Extended Recursion in Operator Space (EROS), a new impurity solver for the single impurity Anderson model

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We have developed a new efficient and accurate impurity solver for the single impurity Anderson model (SIAM), which is based on a non-perturbative recursion technique in a space of operators and involves expanding the self-energy as a continued fraction. The method has no special occupation number or temperature restrictions; the only approximation is the number of levels of the continued fraction retained in the expansion. We also show how this approach can be used as a new approach to Dynamical Mean Field Theory (DMFT) and illustrate this with the Hubbard model. The three lowest orders of recursion give the Hartree-Fock, Hubbard I, and Hubbard III approximations. A higher level of recursion is able to reproduce the expected 3-peak structure in the spectral function and Fermi liquid behavior.

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In the last decade, Dynamical Mean Field Theory (DMFT) \[1,2\] has become a widely used method to study strongly correlated electrons systems. It can be formulated by an action formalism with a self-consistent mapping onto a single impurity Anderson model (SIAM). Because the critical step in this method is the quality of the impurity solvers, there has recently been an increased interest in new and more accurate SIAM solvers. Currently available solvers include: iterated perturbation theory (IPT) \[3\], which works well for small U and single band, the non-crossing approximation (NCA) \[4\], which is able to give the coherent peak but fails to reproduce Fermi liquid behavior, and the equation of motion (EOM) method \[5\], which requires a decoupling scheme involving the self-energy as a continued fraction. The method has no special occupation number or temperature restrictions; the only approximation is the number of levels of the continued fraction retained in the expansion. We also show how this approach can be used as a new approach to Dynamical Mean Field Theory (DMFT) and illustrate this with the Hubbard model. The three lowest orders of recursion give the Hartree-Fock, Hubbard I, and Hubbard III approximations. A higher level of recursion is able to reproduce the expected 3-peak structure in the spectral function and Fermi liquid behavior.

Currently available solvers include: iterated perturbation theory (IPT) \[3\], which works well for small U and single band, the non-crossing approximation (NCA) \[4\], which is able to give the coherent peak but fails to reproduce Fermi liquid behavior. The equation of motion (EOM) method \[5\], which requires a decoupling scheme involving the self-energy as a continued fraction, has also been used but has the limitation that it captures correctly the low energy physics but with a logarithmic divergence instead of the expected Lorentzian shape of a Fermi liquid. It is also inaccurate for high energy physics and is limited at T=0 though finite T is tried to be implemented \[6\]. Quantum Monte Carlo (QMC) \[8\], as a non-perturbative approach, is in principle rigorous and provides good results at high temperatures for static properties but introduces uncertainty for dynamical properties (like spectral density) because of the poorly defined inverse problem, and cannot reach zero temperature.

The purpose of an Extended Recursion method in Operator Space (EROS) is to provide an efficient (rapid) and accurate method to solve the quantum impurity problem. Efficiency is especially important for LDA+DMFT calculations, since most of the computational time is spent on the quantum impurity problem. An accurate solution must include a reliable calculation for both low and high temperatures, low and high-energy physics, as well as any filling factor for the correlated bands. We also intend to extend this method to quantum transport problems for low-dimensional correlated systems (e.g., quantum dots and molecular electronics). As shown below, EROS is able to retrieve well-known approximations such as Hartree-Fock, Hubbard I, and Hubbard III, at the lowest level of recursion and the Fermi liquid regime and metal-insulator transition at higher levels.

The solution involves calculating a retarded Green function \(G(\omega) \equiv \langle \langle A; B \rangle \rangle \omega\), which is the Fourier transform of \(G(t) = -i\theta(t) \langle \{A(t), B(t)\} \rangle\) for the operators A and B. This can be done through a recursion process (RP) (see \[6,13\]), which can be directly seen by examining the coupled equations of motion for the retarded Green function for a Hamiltonian \(H\):

\[
\langle \langle A; B \rangle \rangle \omega = \frac{\{A, B\dagger\}}{\omega} + \frac{\{[A, H], B\dagger\}}{\omega^2} + \frac{\{[[A, H], H], B\dagger\}}{\omega^3} + \ldots \tag{1}
\]

This can be identified with a moment expansion through the definition

\[
\mu_n = \langle \ldots [A, H], H, \ldots, H; B\dagger \rangle >, \tag{2}
\]

where \(H\) appearing \(n\) times introduces a super-operator \(\mathcal{H}\), the ‘Liouvillian’, acting in operator space:

\[
A\mathcal{H} = [A, H] \tag{3}
\]

such that \(\mu_n = \langle \{A\mathcal{H}^n, B\dagger\} \rangle\). From its moment expansion it is possible to reconstruct the Green’s function.
as a continued fraction (CF) \[10\], but a better conditioned approach is to directly obtain the CF coefficients from the recursion method of Haydock \[11\], which can be directly applied in the space of operators, with the Liouvillian playing the role of the Hamiltonian in the standard RP. The more conventional wave-function RP consists in starting from an initial chosen state \( \psi_0 \) and then generating a set of orthonormal states \( \psi_n (n > 0) \) by the recurrence relation \( (b_0 \equiv 0) \):

\[
H \psi_n = a_n \psi_n + b_n \psi_{n-1} + b_{n+1} \psi_{n+1}
\]

(4)

The coefficients \( a_n \) and \( b_{n+1} \) are obtained by the scalar product of \( \psi_n \) by \( H \psi_n \) and with the norm \( \| H \psi_n - a_n \psi_n - b_n \psi_{n-1} \| \) respectively. In the \( \psi_n \) basis, the Hamiltonian has a tridiagonal form, which can be represented as a semi-infinite tight-binding (TB) chain. Once a sufficient number of coefficients pairs have been calculated, the diagonal element of the resolvent \( (\omega - H)^{-1} \) can be expressed as a CF. Standard techniques exist to terminate this expansion \[12\]. The application of this approach to operator space is straightforward, each vector now corresponding with an operator. For our purposes we will be mainly concerned with the local Green function, where \( A = B = c_0 \), the destruction operator of an electron of given spin at site 0. The action of the Liouvillian on any creation or destruction operator (or any combination of them) is then easily computable from its definition, Eq. \[3\]. A natural choice for the scalar product, which is necessary to compute the CF coefficients, is \( (A|B) = \langle A, B^\dagger \rangle \) as suggested by Eq. \[1\], where thermal averages reduce to their ground-state expectation value at zero temperature. Details for computing them will be given in a forthcoming paper. In this formalism, the Green’s function appears as the diagonal element of the resolvent of the Liouvillian:

\[
G(\omega) \equiv \langle c_0|\omega - H\rangle^{-1}|c_0\rangle
\]

(5)

This expression is the origin of the name we have proposed for this approach: the Extended Recursion in Operator Space (EROS); it reduces to the usual RP when only one-body operators appear in the Hamiltonian.

We now apply it to the SIAM Hamiltonian:

\[
H_{SIAM} = \epsilon_0 \sum_{\sigma} n_{\sigma 0} + U n_{0\uparrow} n_{0\downarrow}
\]

\[
+ \sum_{k \sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k \sigma} (V_{k0\sigma} c_{k\sigma}^\dagger c_{k\sigma} + V_{k0\sigma} c_{k\sigma}^\dagger c_{k\sigma}^\dagger)
\]

(6)

which describes a localized orbital 0 that has electronic correlations because of the Coulomb interaction \( U \) and is coupled to itinerant non-interacting electrons of dispersion \( \epsilon_k \); the latter is reflected by an hybridization function \( \Delta(\omega) = \sum_k \frac{\epsilon_k^2}{\omega - \epsilon_k} \), when spin indices are ignored. If we use a conventional RP to tridiagonalize the last 2 terms, we can rewrite Eq. \[6\] as:

\[
H_{imp} = \sum_{\sigma} \epsilon_0 n_{\sigma 0} + \sum_{\sigma} \epsilon_0 n_{\sigma 0} + \sum_{p > 0} (\alpha_p c_{p\sigma}^\dagger c_{p\sigma} + \beta_p c_{p-1\sigma} c_{p\sigma} + \beta_{p+1} c_{p+1\sigma} c_{p\sigma})
\]

(7)

These coefficients \( \{\alpha_p, \beta_{p+1}\} \), are the tight-binding parameters of a semi-infinite chain and also those of the CF expansion considered as a parametrization of the hybridization function \( \Delta(\omega) \), as already often noticed in NRG context \[12\], whereas a RP applied to Hamiltonian \[11\] provides the CF coefficients \( \{a_n, b_{n+1}\} \) of the impurity Green function \( G(\omega) \). Eqs. \[5\] and \[7\] give the action of \( H \) on the basis operators that is necessary to perform an operator RP (where the up-spin is assumed if a spin-index is omitted):

\[
c_0 H = \epsilon_0 c_0 + \beta_1 c_1 + U c_0^\dagger c_0 \uparrow
c_0 H = \alpha_p c_p + \beta_p c_{p-1} + \beta_{p+1} c_{p+1} \quad p > 0.
\]

(8)

(9)

Compared to the “natural” operators \( c_p \), related to a given state \( p \), the local 2-body interaction \( H_{int} \) due to \( U n_{0\uparrow} n_{0\downarrow} \) has generated a new operator \( c_{p\uparrow}^\dagger c_0 \uparrow \), which is the origin of a site representation for 1/8 of a simple tri-dimensional cubic lattice, where each site represents an operator \( c_{p\uparrow}^\dagger c_0 \uparrow \) indexed by 3 positive integers \( p, q, r \) (see Fig. 1). This construction is supported by the following observation, which can be systematically extended:

\[
c_0 n_{0\uparrow} H = U c_0 n_{0\uparrow} + \beta_1 c_1 c_{0\uparrow}^\dagger c_0 - \beta_1 c_0 c_{0\uparrow}^\dagger c_0 - \beta_1 c_0 c_{0\uparrow}^\dagger c_0 + \beta_1 c_0 c_{0\uparrow}^\dagger c_0
\]

(10)

The RP can be performed in this landscape as easily as the regular recursion on a usual lattice through knowing the action of \( H \) on operators like \( c_{p\uparrow}^\dagger c_0 \uparrow \). Special attention should be paid for the case where one or two of the indexes \( p, q, r \) are zero, viz., the 3 faces and the 3 edges of the 1/8 of the cubic lattice, since in these cases \( H_{int} \) has a non-zero effect. For the edges, this operation gives...
either 0 or $U$ for the on-site term, but for the faces, a new kind of operator is generated, which is the product of 5 “natural” operators (3 destruction and 2 creation operators), and the action of the Liouvillian (which are not representable by Fig. 1) can be represented as the sites of 5-dimensional hypercube. These operators correspond to the motion of a hole with 2 electron-hole pairs. In our calculations we did not take them exactly into account, but instead projected them onto existing products of 3 operators (which corresponds to a certain EOM decoupling) or simply neglected them; in term of moments their influence only starts with the 7th moment.

The self-energy, $\Sigma(\omega)$, which is related to the Green’s function through

$$G(\omega) = (\omega - \Sigma(\omega) - \Delta(\omega))^{-1},$$

(11)

can be expanded as a CF:

$$\Sigma(\omega) = A_0 + \frac{B_2}{\omega - A_1} - \cdots.$$  

(12)

To determine the coefficients of this CF, we note that the right hand side of Eq. (11), which includes the sum of $\Delta$ and $\Sigma$ in the denominator, can be expanded in a CF by a RP on their 2 representative chains coupled by their common first site as shown in Fig. 2(a); at the same time this also has to give the the CF expansion for $G$ in Fig. 2(b), which is calculated from the RP in operator space. This enables the coefficients of Eq. (12) for the self-energy $\Sigma$ to be determined.

We now describe an application of our EROS methodology to a DMFT solution of the Hubbard model. An excellent description of the DMFT method is given in 1 and a recent review 2 describes recent developments and extensions. The Hubbard model on a lattice (for site indices $i$ and $j$) can be written as

$$H = \sum_{i\neq j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$  

(13)

The motivation for DMFT arises from the observation based on a diagrammatic analysis that in infinite dimensions the self-energy becomes local, i.e., $k$-independent or simply $\Sigma(\omega)$. In lower dimensions, this is often only approximately true. In the local limit for $\Sigma$ the Hubbard model reduces to the problem of a correlated impurity at site “0” embedded in an effective medium where all the effects of correlation are represented by the self-energy $\Sigma(\omega)$. This can be considered as a complex and energy-dependent on-site energy in terms of a strong analogy with the TB language used in the Coherent Potential Approximation (CPA, for a detailed discussion see [15]), which was developed for studying alloys and has now been further extended for strongly correlated electron systems [19]:

$$H_{DMFT} = Un_0|n_0| + \sum_{i\neq j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum \Sigma(\omega)n_{i\sigma}$$

(14)

It can be shown that this problem maps onto a SIAM model, Eq. (6). To understand this within our approach, we start by noticing that the second term of Eq. (14), the “hopping” term, can be tridiagonalized by a RP to provide the CF expansion of the “bare” hybridization function $\Delta(\omega)$. The last term then functions like a constant on-site energy in a TB Hamiltonian that simply shifts the frequency by $\Sigma(\omega)$. Hence the last two terms of Eq. (14) can be represented by a Green’s function for an effective TB model with the bare hybridization function $\Delta(\omega)$ replaced with an effective $\Delta(\omega) = \Delta(\omega - \Sigma(\omega))$. To complete the DMFT method, we then require that this self-consistent condition be supplemented by the requirement that the local impurity Green’s function, computed from the Hamiltonian of Eq. (14), be equal to the effective lattice Green’s function, which has $\Sigma(\omega)$ on all sites, including site “0”. In RP language, this causes the the local $\Sigma(\omega)$ to be added to the on-site terms $\alpha_p$ in the chain representation for $\Delta(\omega)$. Including this self-energy at site “p” is equivalent to attaching to the TB semi-infinite chain the CF expansion of $\Sigma$ as parameters (see Appendix of [18]), and leads to a comb-shape topology for computing $\Delta(\omega)$. Having performed again a RP on this object provides a CF expansion for $\Delta(\omega)$. The DMFT self-consistency is achieved by simultaneously satisfying all of these CF equations as one steps through the recursion procedure. The first few recursion steps generate the CF coefficients $A_0 \equiv U < n_{0\sigma} >$ of $\Sigma$, corresponding to the Hartree-Fock (HF) energy-independent self-energy, and then $B_1 = Un(n-1)$ and $A_1 = U(1-n)$ gives Hubbard I, which is exact in the atomic limit. If only operators $c_{0\uparrow}^\dagger c_{0\downarrow}$ on one edge of the cubic lattice are retained, Hubbard III is recovered. Further recursions generate approximations that go well beyond these (see below). It is worth mentioning that our approach has some similarities with the approach developed in [20], but our direct use of a RP enables us to go beyond this work by avoiding their requirement to orthogonalize each new operator, which becomes becomes difficult after the first few steps.

We have benchmarked our method on the well-studied half-filled case. For simplicity, all calculations were performed at zero temperature and used as a HF solution of
Eq. (13) as an approximate ground state for computing the scalar products of the operators. In the future we will try to use a better ground state such as a Gutzwiller approximation or an exact diagonalization for a given number of sites. By including approximate excited states in a thermal average, finite-temperature calculations are also possible. For the lattice model that describes the itinerant electrons, we used a semi-elliptic non-interacting density of states, with the energy scale set by the bandwidth. Other lattices would only change the input CF coefficients for the hybridization function. For several different values of $U$, the spectral density is displayed in Fig. 3. One clearly observes the characteristic three-peak features in the Fermi liquid regime: the coherent contribution of the central peak, and the lower and upper Hubbard subbands with a splitting of the order of $U$. One also observes a redistribution of the spectral weight of the coherent central peak as the interaction $U$ increases. The Fermi liquid behavior and the intermediate regime can be better monitored by considering the real and imaginary parts of the self-energy. In the Fermi liquid regime, we have checked that the imaginary part of the self-energy vanishes as it should be at the Fermi level $E_F$, and that it has the usual $(\omega - E_F)^2$ behavior around $E_F$.

We have presented a new impurity self-consistent solver for the SIAM model and a DMFT solution of the Hubbard model using a RP procedure in an operator space. The lowest order approximations to this method generate the Hartree-Fock, Hubbard I, and Hubbard III approximations. Increasing the continued fractions go well beyond these solutions, generating the coherent Kondo peak, for example, and can provide increasingly accurate results. The way that self-consistency is achieved, step by step, makes the method efficient and very promising for its use in DMFT approaches and other more complex correlation problems.

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FIG. 3: RP DMFT calculation of the Hubbard model for the spectral density vs energy for different values of $U$ (color online)