An improved algorithm for the functional renormalization group and its application to the 2D Hubbard model

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Abstract. Among the methods that treat strongly correlated electron systems, the functional renormalization group (fRG) has a desirable feature that it can take account of the shape of the Fermi surface with a systematic inclusion of diagrams. Specifically, the temperature-flow fRG due to Honerkamp et al can be a powerful method. In this method, an even mesh (patch discretization in the Cartesian coordinates) in \( k \) space is desirable in general, but this has remained numerically difficult. To overcome the difficulty we have constructed a fast and stable algorithm, which becomes powerful at lower \( T \) or in the extended Hubbard model.

1. Introduction

Functional renormalization group[1-8] is a numerical method for treating strongly correlated electron systems, where we take account of unbiased inclusion of diagrams up to one-loop level within a rigorous framework of the quantum field theory. In practice, however, errors due to the angular patch discretization of the four-point coupling, and the static approximation (neglect of Matsubara frequencies) have been a problem. Here we have developed a fast and stable algorithm based on box discretization of the four-point coupling.[9] The algorithm has turned out to be (i) stable at lower temperatures, and powerful for treating the extended Hubbard model, and (ii) opens a way to go beyond the static approximation.

In the functional renormalization group a flow parameter depends on the quadratic term of the action but is independent on the interaction part of the action. Derivative of the generating functional with respect to the flow parameter gives the renormalization equation. We can obtain the correlation functions in strongly correlated systems by integrating the renormalization equation from the bare interaction regime.

Three different schemes have been proposed, each corresponding to a generating functional of different Green’s functions or vertex functions. These include Polchinski scheme[1,2], Wick-ordered scheme[3,4], and 1PI-scheme based on the one-particle irreducible vertex functions[5,6,7,8].
For the choice of the flow parameter aside from the standard momentum or energy cutoff, different choices have been proposed, among which are the interaction flow[7] and the temperature flow[8]. Temperature-flow renormalization group is based on the 1PI scheme. A way to overcome the problem of slow convergence in the momentum cutoff method was devised[8], in which temperature \( T \) is used as the flow parameter. In this method the RG equation for the four-point couplings, three-point vertex functions, and susceptibility are integrated from a sufficiently high temperature down to a low temperature to obtain susceptibilities in the strongly correlated regime. We adopt this choice of the flow-parameter in this paper.

2. **Patch discretization of the four-point coupling**

For numerical calculations, coupling constants must be discretized. Cartesian box discretization is preferable, since it can deal with general shapes of the Fermi surface, but is usually not employed because it requires huge CPU times. Here we have overcome the difficulty by developing a fast and stable algorithm for this discretization. The algorithm is accurate when the four-point coupling has a significant momentum dependence in the radial direction, such as lower \( T \), the extended Hubbard model or disconnected Fermi surfaces.

Fig. 1: Angular discretization (left and center panels) and the Cartesian box discretization (right) of the four-point coupling in \( k \)-space. The blue line denotes the Fermi surface.

3. **Improved algorithm for the \( T \)-flow renormalization group**

The RG equation for the four-point coupling is in the form of

\[
\frac{d}{dT}V_T(k_1, k_2, k_3) = -\int dk V_T(k_1, k_2, k) L(k, -k + k_1 + k_2) V_T(k, -k + k_1 + k_2, k_3) + \ldots, \quad (1)
\]

where \( V_T \) is the four-point coupling, \( k, k_1, k_2, k_3 \) are wave vectors, and

\[
L(k, k') = \frac{d}{dT}\left( \sum_n \frac{1}{i\omega_n - \varepsilon_k} \frac{1}{i\omega_n - \varepsilon_{k'}} \right)
\]

is the large-scale propagator.

Next, the wave vectors of the four-point couplings are discretized into \( n \otimes n \) patches. The right-hand side of eqn(1) can be written as

\[
\sum_i V_T(k_1, k_2, k_3) \left[ \int_i dk' L(k_i + k', -k_j - k_j + k_1 + k_2) \right] V(k_i, -k_j + k_1 + k_2, k_3), \text{ where } k \text{ is a wave vector, } k_i \text{ is a wave vector at the center of } i \text{ th patch, } k' = k - k_i, I = \left[ -\frac{\pi}{n}, \frac{\pi}{n} \right] \times \left[ -\frac{\pi}{n}, \frac{\pi}{n} \right].
\]
Fig. 2: Cartesian Box discretization.
We evaluate this quantity as follows:

\[ T_A(i,j) = \left( \int dk' L(p_i + k', p_j - k') \right) V(p_i, p_j, p_k). \]

step2: Evaluate \( \sum_i T_A(i,f(i,1,2))V(p_i, p_2, p_3) \), where \( l, m \) and \( n \) are integers

and \( f \) is defined as \( k_{f(l,m,n)} = -k_i + k_m + k_n \). This reduces the CPU time by \( 1/n^4 \) as compared to the brute-force method for an \( n \times n \) discretization of the four-point coupling. For \( n = 10 \), which is a typical value required for convergence, CPU time is thus reduced by \( 10^4 \). We have also used a special technique in integrating and in the linear interpolation of the four-point coupling to accelerate computations. We have performed exactly the same procedure for particle-hole diagram and three-point vertex functions.

4. Result

4.1. On-site Hubbard model

To check the accuracy of the present method, we first take the standard on-site, repulsive Hubbard model. Our result agrees well with the fRG result with the angular discretization. We have also compared the staggered spin susceptibility at half-filling with a QMC result\(^{10}\). They are almost identical above \( T = 0.5 \) (with the transfer energy \( t \) taken to be the unit of energy). Static approximation proved to be a good approximation above this temperature.

A difference between the Cartesian-box and angular discretizations occurs at lower temperatures. This is because the four-point coupling has a significant momentum dependence in the radial direction, especially along the line between \( q = 0 \) and \( (\pi,\pi) \), which cannot be captured with the angular discretization.

Fig. 3: Spin channel four-point couplings \( V(k_x, k_y, k_z, q) \) averaged over \( k_x, k_y \) is plotted as a function of momentum transfer \( q \) for the \( t-t' \) Hubbard model with \( U = 3, t' = -0.25, \mu = -1.0, T = 0.01 \).
4.2. Extended Hubbard model

Fig. 4: Temperature dependence of the charge susceptibility in the extended Hubbard model at half-filling for the off-site repulsion $V=0.5$ (blue), $V=1.0$ (red), $V=1.25$ (yellow) with $U=4$ for the Cartesian-box discretization (left panel), and for the angular discretization (right).

For the extended Hubbard model, the four-point couplings have strong $q$ dependence in the radial direction in the four-point coupling $V_T$ as well as for the bare couplings, so that the Cartesian-box discretization should definitely be preferred. The result in Fig. 4 indeed indicates this, where the box discretization result is in good agreement with a Monte-Carlo result[11].

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