\mathrm{KS},\lambda} = \frac{\delta\Gamma_{\mathrm{KS},\lambda}}{\delta U_{\mathrm{KS},\lambda}}\cdot\frac{\delta U_{\mathrm{KS},\lambda}}{\delta\bar\rho_\lambda}\cdot\partial_\lambda\bar\rho_\lambda = -\rho\cdot\bar\Gamma^{(2)}_{\mathrm{KS},\lambda}\cdot\partial_\lambda\bar\rho_\lambda\,. \tag{13}$$

As seen from the first term in the right-hand side, the effective one-body term proportional to ρ is properly separated out. Note also that the choice $U_{\mathrm{KS},\lambda=0} = U_{\lambda=0}$ leads to the initial condition $\gamma_{\lambda=0}[\rho] = 0$.

Equations (10), (11), and (12) are the master equations in KS-FRG. To solve them in practice, we expand the correlation part $\gamma_\lambda[\rho]$ around $\bar\rho_\lambda$,

$$\gamma_\lambda[\rho] = \bar\gamma^{(0)}_\lambda + \sum_{n=2}^{\infty}\frac{1}{n!}\int\bar\gamma^{(n)}_\lambda\cdot(\rho-\bar\rho_\lambda)^n\,. \tag{14}$$

On the other hand, we do not introduce the expansion for the mean-field part in Eq. (10). This is in contrast to the case of 2PPI-FRG where the whole $\Gamma_\lambda[\rho]$ is expanded as a power series.

By expanding both sides of Eq. (12) in terms of a dimensionless power counting parameter $(\rho-\bar\rho_\lambda)/\bar\rho_\lambda$, we obtain a set of coupled integro-differential equations in the form of

$$\partial_\lambda\bar\gamma^{(n)}_\lambda = f^{(n)}\left[\bar\gamma^{(0)}_\lambda,\ldots,\bar\gamma^{(n)}_\lambda,\bar\gamma^{(n+1)}_\lambda,\bar\gamma^{(n+2)}_\lambda\right]\,, \tag{15}$$

where $n = 0, 1, 2, 3, \cdots$, and $\bar\gamma^{(1)}_\lambda \equiv 0$. Note that $f^{(n)}$ depends not only on $\bar\gamma^{(0,\ldots,n+2)}_\lambda$ but also on $\bar\Gamma^{(0,\ldots,n+2)}_{\mathrm{KS},\lambda}$ and $\partial_\lambda\bar\rho_\lambda$ originating from the expansion.

A closed set of equations for $\bar\gamma^{(0,\ldots,m)}_\lambda$ and $\bar\rho_\lambda$ is obtained from Eq. (15) under the m-th order truncation, $\bar\gamma^{(n\geq m+1)}_\lambda = 0$. In principle, the uncertainty of the m-th order solution can be checked by solving the $(m+1)$-th order equations. However, it is not always