Functional Renormalization Group and Kohn-Sham scheme in Density Functional Theory

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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 $\varphi^4$ 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.

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with $x = (\tau, \mathbf{x})$, $\int = \int_0^\beta d\tau \int d^d\mathbf{x}$, $d$ the space dimension, $\beta$ the inverse temperature, $\mu$ the chemical potential, and $K = -\nabla^2/2M$. The external potential $U(x)$ 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

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

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

$$\rho(x) = \langle \psi^\dagger(x)\psi(x) \rangle = \frac{\delta W[J]}{\delta J(x)}.$$  \hspace{1cm} (3)

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

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

and the energy density functional at zero temperature is obtained by

$$E[\rho] = \lim_{\beta \to \infty} \frac{\Gamma[\rho]}{\beta}.$$  \hspace{1cm} (5)

In the 2PPI-FRG formalism, a flow parameter $\lambda \in [0, 1]$ is introduced to replace $V$ by $\lambda V$ and $U$ by a given regulator function $U_\lambda$ with the boundary condition $U_{\lambda=1} = U$. Then the $\lambda$-dependent 2PPI effective action is defined by $\Gamma_\lambda[\rho] = \Gamma[\rho; U_\lambda, \lambda V]$ whose renormalization group flow reads \cite{2121},

$$\partial_\lambda \Gamma_\lambda[\rho] = \rho \cdot \partial_\lambda U_\lambda + \frac{1}{2} \rho \cdot V \cdot \rho + \frac{1}{2} \text{Tr} \left\{ V \cdot \left( \Gamma_\lambda^{(2)}[\rho] \right)^{-1} \right\}.$$  \hspace{1cm} (6)

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

$$\Gamma_\lambda^{(n)}[\rho_{x_1,\ldots,x_n}] = \frac{\delta^n \Gamma_\lambda[\rho]}{\delta \rho(x_1) \ldots \delta \rho(x_n)}.$$  \hspace{1cm} (7)

The ground-state density for a fixed $\lambda$ denoted by $\bar{\rho}_\lambda$ is a solution of

$$\left. \frac{\delta \Gamma_\lambda[\rho]}{\delta \rho(x)} \right|_{\rho = \bar{\rho}_\lambda} = 0,$$  \hspace{1cm} (8)

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

$$\Gamma_\lambda[\rho] = \Gamma_\lambda^{(0)}[\bar{\rho}_\lambda] + \frac{1}{2} \int \int \Gamma_\lambda^{(2)}[\bar{\rho}_\lambda](\rho - \bar{\rho}_\lambda)x_1(\rho - \bar{\rho}_\lambda)x_2 + \cdots$$

$$\equiv \Gamma_\lambda^{(0)} + \sum_{n=2}^\infty \frac{1}{n!} \int \Gamma_\lambda^{(n)} \cdot (\rho - \bar{\rho}_\lambda)^n,$$  \hspace{1cm} (9)

where $\Gamma_\lambda^{(n)} \equiv \Gamma_\lambda^{(n)}[\bar{\rho}_\lambda]$. This power series expansion together with the flow equation (6) leads to an infinite hierarchy of coupled integro-differential equations for $\Gamma_\lambda^{(n)}$ and $\bar{\rho}_\lambda$. As shown in some case studies, however, such a “naive” expansion converges rather slowly to the exact results \cite{2324}.

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 \cite{2}. The basic idea is to introduce an effective action for a hypothetical non-interacting system with a mean-field KS potential $U_{KS,\lambda}(x)$ and to split the total effective action into the mean-field part $\Gamma_{KS,\lambda}$ and the correlation part $\gamma_\lambda$,

$$\Gamma_\lambda[\rho] = \Gamma_{KS,\lambda}[\rho] + \gamma_\lambda[\rho],$$  \hspace{1cm} (10)

with $\Gamma_{KS,\lambda}[\rho] \equiv \Gamma[\rho; U_{KS,\lambda}, 0]$. 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 $\Gamma_{KS,\lambda}[\rho]$ through $U_{KS,\lambda}$ is

$$\left. \frac{\delta \Gamma_{KS,\lambda}[\rho]}{\delta \rho(x)} \right|_{\rho = \bar{\rho}_\lambda} = 0.$$  \hspace{1cm} (11)

This implies that $\bar{\rho}_\lambda$ is a common stationary point for both $\Gamma_{KS,\lambda}[\rho]$ and $\gamma_\lambda[\rho]$. Equation (11) is equivalent with the standard KS equation $\gamma_\lambda = 0$ 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

$$\partial_\lambda \gamma_\lambda[\rho] = \rho \cdot \left( \partial_\lambda U_\lambda + \Gamma_{KS,\lambda}^{(2)} \cdot \partial_\lambda \bar{\rho}_\lambda \right) + \frac{1}{2} \rho \cdot V \cdot \rho$$

$$+ \frac{1}{2} \text{Tr} \left\{ V \cdot \left( \Gamma_{KS,\lambda}^{(2)}[\rho] + \gamma_\lambda^{(2)}[\rho] \right)^{-1} \right\}.$$  \hspace{1cm} (12)

Here we have used the following chain rule,

$$\partial_\lambda \Gamma_{KS,\lambda} = \frac{\delta \Gamma_{KS,\lambda}}{\delta U_{KS,\lambda}} \delta U_{KS,\lambda} \cdot \partial_\lambda \bar{\rho}_\lambda = -\rho \cdot \Gamma_{KS,\lambda}^{(2)} \cdot \partial_\lambda \bar{\rho}_\lambda.$$  \hspace{1cm} (13)

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

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 $\bar{\rho}_\lambda$,

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

On the other hand, we do not introduce the expansion for the mean-field part in Eq. (11). This is in contrast to the case of 2PPI-FRG where the whole $\Gamma_\lambda[\rho]$ is expanded as a power series.
Here we introduce a simple uncertainty estimate by going higher orders in physical systems, so that a practical 0th-order flow equations to obtain updated γ and ∂γ /∂ρ originating from the expansion.

A closed set of equations for Gm,Gn are obtained from Eq. (13) under the m-th order truncation, γm,n+1 = 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 possible to go higher orders in physical systems, so that a practical method of uncertainty quantification would be desirable. Here we introduce a simple uncertainty estimate by taking only a first iteration of solving the (m+1)-th order equations. First, we insert the m-th order results into the flow equation for γm+1. Then we obtain an approximate solution, γm+1,appr. We plug this into the m-th order flow equations to obtain updated m-th order solutions. The difference from the original ones is an uncertainty measure. We will discuss an actual procedure to assign error bars to γm,n by using a simple model below.

0-D $\varphi^4$ theory.—Let us now demonstrate how the KS-FRG works for obtaining energy functional in a simple 0-D bosonic model with the classical action,

$$S[\varphi] = \frac{1}{2} \omega^2 \varphi^2 + \frac{1}{4!} v \varphi^4.$$  

Its generating function is just obtained by an ordinary integral

$$e^{W[\varphi]} = \sqrt{\frac{\omega^2}{2\pi}} \int_{-\infty}^{\infty} d\varphi \exp \left( -S[\varphi] + J\varphi^2 \right).$$  

The exact solutions for the ground-state energy $E_{gs}$ and the density $\rho_{gs} = \langle \varphi^2 \rangle$ are known to be written in terms of the modified Bessel functions $\bar{\Gamma}$. By taking $U_{KS,\lambda} = (\omega_{KS,\lambda})^2/2$ with $\bar{\omega}_{KS,\lambda=0} = \omega$, the mean-field part of the effective action becomes

$$\Gamma_{KS,\lambda}[\rho] = \frac{1}{2} \left[ -\ln(\omega^2 \rho) - 1 + (\bar{\omega}_{KS,\lambda})^2 \right].$$  

In this case, Eq. (14) can be solved analytically to obtain $\bar{\rho}_\lambda = (1/\omega_{KS,\lambda})^2$. On the other hand, the flow equation (12) for the correlation part reads

$$\partial_\lambda \gamma_\lambda[\rho] = \rho \bar{\Gamma}^{(2)}_{KS,\lambda}[\bar{\rho}_\lambda + \frac{v}{4!} \rho^2 + (\bar{\Gamma}^{(2)}_{KS,\lambda}[\rho] + \gamma_\lambda^{(2)}[\rho])^{-1}].$$  

Combining Eqs. (13) and (14), the ground-state energy of the system becomes

$$E_{gs} = \left[ -\frac{1}{2} \ln(\omega^2 \bar{\rho}_\lambda) + \gamma_\lambda^{(0)} \right]_{\lambda=1}.$$  

Here $\bar{\rho}_\lambda$ and $\gamma_\lambda^{(0)}$ are obtained by solving the flow equation (14) up to a certain order. For example, the equations up to $n = 4$ are

$$\begin{align*}
\partial_\lambda \gamma_\lambda^{(0)} &= \frac{v}{4!} \left( \bar{\rho}_\lambda^2 + \bar{G}_\lambda \right) + \frac{1}{2 \bar{\rho}_\lambda} (\partial_\lambda \bar{\rho}_\lambda), \\
0 &= \frac{v}{4!} \left( 2 \bar{\rho}_\lambda \bar{G}_\lambda - \bar{\Gamma}^{(3)}_\lambda (\bar{G}_\lambda)^3 \right) + \partial_\lambda \bar{\rho}_\lambda, \\
\partial_\lambda \gamma_\lambda^{(2)} &= \frac{v}{4!} \left( 2 - \bar{\Gamma}^{(4)}_\lambda (\bar{G}_\lambda)^2 + 2 (\bar{\Gamma}^{(2)}_\lambda)^2 (\bar{G}_\lambda)^3 \right) + \bar{\gamma}_\lambda^{(3)} (\partial_\lambda \bar{\rho}_\lambda), \\
\partial_\lambda \gamma_\lambda^{(3)} &= \frac{v}{4!} \left( \bar{G}_\lambda^4 - 6 \bar{\Gamma}^{(5)}_\lambda (\bar{G}_\lambda)^4 - 6 (\bar{\Gamma}^{(3)}_\lambda)^3 (\bar{G}_\lambda)^4 \right) + \bar{\gamma}_\lambda^{(4)} (\partial_\lambda \bar{\rho}_\lambda), \\
\partial_\lambda \gamma_\lambda^{(4)} &= \frac{v}{4!} \left( -\bar{G}_\lambda^4 + 8 \bar{\Gamma}^{(5)}_\lambda (\bar{G}_\lambda)^5 + 6(\bar{\Gamma}^{(4)}_\lambda)^2 (\bar{G}_\lambda)^5 - 36 (\bar{\Gamma}^{(3)}_\lambda)^4 (\bar{G}_\lambda)^5 \right) + \bar{\gamma}_\lambda^{(5)} (\partial_\lambda \bar{\rho}_\lambda). 
\end{align*}$$
where \( \Gamma^{(n)}_\lambda = \Gamma^{(n)}_{\text{KS},\lambda} + \bar{\zeta}^{(n)}_\lambda \) and \( G_\lambda \equiv (\bar{\Gamma}^{(2)}_{\text{KS},\lambda} + \bar{\gamma}^{(2)}_\lambda)^{-1} \), with initial conditions \( \bar{\rho}_\lambda = n = (1/\omega)^2 \) and \( \bar{\gamma}^{(n)}_\lambda = 0 \).

Let us now discuss the uncertainty quantification by taking the third-order truncation as an example. In this case, we first solve Eqs. (21a)–(21d) with \( \bar{\gamma}^{(n \geq 4)}_\lambda = 0 \). Then, the solutions \( \bar{\zeta}^{(0 \ldots 3)}_\lambda \) and \( \bar{\rho}_\lambda \) together with \( \bar{\gamma}^{(5,6)}_\lambda = 0 \) are used in the right-hand side of Eq. (21b) to obtain an approximate solution \( \bar{\zeta}^{(4)}_{\lambda,\text{app}} \). Next we introduce an ansatz \( g^{(4)}_\lambda \) that satisfies

\[
c_L g^{(4)}_\lambda \leq \bar{\zeta}^{(4)}_{\lambda,\text{app}} \leq c_U g^{(4)}_\lambda
\]

in the interval \( \lambda \in [0,1] \). Since we know \( \bar{\zeta}^{(4)}_{\lambda=0} = 0 \), we separate out the factor \( \lambda \) explicitly in the ansatz. The constants \( c_{L,U} \) are defined by

\[
c_L = \inf \lambda (\bar{\zeta}^{(4)}_{\lambda,\text{app}} / g^{(4)}_\lambda) \quad \text{and} \quad c_U = \sup \lambda (\bar{\zeta}^{(4)}_{\lambda,\text{app}} / g^{(4)}_\lambda) .
\]

Natural choice of the ansatz in the present model is \( g^{(n)}_\lambda = v \bar{\rho}^{2-n}_\lambda \) obtained by inspecting the \( v \) and \( \bar{\rho}_\lambda \) dependence of the right-hand sides of Eqs. (21) and (18). By substituting \( c_L g^{(4)}_\lambda, c_U g^{(4)}_\lambda \), and \( c_M g^{(4)}_\lambda \) with \( c_M \equiv \bar{\gamma}^{(4)}_{\lambda,\text{app}} / g^{(4)}_\lambda \) for \( \bar{\gamma}^{(4)}_\lambda \) in Eqs. (21a)–(21d), we end up with most probable solutions for \( \bar{\zeta}^{(0 \ldots 3)}_\lambda \) from \( c_M \) and their errors from \( c_{L,U} \). (In practice, we use \( 2c_{L,U} \) for conservative uncertainty estimates to take into account the effects from \( \bar{\gamma}^{(n \geq 6)}_\lambda \), guided by the idea of effective field theory that the effects from higher orders should not be larger than those from the leading orders.)

**Numerical results.**—We take three typical cases: a weak coupling \( (\omega, v) = (1,0.01) \), an intermediate coupling \( (\omega, v) = (1,1) \), and a strong coupling \( (\omega, v) = (1,100) \). The last case has barely been discussed before in FRG. The ground-state density \( \rho_{gs} = \bar{\rho}_{\lambda=1} \) and energy \( E_{gs} \) obtained by KS-FRG in the first-, second-, and third-order truncations are listed in Table 1 for the three cases. Corresponding effective actions \( \Gamma[\rho] \) as a function of \( \rho \) are shown in Fig. 1 with error bands at each order of truncation. The exact solutions are shown by the solid lines for comparison.

In the weak-coupling case, the accuracy for \( \rho_{gs} \) and \( E_{gs} \) in the first-order calculation are already at \( O(10^{-6}) \) and \( O(10^{-7}) \), respectively, as shown in Table 1. Also, \( \Gamma[\rho] \) in the first order is already on top of the exact solution in a very wide density range with invisible theoretical uncertainty as shown in Fig. 1(a).

In the intermediate-coupling case, an order of magnitude improvement of the accuracy of \( \rho_{gs} \) and \( E_{gs} \) is seen by increasing the order of truncation. The third-order calculation of \( E_{gs} \) reaches to \( O(10^{-4}) \) accuracy in KS-FRG as shown in Table 1. This is in contrast to the conventional FRG calculation which gives only \( O(10^{-2}) \) accuracy even with a 6th-order calculation. The rapid convergence and the rapid shrinking of the error in KS-FRG are also found for \( \Gamma[\rho] \) as shown in Fig. 1(b).

Even in the strong-coupling case, an order of magnitude improvement of the accuracy is achieved by increasing the order of truncation. The third-order results of \( \rho_{gs} \) and \( E_{gs} \) reach to \( O(10^{-2}) \) accuracy as shown in Table 1. The convergence of \( \Gamma[\rho] \) to the exact result is also seen clearly in Fig. 1(c).
the exact value is shown with the star.

\[ \lambda \] and 3rd-order KS-FRG calculations are shown as the square, diamond, and circle with the theoretical uncertainties, while the results by the 1st-, 2nd-, and 3rd-order KS-FRG calculations are shown by the green and blue bands, respectively.

**Summary.**—In this Letter, we have proposed a novel optimization method of FRG in analogy with the Kohn-Sham scheme of DFT. Essential idea of our method, called KS-FRG, is to separate the full effective action into the mean-field (KS) part and the correlation part at each flow parameter \( \lambda \). Then the KS equation for the mean field and the FRG flow equation for the correlation are solved self-consistently. In practice, the correlation part is expanded in Taylor series around the stationary point \( \bar{\rho}_\lambda \), controlled by the power counting \([\rho - \bar{\rho}_\lambda]/\bar{\rho}_\lambda]^m\). The speed of propagation depends on the strength of interaction.

Such a rapid convergence in our KS-FRG scheme, as also illustrated in Fig. 2 for the strong-coupling case, stems from the facts that significant part of \( \Gamma_\lambda[\rho] \) is already taken into account in the mean-field part \( \Gamma_{KS,\lambda}[\rho] \) which evolves with \( \lambda \), and the correlation part \( \gamma_{KS,\lambda}[\rho] \) can be treated well as small fluctuations around the mean-field part.

In Fig. 3 we show how the effective action \( \Gamma_\lambda[\rho] \) and its uncertainty in the strong-coupling case evolve under the FRG flow from the non-interacting system at \( \lambda = 0 \) to the fully interacting system at \( \lambda = 1 \). Due to the repulsive nature of the interaction, the effective action increases as \( \lambda \) increases. Also, the uncertainty grows as \( \lambda \) increases because of the truncation of the coupled flow equations. From Eq. (13) it is seen that the uncertainties in \( \gamma^{(n+1)}_{\lambda} \) and \( \gamma^{(n+2)}_{\lambda} \) propagate to \( \gamma^{(n)}_{\lambda} \) with the flow evolution. In such a way, the total truncation uncertainties in \( \Gamma_\lambda[\rho] \) propagate from high- and low-density regions towards the stationary point \( \bar{\rho}_\lambda \) controlled by the power counting \([\rho - \bar{\rho}_\lambda]/\bar{\rho}_\lambda]^m\).

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