Eur. Phys. J. B **51**, 189–193 (2006)
DOI: 10.1140/epjb/e2006-00212-0

THE EUROPEAN
PHYSICAL JOURNAL B

Construction of localized basis for dynamical mean field theory

I. Paul[1,a] and G. Kotliar[2]

[1] SPhT, CEA-Saclay, L'Orme des Merisiers, 91191 Gif-sur-Yvette, France
[2] Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

Received 22 March 2005 / Received in final form 7 April 2006
Published online 1st June 2006 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2006

Abstract. Many-body Hamiltonians obtained from first principles generally include all possible non-local interactions. But in dynamical mean field theory the non-local interactions are ignored, and only the effects of the local interactions are taken into account. The truncation of the non-local interactions is a basis dependent approximation. We propose a criterion to construct an appropriate localized basis in which the truncation can be carried out. This involves finding a basis in which a functional given by the sum of the squares of the local interactions with appropriate weight factors is maximized under unitary transformations of basis. We argue that such a localized basis is suitable for the application of dynamical mean field theory for calculating material properties from first principles. We propose an algorithm which can be used for constructing the localized basis. We test our criterion on a toy model and find it satisfactory.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 71.10.-w Theories and models of many-electron systems

1 Introduction

In the last decade and a half dynamical mean field theory (DMFT) has emerged as an important tool for studying condensed matter systems with strong correlation [1]. The principal difficulty in understanding these systems is the non-perturbative character of such systems, for which the physical properties cannot be understood by expanding various quantities in powers of the interaction. In this respect DMFT is a powerful tool for studying problems of interacting electrons on a lattice. It is a non-perturbative technique which is able to capture fully the local dynamical correlations in the system. Single site DMFT, as an approximation scheme, is controlled in that the result is exact in the limit of large coordination numbers [1]. Recent extensions of DMFT to clusters seem to be rapidly convergent for local observables [2]. Other cluster schemes such as cluster perturbation theory and dynamical cluster approximation are also being used to study problems of strong electron correlation [3]. Recently it has also been recognized that DMFT can be used as a powerful tool for the realistic computation of properties of materials as in the LDA+DMFT scheme [4–6]. Indeed results for a large variety of materials ranging from Cerium [7], Iron and Nickel [8], Plutonium [9] and many other oxides have been successfully studied with this method starting from first principles.

A common way to utilize DMFT in first principles calculations is to first derive a Hamiltonian with a kinetic energy part and a general short-range interaction part. This Hamiltonian, which will be the starting point of this paper in equation (1), is subsequently studied by DMFT. The long-range part of the Coulomb interaction can be taken into account by several means. For example, in extended DMFT this is done by coupling the electron at the impurity site to a bath of bosons whose spectral function is determined self-consistently [10,11]. This is equivalent to treating the electrons in the presence of a fluctuating electric field (long range interaction). Another possibility is to follow along the lines of Bohm and Pines [12]. In this method, starting with the charged electron gas, one performs canonical transformations to screen the electrons. In the resulting Hamiltonian the excitations are no longer the bare charged electrons, but screened neutral quasi-particles. There are various methods to obtain the starting Hamiltonian for DMFT. (1) In one of the approaches the kinetic energy term is the Kohn Sham Hamiltonian of a density functional theory calculation written in a local basis set. The interaction terms, which can include on-site (Hubbard) as well as the short range part of the Coulomb interaction, is evaluated using constrained LDA [4]; (2) in an alternative procedure, as mentioned above, one could start with the electron gas Hamiltonian and the periodic potential, and perform the Bohm-Pines canonical transformation [12] to reduce the range of the Coulomb interactions,

---

[a] e-mail: `ipaul@anl.gov`

and then write the transformed Hamiltonian in a local basis set; (3) a third approach proposed recently [13] uses the GW approach to obtain the interaction strength.

The next step is the study of the resulting Hamiltonian with a short-range interaction using DMFT. This involves local approximations, and the notion of locality depends explicitly on the basis set considered. To illustrate the point, if we perform an invertible transformation of the original basis, we merely re-express the original Hamiltonian in a new basis, provided we keep all the terms in the Hamiltonian. The full electron Green's function is obtained by applying the same transformation to the creation and destruction operators. But in practice, one performs two approximations that explicitly depend on the basis set. The first one is to neglect interactions whose range exceeds the cluster size (truncation). The second (local approximation) consist of setting equal to zero the elements of the self energy which exceeds that size. These two approximations explicitly depend on the definition of locality which is encoded in the basis set. In this paper we address only the first issue, and argue that truncating non-local interactions is appropriate when the wave-functions of the basis are well localized. As DMFT techniques are beginning to be applied to Hamiltonians with realistic interactions involving non-local terms [14], there is need for well-defined criteria for choosing optimal bases for computations. The purpose of this paper is to propose one criterion which can be used to construct a localized basis for DMFT computations.

The method of choosing a suitable localized basis of wave-functions has been studied earlier in quantum chemistry and in band structure theory [15]. The formulation of the problem consists of two steps. First, one identifies a certain group of transformations of the basis states, say for example, unitary transformations. Second, one identifies a criterion that picks out one basis out of all possible choices that are connected by the transformations. The criterion is a basis dependent quantity, and therefore is a functional in the space of the transformations. It is a measure of the amount of localization of the wave-functions in a given basis. For example, in quantum chemistry "energy localized molecular orbitals" have been studied [16]. These are obtained by maximizing under unitary transformations a functional given by the sum of the Coulomb self-interaction of the orbitals. Similarly, for band structure calculations the use of "maximally-localized" Wannier functions has been proposed [15]. The idea is to exploit the freedom that is present in the choice of the phases of the Bloch orbitals. With a given set of Bloch orbitals one can define a new set by a unitary transformation. From each such set of Bloch orbitals one can obtain a corresponding set of Wannier functions by Fourier transformation. The maximally-localized Wannier functions are obtained by minimizing the spread functional, which is the sum of the second moments of the Wannier functions, in the space of unitary transformations. More recently, the construction of localized basis states has been extended to include non-orthogonal molecular orbitals [17].

The rest of the paper is organized as follows. In Section 2 we identify a criterion for choosing a basis suitable for DMFT. We construct a functional which is maximum in the preferred basis. We discuss the properties of such a basis by studying linear variations of the functional under unitary transformations. We also propose a method for constructing the preferred basis. In Section 3 we test the criterion on a Hamiltonian whose interaction is taken to be simple but non-trivial. We find that the criterion and the associated functional is well-behaved. In conclusion, we summarize our main results.

2 Localized basis for DMFT

To keep the discussion general, in the following we formulate the problem in a basis which is non-orthogonal. For this purpose we consider a system of interacting electrons on a lattice whose Hamiltonian is expressed in a basis of atomic orbitals. The single particle states are denoted by $\phi_\alpha(\mathbf{r}-\mathbf{R}_n) \equiv \langle \mathbf{r}|n\alpha\rangle$, where α is a symmetry related index (say, orbital) and $\mathbf{R}_n$ is a lattice position. We suppose there are m orbitals per site such that the index $\alpha = 1,\ldots,m$, and there are N lattice sites with the index $n = 0,\ldots,N-1$. We also impose periodic boundary condition $|n,\alpha\rangle = |n+N,\alpha\rangle$. The states defining the basis, unlike those in a Wannier basis, are not orthogonal. We denote the overlap between any two states by $O_{\alpha\beta}(n-m) \equiv \langle n\alpha|m\beta\rangle$. The second quantized many-body Hamiltonian can be written as

$$\mathcal{H} = \sum_{\substack{nm\\ \alpha\beta}} t^{nm}_{\alpha\beta} c^\dagger_{n,\alpha} c_{m,\beta} + \sum_{\substack{nmlk\\ \alpha\beta\gamma\delta}} V^{nmkl}_{\alpha\beta\delta\gamma} c^\dagger_{n,\alpha} c^\dagger_{m,\beta} c_{k,\delta} c_{l,\gamma}. \quad (1)$$

We assume that the matrix elements $t^{nm}_{\alpha\beta} \equiv \langle n\alpha|\mathcal{H}_0|m\beta\rangle$ for the non-interacting part, and $V^{nmkl}_{\alpha\beta\delta\gamma} \equiv \langle n\alpha, m\beta|\hat{V}|l\gamma, k\delta\rangle$ for the interacting part are known from first principles studies such as band structure calculations. It is useful to bear in mind that the anti-commutation relation between the creation and annihilation operators in a non-orthogonal basis is given by $\{c^\dagger_{n,\alpha}\ ,\ c_{m,\beta}\} = O^{-1}_{\alpha\beta}(n-m)$ [18]. We now consider an invertible transformation of the single particle basis that preserves the lattice translation invariance, $|n\alpha\rangle \to |n'\alpha'\rangle = \sum_{m\beta} T_{\beta\alpha'}(m-n')|m\beta\rangle$. Expressed in the new basis the Hamiltonian, say $\mathcal{H}'$, has the same form as in equation (1) except with all the indices primed. We know that $\mathcal{H}' = \mathcal{H}$, since it is the same operator expressed in two different bases. However, when we truncate all the non-local interactions, we deal with a model Hamiltonian of the form

$$\mathcal{H}_{\rm tr} = \sum_{\substack{nm\\ \alpha\beta}} t^{nm}_{\alpha\beta} c^\dagger_{n,\alpha} c_{m,\beta} + \sum_{\substack{n\\ \alpha\beta\gamma\delta}} V^{nnnn}_{\alpha\beta\delta\gamma} c^\dagger_{n,\alpha} c^\dagger_{n,\beta} c_{n,\delta} c_{n,\gamma}. \quad (2)$$

But the process of truncation is a basis dependent step. If we perform the truncation in the new basis, i.e., on $\mathcal{H}'$, the resulting new truncated Hamiltonian $\mathcal{H}'_{\rm tr} \neq \mathcal{H}_{\rm tr}$. This observation implies that ignoring non-local interactions is a good approximation only if the single particle basis is sufficiently localized. In the following we develop a systematic criterion for constructing such a basis.

Here we consider only unitary transformations of basis. Later we comment about the possibility of extending the scheme to include non-unitary invertible transformations as well. We start from an initial basis $\{|n\alpha\rangle\}$, and consider unitary transformations

$$|n\alpha\rangle \rightarrow |n'\alpha'\rangle = U|n\alpha\rangle = \sum_{m\beta} U_{\beta\alpha}(m-n)|m\beta\rangle \qquad (3)$$

to new basis states $\{|n'\alpha'\rangle\}$. In order to find a criterion to choose the most localized basis among the possible bases $\{|n'\alpha'\rangle\}$, we first identify a quantity which is invariant under unitary transformations. The trace of any operator has this property. Since we are concerned about truncating the interacting part of the Hamiltonian, we consider the trace of the square of the interaction operator. In terms of the overlap matrix and the interactions expressed in the $\{|n\alpha\rangle\}$ basis this is given by

$$\begin{aligned} I = \mathrm{Tr}(\hat{V}^2) = {} & O^{-1}_{\alpha\beta}(n-m)O^{-1}_{\gamma\delta}(l-k)O^{-1}_{\sigma\rho}(r-s) \\ & \times O^{-1}_{\eta\nu}(p-q)V^{mkpr}_{\beta\delta\eta\sigma}V^{sqln}_{\rho\nu\gamma\alpha}. \end{aligned} \qquad (4)$$

Here, and in the rest of the paper we adopt the convention that repeated indices are summed. The invariant defined above has two basis dependent parts, namely, terms that involve only the local interactions and those involving non-local interactions. Keeping only the local interactions in a given basis, we define the "local interaction functional". For example, in the basis $\{|n\alpha\rangle\}$ the functional has the value

$$F[\{|n\alpha\rangle\}] = O^{-1}_{\alpha\beta}(0)O^{-1}_{\gamma\delta}(0)O^{-1}_{\sigma\rho}(0)O^{-1}_{\eta\nu}(0)V^{0000}_{\beta\delta\eta\sigma}V^{0000}_{\rho\nu\gamma\alpha}.$$

To elucidate the structure of the functional we first note that the overlap matrix remains unchanged under unitary transformations, i.e.,

$$\langle n'\alpha'|m'\beta'\rangle = O_{\alpha'\beta'}(n'-m') = \langle n\alpha|m\beta\rangle = O_{\alpha\beta}(n-m). \qquad (5)$$

Next, the transformation of the interaction terms is given by

$$\begin{aligned} V^{nmkl}_{\alpha\beta\delta\gamma} \rightarrow V^{n'm'k'l'}_{\alpha'\beta'\delta'\gamma'} = {} & U^*_{\sigma\alpha}(r-n)U^*_{\rho\beta}(s-m)V^{rsqp}_{\sigma\rho\nu\eta} \\ & \times U_{\eta\gamma}(p-l)U_{\nu\delta}(q-k). \end{aligned} \qquad (6)$$

In terms of the unitary transformations the local interaction functional can be written as

$$\begin{aligned} F[\{|n'\alpha'\rangle\}] = {} & \\ & O^{-1}_{\alpha'\beta'}(0)O^{-1}_{\gamma'\delta'}(0)O^{-1}_{\sigma'\rho'}(0)O^{-1}_{\eta'\nu'}(0)V^{0000}_{\beta'\delta'\eta'\sigma'}V^{0000}_{\rho'\nu'\gamma'\alpha'} \\ & = \left[O^{-1}_{\alpha\beta}(0)O^{-1}_{\gamma\delta}(0)O^{-1}_{\sigma\rho}(0)O^{-1}_{\eta\nu}(0)\right] \\ & \quad \times \left[U^*_{\mu\beta}(r)U^*_{\kappa\delta}(s)V^{rsqp}_{\mu\kappa\lambda\tau}U_{\tau\sigma}(p)U_{\lambda\eta}(q)\right] \\ & \quad \times \left[U^*_{\pi\rho}(n)U^*_{\phi\nu}(m)V^{nmkl}_{\pi\phi\omega\theta}U_{\theta\alpha}(l)U_{\omega\gamma}(k)\right]. \end{aligned} \qquad (7)$$

The inverse of the overlap matrix enters as weight factor, and the interaction terms in the starting basis $\{|n\alpha\rangle\}$ serve as parameters of the functional. The desired basis is the one in which the functional is maximum in the space of unitary transformations. This criterion also implies that, in the chosen basis, the part of the invariant I that contains non-local interactions is minimized.

In order to study the property of the preferred basis we consider infinitesimal unitary transformation given by $U = e^{i\epsilon H}$, where H is hermitian and ϵ is a small parameter. The action of H on the single particle wave-functions is given by $H|n\alpha\rangle = H_{\beta\alpha}(m-n)|m\beta\rangle$, such that

$$\begin{aligned} U_{\alpha\beta}(n-m) = {} & \delta_{\alpha\beta}\delta_{nm} + (i\epsilon)H_{\alpha\beta}(n-m) \\ & + \frac{(i\epsilon)^2}{2!}H_{\alpha\gamma}(n-l)H_{\gamma\beta}(l-m) + \ldots \end{aligned}$$

The hermiticity of H implies that

$$[\langle n\alpha|H|m\beta\rangle]^* = \langle m\beta|H|n\alpha\rangle,$$

i.e.,

$$H^*_{\gamma\beta}(l-m)O_{\gamma\alpha}(l-n) = O_{\beta\gamma}(m-l)H_{\gamma\alpha}(l-n).$$

For a lattice of N sites with periodic boundary condition and m orbitals per site, we note that the transformation matrix H has Nm^2 real independent parameters. In the following we assume that $\hat{V}(\mathbf{r}_1, \mathbf{r}_2) = \hat{V}(\mathbf{r}_2, \mathbf{r}_1)$, so that $V^{nmkl}_{\alpha\beta\delta\gamma} = V^{mnlk}_{\beta\alpha\gamma\delta}$. For the convenience of notation we define the quantity

$$L_{\sigma\mu}(t) \equiv O^{-1}_{\sigma\rho}(0)O^{-1}_{\alpha\beta}(0)O^{-1}_{\gamma\delta}(0)O^{-1}_{\eta\nu}(0)V^{0000}_{\rho\nu\gamma\alpha}V^{000t}_{\beta\delta\eta\mu}. \qquad (8)$$

To $\mathcal{O}(\epsilon)$ the variation of the functional can be written as

$$\begin{aligned} \delta F & = (-4i\epsilon)\left[L^*_{\sigma\mu}(t)H^*_{\mu\sigma}(t) - L_{\sigma\mu}(t)H_{\mu\sigma}(t)\right] \\ & = (-4i\epsilon)\Big[O^{-1}_{\sigma\beta}(m-n)L^*_{\alpha\beta}(N-m)O_{\alpha\mu}(n-t) \\ & \quad -L_{\sigma\mu}(t)\Big]H_{\mu\sigma}(t). \end{aligned} \qquad (9)$$

We define

$$A_{\sigma\mu}(t) \equiv L_{\sigma\mu}(N-t) - O^{-1}_{\sigma\beta}(m-n)L^*_{\alpha\beta}(N-m)O_{\alpha\mu}(n+t), \qquad (10)$$

and we note that A is anti-hermitian, i.e.,

$$O_{\beta\gamma}(m-l)A_{\gamma\alpha}(l-n) = -A^*_{\gamma\beta}(l-m)O_{\gamma\alpha}(l-n). \qquad (11)$$

The condition for the functional F to have a local maximum is

$$\frac{\delta F}{\delta H_{\mu\sigma}(t)} = A_{\sigma\mu}(N-t) = 0. \qquad (12)$$

The above anti-hermitian condition has to be satisfied by the preferred basis. In other words, the preferred basis is the one in which $L_{\sigma\mu}(t)$ is hermitian. The above condition gives Nm^2 real independent equations, which is the same as the number of real independent parameters in the transformation matrix H.

The following is a simple ansatz for maximizing F by successive unitary transformations. We start with an initial basis $\{|n\alpha\rangle\}$, and we calculate $A_{\mu\sigma}(t)$ using equations (8) and (10). We then change the basis using the transformation

$$H_{\mu\sigma}(t) = iA_{\mu\sigma}(t), \tag{13}$$

and iterate this procedure until the condition for the maximum is achieved. We assert (proved in the appendix) that with this ansatz, to $\mathcal{O}(\epsilon)$

$$\delta F = -(4\epsilon)A_{\sigma\mu}(N-t)A_{\mu\sigma}(t) \geq 0. \tag{14}$$

This ensures that with successive transformations the value of the functional increases (provided ϵ is small enough) until it reaches a local maximum.

Our method for constructing a localized basis is similar to Wegner's flow equation [19] and Glazek and Wilson's similarity renormalization scheme [20] approaches where small unitary transformations are used to reduce non-diagonal elements of a Hamiltonian. In our case, we use unitary transformations to reduce the strength of non-local interactions and increase the value of the functional F.

3 Discussion and conclusion

We test our criterion on a lattice Hamiltonian with an interaction of the form

$$\mathcal{H}_{\text{int}} = \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l, \tag{15}$$

where

$$U_{ijkl} = \sum_{\mathbf{R}} \phi^*(i-\mathbf{R})\phi^*(j-\mathbf{R})\phi(k-\mathbf{R})\phi(l-\mathbf{R}). \tag{16}$$

Here $\phi(i-\mathbf{R}) \equiv \phi(\mathbf{R}_i-\mathbf{R})$ is an orbital on lattice site $\mathbf{R}_i$, which defines a one-particle starting basis $\{\phi(n-\mathbf{R})\}$. The interaction described above is local in configuration space, but in the basis of $\{\phi(n-\mathbf{R})\}$ it has non-local terms as well. For simplicity we consider one orbital per site, and assume that the starting basis is orthonormal. In this basis the local interaction functional is given by

$$F = \frac{1}{\mathcal{N}_s} \sum_{n,\mathbf{R},\mathbf{R}'} |\phi(n-\mathbf{R})|^4 \, |\phi(n-\mathbf{R}')|^4, \tag{17}$$

where $\mathcal{N}_s$ is the number of lattice sites. We note that the above functional has a form similar to the (square of the) inverse participation ratio that is studied in the context of Anderson localization [21]. We perform a unitary transformation of the basis of the form $\phi(n-\mathbf{R}) \to \phi(n-\mathbf{R}) + \delta\phi(n-\mathbf{R})$, where

$$\delta\phi(n-\mathbf{R}) = (i\epsilon)\sum_m h_{mn}\phi(m-\mathbf{R}) + \mathcal{O}(\epsilon^2).$$

The coefficients h_{mn} are hermitian such that $h_{mn}^* = h_{nm}$. The variation of the functional F can be written as

$$\delta F = \frac{4\mathcal{C}}{\mathcal{N}_s} \sum_{n,\mathbf{R}} |\phi(n-\mathbf{R})|^2 \left\{\phi^*(n-\mathbf{R})\delta\phi(n-\mathbf{R}) + \text{h.c.}\right\},$$

where $\mathcal{C} = \sum_{\mathbf{R}} |\phi(n-\mathbf{R})|^4$ is a site independent constant. Using the above form for $\delta\phi$ and the unitarity of the transformation, we get to $\mathcal{O}(\epsilon)$

$$\delta F = \frac{4i\epsilon\mathcal{C}}{\mathcal{N}_s} \sum_{n,m,\mathbf{R}} h_{nm}\phi^*(m-\mathbf{R})\phi(n-\mathbf{R}) \times \left[|\phi(m-\mathbf{R})|^2 - |\phi(n-\mathbf{R})|^2\right]. \tag{18}$$

The extrema of the functional is given by

$$\sum_{\mathbf{R}} \phi^*(m-\mathbf{R})\phi(n-\mathbf{R}) \left[|\phi(m-\mathbf{R})|^2 - |\phi(n-\mathbf{R})|^2\right] = 0, \tag{19}$$

for all sites (n,m). By inspection, there are two solutions to the above equation. (1) $|\phi(n-\mathbf{R})|^2 = 1/\mathcal{N}_s, \forall n$, which is the limit of delocalized states, for which $F = 1/\mathcal{N}_s^2$ (minimum); (2) $|\phi(n-\mathbf{R})|^2 = \delta_{n,\mathbf{R}}$, which is the limit of localized states. In this case $F = 1$ (maximum), and the interaction is entirely on-site. Starting with the original basis $\{\phi(n-\mathbf{R})\}$, and the ansatz

$$h_{nm} = i\sum_{\mathbf{R}} \phi^*(n-\mathbf{R})\phi(m-\mathbf{R}) \times \left[|\phi(n-\mathbf{R})|^2 - |\phi(m-\mathbf{R})|^2\right], \tag{20}$$

we get to $\mathcal{O}(\epsilon)$

$$\delta F = \frac{4\epsilon\mathcal{C}}{\mathcal{N}_s} \sum_{n,m,\mathbf{R}} |\phi^*(n-\mathbf{R})\phi(n-\mathbf{R})|^2 \times \left[|\phi(m-\mathbf{R})|^2 - |\phi(n-\mathbf{R})|^2\right]^2 \geq 0. \tag{21}$$

Provided ϵ is chosen small enough (to justify the neglect of higher order variations), with the above ansatz it is possible to increase the value of F with successive unitary transformations until the limit of localization is attained. This simple example illustrates how the local interaction functional can be used to construct a basis of localized one-particle states. For interactions which are more complicated and realistic, it is unlikely that unitary transformations can make the interactions entirely on-site. However, the strengths of the non-local terms can be reduced (quantitatively defined by maximization of functional F) in a more localized basis.

Two more comments are of relevance. First, our criterion ignores the non-interacting part of the Hamiltonian. If one starts with nearest neighbour hopping in the original basis, in the localized basis the hopping will be more complicated. But the point of view adopted here is that the non-interacting part can still be solved exactly. Second, in this paper we consider only unitary transformations of basis. This implies that one maximizes the local interaction functional within a family of bases with the same overlap matrix (say, orthonormal bases, if the original basis is orthonormal). In principle one could probe for bases with different overlap matrices by general invertible transformations. Such a group is non-compact and one needs to impose constraints such that the functional is bounded from above. One possible constraint can be imposed in terms of the singular value decomposition of the transformation matrix, say, the ratio of the maximum and the minimum singular values be within a specified bound.

In conclusion, we propose a criterion for constructing a localized single particle basis where non-local interactions can be truncated. Such a basis is appropriate for using DMFT for the calculation of material properties. We suggest a simple algorithm by which the construction of the localized basis can be carried out. By testing the criterion on a toy Hamiltonian we conclude that the criterion and the associated functional is well-behaved.

We thank D. Vanderbilt, S. Savrasov, V. Oudovenko, and H. Jeschke for stimulating discussions and useful suggestions.

Appendix

In this appendix we prove the assertion in equation (14).

First, if the basis is orthonormal to begin with, i.e., $O_{\alpha\beta}(n-m) = \delta_{\alpha\beta}\delta_{nm}$, it is easy to see that

$$A_{\mu\sigma}(t) = L_{\mu\sigma}(N-t) - L^*_{\sigma\mu}(t) = -A^*_{\sigma\mu}(t). \tag{22}$$

Then, $\delta F = (4\epsilon)\left|A_{\sigma\mu}(N-t)\right|^2 \geq 0$.

If the basis $\{|n\alpha\rangle\}$ is non-orthogonal, we assume there exists an orthonormal basis $\{|a\tau\rangle\rangle\}$ (say, a Wannier basis) to which it is related by $|a\tau\rangle\rangle = S(n,\alpha;a\tau)|n\alpha\rangle$ and $\langle\langle a\tau| = \langle n\alpha|S(n,\alpha;a,\tau)^*$. One can show that

$$O^{-1}_{\alpha\beta}(n-m) = S(n,\alpha;a,\tau)S(m,\beta;a,\tau)^*. \tag{23}$$

Using the above relation and equation (11) one can show that

$$\begin{aligned}\delta F &= (4\epsilon)O^{-1}_{\sigma\beta}(m-n)A^*_{\alpha\beta}(m)O_{\alpha\mu}(n-t)A_{\mu\sigma}(t)\\ &= \frac{4\epsilon}{N}\sum_{\substack{ab\\ \tau\kappa}}\left|\sum_{\substack{tm\\ \mu\sigma}} S^{-1}(b,\kappa;t,\mu)A_{\mu\sigma}(t-m)S(m,\sigma;a,\tau)\right|^2\\ &\geq 0. \end{aligned} \tag{24}$$

References

1. For reviews see, e.g., A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996); T. Pruschke, M. Jarrell, J.K. Freericks, Adv. Phys. **44**, 187 (1995)
2. G. Biroli, G. Kotliar, Phys. Rev. B **65**, 155112 (2002)
3. For review see, e.g., T. Maier, M. Jarrell, T. Pruschke, M.H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005)
4. V.I. Anisimov, A.I. Poteryaev, M.A. Korotin, A.O. Anokhin, G. Kotliar, J. Phys.: Condens. Mat. **9**, 7359 (1997)
5. K. Held, I.A. Nekrasov, N. Blumer, V.I. Anisimov, D. Vollhardt, Intnl. J. Mod. Phys. B **15**, 2611 (2001)
6. A.I. Lichtenstein, M.I. Katsnelson, Phys. Rev. B **57**, 6884 (1998)
7. K. Held, A.K. McMahan, R.T. Scalettar, Phys. Rev. Lett. **87**, 276404 (2001)
8. I. Yang, S.Y. Savrasov, G. Kotliar, Phys. Rev. Lett. **87**, 216405 (2001)
9. S. Savrasov, G. Kotliar, E. Abrahams, Nature **410**, 793 (2001)
10. Q. Si, J.L. Smith, Phys. Rev. Lett. **77**, 3391 (1996)
11. R. Chitra, G. Kotliar, Phys. Rev. Lett. **84**, 3678 (2000)
12. D. Bohm, D. Pines, Phy. Rev. **92**, 609 (1953)
13. F. Aryasetiawan, S. Biermann, A. Georges, e-print `arXiv:cond-mat/0401626`
14. A. Schiller, Phys. Rev. B **60**, 15 660 (1999)
15. N. Marzari, D. Vanderbilt, Phys. Rev. B **56**, 12 847 (1997), and references therein
16. C. Edmiston, K. Ruedenberg, Rev. Mod. Phys. **35**, 457 (1963)
17. S. Liu, J.M. Pérez-Jordá, W. Yang, J. Chem. Phys. **112**, 1634 (2000)
18. T. Wegner, M. Potthoff, W. Nolting, Phys. Rev. B **61**, 1386 (2000)
19. F. Wegner, Ann. Phys. (Leipzig) **3**, 77 (1994)
20. S.D. Glazek, K.G. Wilson, Phys. Rev. D **49**, 4214 (1994)
21. see e.g., D.J. Thouless, Phys. Rep. **13**, 93 (1974)