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Renormalization Group Approach to Self-Consistent-Field Approximation for the Interacting Electrons

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Due to the retarded nature of the phonon-mediated electron-electron interaction, neither fast Fourier transform (FFT) nor previously developed NRG methods for Hubbard-type purely electronic models are applicable, while brute-force solutions are limited by the demands on computational time and storage which increase rapidly at low temperature T. A new numerical renormalization group (NRG) approach to the solution of self-consistent-field equations for correlated lattice electrons is illustrated for the two-dimensional Hubbard-type model. This approach allows us to handle the fermion frequency matrix inversions in the FLEX equations efficiently. Several orders of magnitude of CPU time and storage can be saved at the temperature scales relevant to electronic phase transitions.

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In the past decade, self-consistent field (SCF) theory, such as the fluctuation exchange (FLEX) approximation [1-8] and parquet approximation [2, 9-11] have been used to study antiferromagnetic (AF) spin fluctuation (SF) exchange within the framework of microscopic correlated electron models with only a few orbitals per unit cell. While model parameters are on the order of electron-volt scale, the energy scales of electronic phase transitions are typically on the order of 100 K or smaller. Most of the SGF techniques require to solve a set of nonlinear integral equations in the lattice of suitable meshes of momenta $\mathbf{k}$ and imaginary frequencies $i\omega_n$. The numerical problems of the SCF approaching are the extreme magnification of the momentum and frequency spaces required for the accuracy at the low temperature of the phase transition. Both numerical renormalization group [5] (NRG) and fast Fourier transform [3] (FFT) methods have been developed and successfully applied to the Hubbard model within the FLEX approximation. Due to the instantaneous interaction in the Hubbard model, the FLEX equations are greatly simplified. For more general interactions depending on the frequency [$e.g.$, the electron-phonon (EP) interaction] or momentum ($e.g.$, the long-range Coulomb interaction), neither FFT [3] approaches nor the original form of the NRG method [S] can be used to reduce the numerical problems.

When the interaction is not instantaneous, an inversion of large fermion frequency matrices would increase the demands on CPU time and memory consumption to several orders of magnitude relative to the purely Hubbard model in the FLEX approximation. Also, this fermion matrix inversion problem can not be avoided for the self-consistent calculation of the two-particle vertex functions, for example the parquet approximation. We present below an extension of the NRG

approach which allow us to incorporate EP interaction into a Hubbard-type correlated electron model. This approach provides accurate results with a highly efficient way to do the matrix inversion. Both CPU time and memory storage required can be greatly reduced by several order of magnitudes to reach a specified low temperature.

We start from the simplest microscopic model, including both an on-site Hubbard U Coulomb repulsion and a local Holstein-type EP coupling to an Einstein phonon branch, The Hamiltonian of this Holstein-Hubbard model [12-14] can be written as:

$$\begin{aligned} H = & -t \sum_{\hbar i j \imath \sigma} \left[c_{i\sigma}^{\jmath} c_{j\sigma} + HC \right] - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i"} n_{i\#} \\ & + \sum_{i} \left[\frac{p_i^2}{2M} + \frac{1}{2} K u_i^2 \right] - C \sum_{i\sigma} u_i \left(n_{i\sigma} - \frac{1}{2} \right), \end{aligned} \tag{1}$$

with a nearest neighbor hopping t, chemical potential μ, on-site Coulomb repulsion U, onsite EP coupling constant C, harmonic restoring force constant K, and ionic oscillator mass M. The $c_{i\sigma}^{\jmath}$ $(c_{i\sigma})$ is the electron creation (annihilation) operator at site i and spin σ; $n_{i\sigma}$ is the number operator; and u_i is the local ionic displacement at lattice site i. The dispersionless bare phonon frequency is $_p = (K/M)^{1/2}$ and the phonon-mediated on-site attraction is $U_p = C^2/K$.

Under the FLEX approximation [1], the diagrammatic method reduced the one-particle Green's function and two-particle vertex function into a set of nonlinear integral equations [15]. At high temperatures accurate results may be obtained using a sparse momentum and frequency mesh. As the temperature is lower, the correlation functions at high frequencies remain essentially constant. A temperature dependent cut-off may be introduced to separate the frequency space into "low" and "high" regions. The principal concept of the NRG is that after calculating at a given temperature, the high region of the space may be eliminated from further calculation. The low region may be regrained in lower temperature calculation. We can then solve the problem effectively within the "low" region only without losing the accuracy. Repeating this operation we may study the instabilities at low temperatures. During the NRG technique, the corresponding fermion Matsubara frequency grids are given by $i\omega_n^{(i)} = (2n+1)\pi T_i$, where i denotes the i-th RG operation. These grids form the basic summation domains. A typical example of this domain is shown in Fig. 1. Within this NRG frequency grid, the dimension of fermion matrix for calculating the effective potential will be greatly reduced such that the low temperature phase transition may be studied.

In order to test the accuracy of the NRG approach we have carried out the calculations based on (a) brute-force solution of the FLEX equations, (b) the factor-of-2 NRG operation describing in Fig. 1. We plot the self-energy and Green's function in Fig. 2 for $\mathsf{k} = (2.95, 0.20)$. The brute-force results obtained for Matsubara cutoff $_0/t = 25.13$ and $T/t = 0.125$. The NRG calculation has initial temperature $T_0/t = 1.0$ with 8 fermion Matsubara frequency (from $-7\pi T_0$ to $+7\pi T_0$). After three stages of factor-of-2 NRG operation, we reach the same temperature as the brute-force results. The remarkable agreement between these two methods. The NRG metllod only uses 8 ferrnion Matsubara frequencies at each temperature. Note that 64 fermion Matsubara frequencies are employed in the brute-force results at $T/t = 0.125$. In Table I, we list the memory and CPU time per iteration for both approaches. Saving of memory and CPU time of about two orders of magnitudes are achieved by the NRG approach, without loss accuracy.

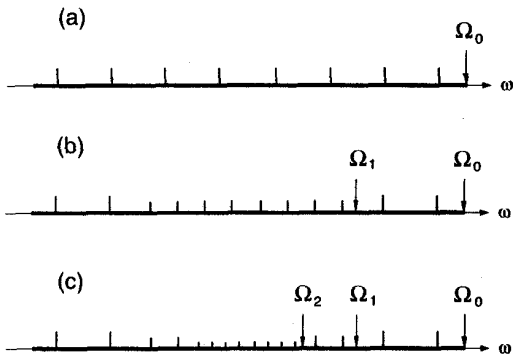

FIG. 1. Imaginary frequency discretization for the frequency NRG space. (a) Initial stage of the frequency space with cutoff $_0$, including four positive and four negative fermion frequencies, corresponding to $N_0 = 4$. (b) After one "factor-2" NRG operation, the lower cutoff is $_1 = _0/2$ There are eight frequencies in "L_1" and four frequencies in "H_1". (c) After two "factor-2" NRG operations, the lower cutoff becomes $_2 = _0/4$. There are 8 frequencies in "L_2" and eight frequencies in "H_2".

TABLE I. Comparison of memory and CPU time requirements between brute-force and frequency NRG calculations. Parameters are the same as in Fig. 2. The calculations were performed on an IBM RS6000/397 workstation.

	memory	CPU time per iteration
brute-force	105 MB	78.1 sec
frequency NRG	9 MB	0.6 sec

In summary, we have developed an important generalization of the NRG technique for solving the SCF equations of the fluctuation exchange (FLEX) approximation in the presence of the on site EP and Coulomb interactions. Because of the frequency dependence of the bare interactions neither fast Fourier transform [3] nor the previously developed NRG approach [5, 6] can be employed. On the other hand, our generalized "fermion frequency matrix" NRG technique, produces large gains in computational efficiency, both in terms of CPU time and memory requirements. This suggests possible way for solving two-particle vertex function self-consistently, such the parquet approximation [2, 9-11].

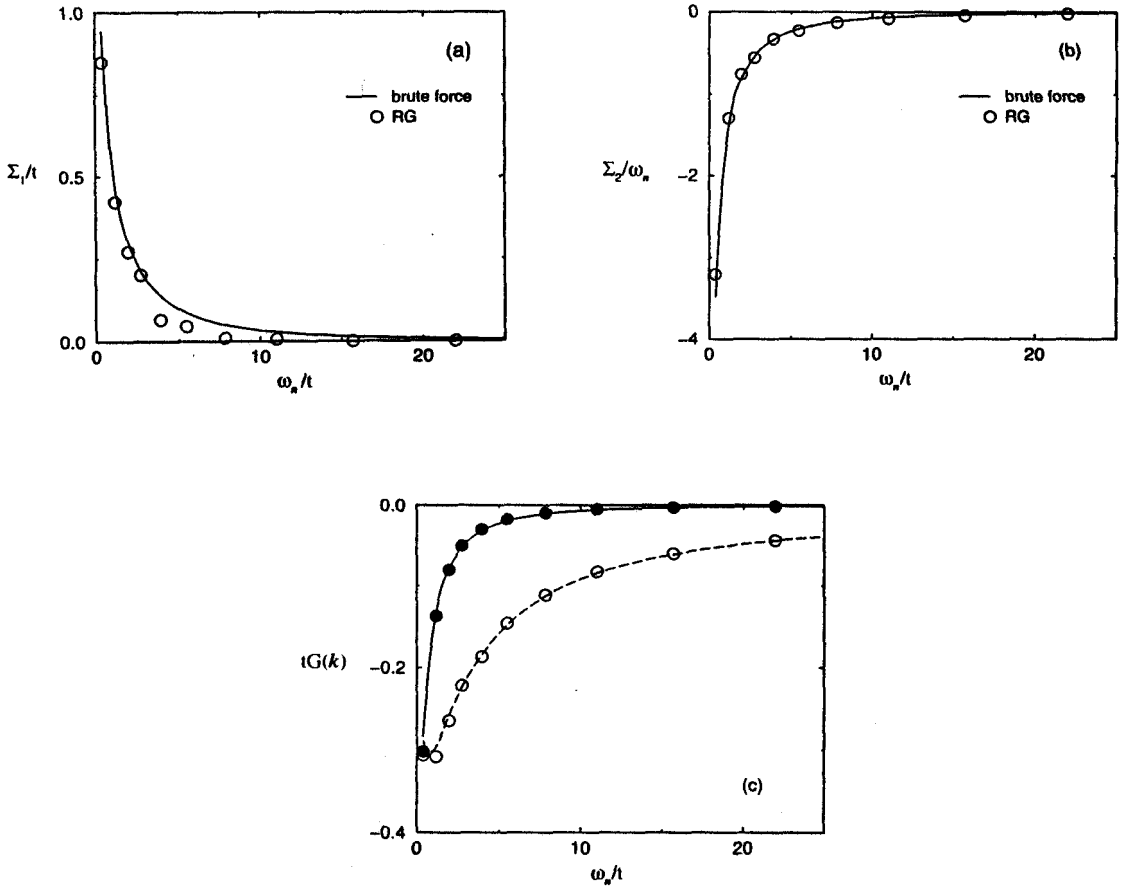

FIG. 2. Comparison of the self-energy $\sum(k) = \sum_1(k) + i\sum_2(k)$ [(a) for real part and (b) for imaginary part] and Green's function $G(k)$ [(c) solid line for real part and dashed lines for imaginary part] using factor-2 frequency NRG and a brute-force approach. Results from 3 stages of NRG are represented by symbols. Results from brute-force are represented by lines. The parameters are: $_0/t = 25$, $_p = 1.0$, $U_p/t = 4.0$, $U/t = 0$, and $\langle n\rangle = 1.0$.

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