Boosting unitary renormalization group with exact diagonalization

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Any fermionic Hamiltonian composed of electronic states from $1, .., N$ can very generally, be decomposed into three parts

$$H = H^D_{(N)} + H^{X,N}_{(N)} + H^{X,\bar{N}}_{(N)} \ , \tag{1}$$

where the number diagonal part of the Hamiltonian ($H^D_{(N)}$) is associated with n-particle self/correlation energies, while the term $H^{X,N}_{(N)}$ represents quantum fluctuations in the occupation number of state N, i.e., n-particle scattering induced coupling between the state N and the other $\{1, \ldots, N-1\}$ states. Finally, the term $H^{X,\bar{N}}_{(N)}$ represents coupling only among the other degrees of freedom $\{1, \ldots, N-1\}$. We provide a prescription for iteratively block diagonalizing a Hamiltonian in Fock space via unitary rotations. This corresponds to the renormalization of the Hamiltonian. At the first step an unitary rotation $U_{(N)}$ of the Hamiltonian $U_{(N)} H U^\dagger_{(N)}$ causes decoupling of the electronic degree of freedom labelled N such that,

$$[U_{(N)} H U^\dagger_{(N)}, \hat{n}_N] = 0 \tag{2}$$

Therefore the occupation numbers $1_N, 0_N$ of the state N becomes good quantum nos. Similarly the renormalized Hamiltonian $H_{(j-1)} = U_{(j)} H_{(j)} U^\dagger_{(j)}$ has integrals of motion $\hat{n}_N, \ldots, \hat{n}_{j+1}$. The decoupling condition eq.(2) at the RG step j demands that in the new Hamiltonian ($H_{(j-1)}$), the off-diagonal blocks in the occupation number basis of state j must vanish $H^{X,j}_{(j-1)} \equiv 0$. Therefore the Hamiltonians at the jth ($H_{(j)}$) and $j-1$th ($H_{(j-1)}$) RG steps satisfy the condition

$$(H^D_{(j)} + H^{X,j}_{(j)} + H^{X,\bar{j}}_{(j)})|\Psi_{(j)}\rangle = (H^D_{(j-1)} + H^{X,\bar{j}}_{(j-1)})|\Psi_{(j)}\rangle \ . \tag{3}$$

We can write the state $|\Psi_{(j)}\rangle$ as a linear superposition of states labelled by the occupation number of state j

$$|\Psi_{(j)}\rangle = a_{1_j}|\Psi_{(j),1_j}\rangle + a_{0_j}|\Psi_{(j),0_j}\rangle \ , \tag{4}$$

where 1_j and 0_j correspond to the jth state being occupied and unoccupied respectively. The decoupling equation (eq(2)) can then be represented in terms of electron-hole transition relations connecting the two members of the superposition in $|\Psi_{(j)}\rangle$ marked by electron occupation number of state j

$$\begin{aligned} a_{1_j}(\hat{\omega}_{(j)} - H^D_{(j)})|\Psi_{(j),1_j}\rangle &= a_{0_j} H^{X,j}_{(j)}|\Psi_{(j),0_j}\rangle \ , \\ a_{0_j}(\hat{\omega}_{(j)} - H^D_{(j)})|\Psi_{(j),0_j}\rangle &= a_{1_j} H^{X,j}_{(j)}|\Psi_{(j),1_j}\rangle . \end{aligned} \tag{5}$$

Using these equations, we can obtain a relation for the effective Hamiltonian

$$\begin{aligned} \Delta H_{(j)}|\Psi_{(j),1_j}\rangle &= (\hat{\omega}_{(j)} - H^D_{(j)})|\Psi_{(j),1_j}\rangle, \\ \Delta H_{(j)} &= H^{X,j}_{(j)} \frac{1}{\hat{\omega}_{(j)} - H^D_{(j),1_j}} H^{X,j}_{(j)} \end{aligned} \tag{6}$$

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In the above, $H^D_{(j)}$ corresponds to the diagonal energies of the occupied and unoccupied configuration for state j. Further, $H^{X,j}_{(j)}$ represents the scattering processes that cause transitions between the occupied and unoccupied configurations of state j (i.e., via its coupling with other states $\{1, \ldots, j-1\}$). Finally, $\Delta H_{(j)}$ represents the renormalization of the Hamiltonian upon the decoupling of a single degree of freedom.

These relations are a many-body analog of the Feshbach-Lowdin partitioning scheme with respect to the two subspaces of the j state ($I \otimes \hat{n}_j$ and $I \otimes (1 - \hat{n}_j)$). A similar decoupling condition is found within the coupled-cluster formalism [prasad1985some], where the transitions give rise to 1, 2 and higher order electron-hole excitations.
An explicit form for the quantum fluctuation operator $\hat{\omega}_j$ is derived using $\Delta H_{(j)} = \Delta H^{D}_{(j)} + \Delta H^{X,\bar{j}}_{(j)}$ together with eq.(6)

$$\hat{\omega}_{(j)} = H^{D}_{(j-1)} + \Delta H^{X,\bar{j}}_{(j)} \ , \tag{7}$$

The two components of $\hat{\omega}_j$ encode the renormalisation of different aspects of the remaining coupled degrees of freedom $\{1, j-1\}$: the first ($\Delta H^{X,\bar{j}}_{(j)} = H^{X,\bar{j}}_{(j-1)} - H^{X,\bar{j}}_{(j)}$) corresponds to the renormalization of various scattering vertices, and the second ($H^{D}_{(j-1)}$) to the renormalization of various n-particle self energies.
Another important outcome of the decoupling procedure can now be understood. The vanishing of the off-diagonal scattering processes via, say,

$$H^{X,j,0\to 1}_{(j*)} |\Psi_{(j),0_j}\rangle = 0 \tag{8}$$

at RG step j and fluctuation scale $\omega^{i}_{(j)} = E^{i}_{(j),1_j}$ leads to $E^{i}_{(j),1_j}$ becoming the exact eigenvalue of $H^{D}_{(j),1_j}$ containing all n-particle self energies of the state j. No further decoupling of states can take place at this energyscale, signalling that a fixed point of the RG transformations has been reached. It can be checked that the same condition is reached from the vanishing of the other member of the decoupling equations in eq.(5). Indeed, this is the many-body analog of the fixed point condition obtained from the non-perturbative similarity RG flow by Glazek and Wilson [glazek2004universality] for the case of a simple discrete Hamiltonian.

In order to connect our iterative procedure with pure diagonalization of a Hamiltonian we now write down the time independent Schröedinger equation with the decomposition given above eq(1),

$$(H^{D}_{(N)} + H^{X,N}_{(N)} + H^{X,\bar{N}}_{(N)})|\Psi\rangle = E|\Psi\rangle \ . \tag{9}$$

By taking the $|\Psi\rangle = a_{1_N}|\Psi_{1_N}\rangle + a_{0_N}|\Psi_{0_N}\rangle$ and placing it in the above eigenvalue equation leads to,

$$\begin{aligned} a_{1_N}(E - H^{D}_{(N)} - H^{X,\bar{N}}_{(N)})|\Psi_{1_N}\rangle &= a_{0_N} H^{X,N}_{(N)}|\Psi_{0_N}\rangle, \\ a_{0_N}(E - H^{D}_{(N)} - H^{X,\bar{N}}_{(N)})|\Psi_{0_N}\rangle &= a_{1_N} H^{X,N}_{(N)}|\Psi_{1_N}\rangle \ . \end{aligned} \tag{10}$$

From the above equation and eq(5) we obtain a identification of the quantum fluctuation energy scale projected onto the eigenstate $|\Psi\rangle$,

$$\begin{aligned} \langle\Psi_{1_N}|\hat{\omega}|\Psi_{1_N}\rangle &= \langle\Psi_{1_N}|H^{D}_{(N)}|\Psi_{1_N}\rangle + \frac{a_{0_N}}{a_{1_N}}\langle\Psi_{1_N}|H^{X,N}_{(N)}|\Psi_{0_N}\rangle \ , \\ \langle\Psi_{0_N}|\hat{\omega}|\Psi_{0_N}\rangle &= \langle\Psi_{0_N}|H^{D}_{(N)}|\Psi_{0_N}\rangle + \frac{a_{1_N}}{a_{0_N}}\langle\Psi_{0_N}|H^{X,N}_{(N)}|\Psi_{1_N}\rangle \ , \\ \langle\Psi_{1_N}|\hat{\omega}|\Psi_{0_N}\rangle &= 0\rangle \ , \\ \langle\Psi_{0_N}|\hat{\omega}|\Psi_{1_N}\rangle &= 0 \end{aligned} \tag{11}$$

By performing exact diagoanalization we can obtain the eigenstates and eigenvalues of a Hamiltonian. This can be numerically implemented for a small system size say 4×4 cluster. Using the eigenstates the RHS of eq(11) can determine the ω eigenvalues. This then can be fed into a RG prescription for a large system with initial ω values exactly determined.