

Exact Diagonalization Approach to Correlated Fermions in Infinite Dimensions: Mott Transition and Superconductivity

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We present a powerful method for calculating the thermodynamic properties of infinite-dimensional Hubbard-type models using an exact diagonalization of an Anderson model with a finite number of sites. The resolution obtained for Green's functions is far superior to that of quantum Monte Carlo calculations. We apply the method to the half-filled Hubbard model for a discussion of the metal-insulator transition, and to the two-band Hubbard model where we find direct evidence for the existence of a superconducting instability at low temperatures.

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Following the pioneering work of Metzner and Vollhardt [1], the limit of large dimensions for models of strongly correlated fermions has received much attention. In this limit, the highly intricate quantum many-body problem simplifies considerably and leads to a nontrivial mean-field theory [2]. Remarkably, this limit captures many features of the physics in finite dimensions and gives a very successful description of quantum fluctuations.

In spite of the considerable simplification obtained in taking the large D limit, the mean-field equations still have to be solved numerically. Up to now, all calculations [3–5] have relied on the Hirsch-Fye quantum Monte Carlo (QMC) algorithm [6]. A major limitation of this scheme is the difficulty of accessing low temperatures, where statistical and finite time-step discretization errors of the QMC algorithm become very important.

In this paper, we present a powerful exact diagonalization method for solving these mean-field equations. We find that the resolution obtained for thermodynamic Green's functions is far superior to that of QMC calculations and that essentially the exact solution of the model is obtained, except at very small frequencies. Having at our disposal such a unique method, we investigate two important physical issues for which no definite answers have been given so far. *First*, we consider the metal-insulator transition in the half-filled Hubbard model, where our numerical results are indicative of a second-order transition at zero temperature. *Second*, we establish the instability of the normal state of the two-band Hubbard model [7] with respect to singlet superconductivity at large U and small doping (the regime of relevance for high- T_c superconductors) and also an instability towards triplet superconductivity in the large doping regime $n \sim 2$.

For concreteness, we explain the method in the single-band Hubbard model on a Bethe lattice of infinite con-

nectivity $z \rightarrow \infty$. The Hamiltonian is written as

$$H = - \sum_{(ij)\sigma} \frac{1}{\sqrt{2z}} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

The calculation of the single-site properties of the Hubbard model, in this limit reduces to the self-consistent determination of the on-site Green's function $G(i\omega)$ of the Hubbard model and of a bath Green's function $G_0(i\omega)$, which describes the interaction on the single site with the external environment. $G(i\omega)$ and $G_0(i\omega)$ are related by a self-consistency condition which (in the paramagnetic normal state, on the Bethe lattice) reads

$$G_0^{-1}(i\omega) = i\omega + \mu - G(i\omega)/2. \quad (2)$$

As is well known [8], the on-site Green's function of the Hubbard model may be interpreted as the Green's function of an Anderson model

$$H_{\text{And}} = \epsilon_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + \sum_{\sigma, l=2}^{n_s} \epsilon_l a_{l\sigma}^\dagger a_{l\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\sigma, l=2}^{n_s} (V_l a_{l\sigma}^\dagger d_{\sigma} + \text{H.c.}), \quad (3)$$

the function $G_0(i\omega_n)$ being given by the $U = 0$ Green's function of the impurity

$$G_0(i\omega_n) = G_0^{\text{And}}(i\omega_n) = \left(i\omega_n - \epsilon_d - \mu - \sum_{l=2}^{n_s} \frac{V_l^2}{i\omega_n - \epsilon_l} \right)^{-1}. \quad (4)$$

Given the infinite number of degrees of freedom of the models defined in Eq. (1) and Eq. (3), it is evident that strict self-consistency can only be obtained with a continuous Anderson model, i.e., with $n_s = \infty$. Our algorithm is based on the observation that a *systematic* approximation (i.e., fit) of $G_0(i\omega)$ with a finite- n_s Anderson model

gives extremely good results. We stress from the beginning that we perform a fit of the imaginary-frequency Green's functions only.

In practice, we approximate any $G_0^{-1}(i\omega)$ by a function $G_0^{-1 \text{ And}}(i\omega)$ with a finite number n_s of sites. This can be cast into a minimization problem in the variables ϵ_l and V_l . In this work, we choose the following cost function:

$$\chi^2 = \frac{1}{n_{\max} + 1} \sum_{n=0}^{n_{\max}} |G_0^{-1}(i\omega_n) - G_0^{-1 \text{ And}}(i\omega_n)|^2, \quad (5)$$

where n_{\max} is chosen sufficiently large [$\omega_{n_{\max}} \gg \max_l(\epsilon_l)$] [9]. We search for the parameters ϵ_l and V_l minimizing the χ^2 in Eq. (5) with a standard conjugate gradient method.

For a small number of sites, $n_s \leq 6$, the Green's function $G(i\omega_n)$ can be obtained exactly from the complete set of eigenvectors and eigenvalues of the Anderson Hamiltonian equation (3). The procedure

$$G_0^{-1}(i\omega) \xrightarrow{\text{Eq. (5)}} G_0^{-1 \text{ And}}(i\omega) \xrightarrow{\text{Eq. (3)}} G(i\omega) \xrightarrow{\text{Eq. (2)}} G_0^{-1}(i\omega) \quad (6)$$

is then iterated to convergence.

Beyond $n_s = 6$, the size of the Hilbert space becomes too large for an explicit diagonalization of the Anderson Hamiltonian. However, the calculation of *zero-temperature* Green's functions is still possible by means of the Lancz\`os algorithm [10], which allows us to easily calculate $G(i\omega)$ and $G_0(i\omega)$ up to $n_s \sim 10$ on a work station. The fit with the Anderson model is performed as before. We simply replace the Matsubara frequencies by a fine grid of imaginary frequencies, which correspond to a "fictitious" inverse temperature $\tilde{\beta}$ ($\omega_n = (2n+1)\pi/\tilde{\beta}$). $\tilde{\beta}$ introduces a low-frequency cutoff in an obvious way.

The following observations are made:

(1) We notice in general very small differences between $G_0^{-1}(i\omega)$ and $G_0^{-1 \text{ And}}(i\omega)$ as expressed by small minimal values of χ^2 in Eq. (5). χ^2 decreases by approximately a constant factor each time we add one more site. This means that *exponential* convergence in n_s is observed.

(2) The extensive comparisons with QMC [5] which we have undertaken indicate that, even at finite temperature, exact diagonalization is by far the superior method for this problem. Using exact diagonalization at $n_s = 3, \dots, 6$, very precise values of the Green's function $G(\tau)$ can be obtained in a few minutes on a work station, which it has taken us days to check by QMC [11].

(3) Using the Lancz\`os algorithm at $T = 0$ we can go higher in n_s , and the quality of fit can be ameliorated by another 2 orders of magnitude. To illustrate, we display in Fig. 1(a) the low-frequency part of $G_0^{-1}(i\omega)$ and $G_0^{-1 \text{ And}}(i\omega)$ for $U = 2$ at $\tilde{\beta} = 200$ [see also Fig. 3(a) for the two-band Hubbard case]. Notice the *systematic* amelioration of the fit. Furthermore, the bath Green's function G_0^{-1} [the Green's function obtained from Eq. (2), once $G(i\omega)$ has been computed] is extremely independent of n_s , especially at high frequency. Already at $\omega = 0.11$, e.g., G_0^{-1} varies by less than 0.0001 between

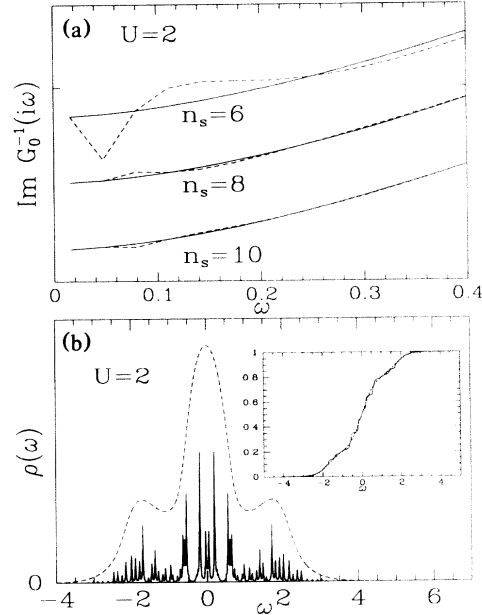


FIG. 1. (a) $G_0(i\omega)^{-1}$ and $G_0^{-1 \text{ And}}$ in the Hubbard model at $U = 2$ at small frequency for $n_s = 6, 8, 10$. Note the systematic improvement of the solution. The maximal misfit between the two functions is 0.082 for $n_s = 6$. (b) Density of states $\rho(\omega)$ for $U = 2$ ($\epsilon = 0.01$). We compare with the IPT density of states [12]. Inset: Comparison of the integrated densities of states between exact diagonalization and IPT.

$n_s = 6, 8$, and 10. The same convergence is observed for the physical Green's function $G(i\omega)$ in which we are ultimately interested.

(4) Even though the method has been geared exclusively at the calculation of thermodynamic Green's quantities, it is very interesting to consider the dynamic properties, e.g., the one-particle spectral densities $\rho(\omega) = -\text{Im}G(\omega + i\epsilon)/\pi$. We have computed $\rho(\omega)$ ($n_s=10$) for different values of U . In the Fermi-liquid regime at moderate U , the excitation spectrum of our finite-size Anderson model consists of a large number of peaks, which are grouped into three well-separated structures: a central quasiparticle peak and two broad high-energy satellite features, corresponding to the formation of the upper and lower Hubbard bands. At sufficiently large U a Mott insulator gap is observed, and far fewer peaks contribute to the spectrum. Figure 1(b) gives the spectral density as obtained at $U = 2$. The dashed line represents the results given by the iterated perturbation theory (IPT) approximation. This method is based essentially on the use of a weak coupling calculation to second order in U of Σ which gives an interpolation between the small and large U limits (exclusively at half filling and in the paramagnetic phase) [8,12,13]. We also present the *integrated* density of states corresponding to Lancz\`os and IPT. The agreement between both curves is seen to be excellent, provided we average over a small frequency interval. This indicates that the spectral density, as calculated by our

method, contains coarse-grained information about the exact solution, and can be very useful in cases in which IPT cannot be applied.

Let us now give a more quantitative discussion of the metal-insulator transition. Figure 2 presents some results for the quasiparticle spectral weight Z calculated from the slope of the self-energy $\Sigma = G_0^{-1} - G^{-1}$. In the inset of Fig. 2 we present the data for $\text{Im}\Sigma(i\omega)$ at small frequencies from which the spectral weight is extracted [$\text{Im}\Sigma(i\omega) \sim (1 - 1/Z)\omega + \dots$]. To get a truly stabilized slope of Σ we have found it necessary to reach very large values of $\tilde{\beta}$. The main plot compares the results at $n_s = 10$ with IPT. On a few points we give in addition the results at $n_s = 6$ and $n_s = 8$. Given the extremely good agreement between the values of Z calculated with $n_s = 8$ and 10, we are very confident of the numerical values presented.

As discussed in Ref. [12], the IPT approximation leads to a first-order Mott-Hubbard transition (cf. Fig. 2), and the quasiparticle weight Z jumps discontinuously at $U \sim 3.6$. We have only found limited evidence for such a scenario within the present approach. At $n_s = 6$, we are unable to stabilize two solutions at the same values of the physical parameters (the coexistence of two solutions is indicative of a first-order phase transition). At $n_s = 8$, and using a fictitious temperature of $\tilde{\beta} = 120$, we find a coexistence region within a very small interval of U : $4.45 \leq U \leq 4.60$ [14]. Even though the question of the order of the transition will have to await a more detailed investigation, it seems to us to be difficult to reconcile our numerical results with an abrupt zero-temperature transition anywhere close to $U = 3.6$. Let us reiterate the fact that the results presented in Fig. 2 are at zero temperature and that $\tilde{\beta}$ only serves as a frequency cutoff.

We now consider the very important issue of supercon-

ductivity in Hubbard-type models in infinite D . We have looked for it in the single-band model defined above, and in the two-band Hubbard model defined by the Hamiltonian [7]

$$\mathcal{H} = - \sum_{i \in D, j \in P, \sigma} t_{ij} d_{i\sigma}^\dagger p_{j\sigma} + \text{H.c.} + \epsilon_p \sum_{j \in P, \sigma} p_{j\sigma}^\dagger p_{j\sigma} + \epsilon_d \sum_{i \in D, \sigma} d_{i\sigma}^\dagger d_{i\sigma} + U_d \sum_{i \in D} n_{i\uparrow}^d n_{i\downarrow}^d, \quad (7)$$

where the hopping is scaled as $t_{ij} \sim 1/\sqrt{2z}$. In Eq. (7) (d_σ, p_σ) represent two atomic orbitals on different sublattices (D, P) of a bipartite lattice with $z \rightarrow \infty$ which, as before, is taken to be the infinitely connected Bethe lattice.

In the standard Nambu notation, $\Psi_d^\dagger \equiv (d_\uparrow^\dagger, d_\downarrow)$ (equivalently for Ψ_p) the d -orbital Green's function can be written as a 2×2 matrix

$$\mathbf{D}(\omega) \equiv -T \langle \Psi_d(\omega) \Psi_d^\dagger(\omega) \rangle = \begin{pmatrix} G_d(\omega) & F_d(\omega) \\ F_d(\omega)^* & -G_d(-\omega) \end{pmatrix} \quad (8)$$

and the self-consistency equations for the Green's functions are given by [7]

$$\begin{aligned} \mathbf{D}_0^{-1}(i\omega_n) &= i\omega_n + (\mu - \epsilon_d)\sigma_3 - t_{pd}^2 \sigma_3 \mathbf{P}(i\omega_n) \sigma_3, \\ \mathbf{P}^{-1}(i\omega_n) &= i\omega_n + (\mu - \epsilon_p)\sigma_3 - t_{pd}^2 \sigma_3 \mathbf{D}(i\omega_n) \sigma_3 \end{aligned} \quad (9)$$

(note that \mathbf{D}_0 and \mathbf{D} are 2×2 matrices and that \mathbf{D}_0^{-1} denotes the matrix inverse).

In the presence of superconducting order, the Green's functions $D(i\omega_n)$ and $D_0(i\omega_n)$ may be viewed as impurity Green's functions of an effective Anderson model in a superconducting medium, which we fit by a generalization of Eq. (4), modified by an explicit pairing between all the sites [11].

We are interested in the normal state exclusively as a starting point for a linear stability analysis and investigate the regime close to the normal solution. An example of the excellent quality of the normal state solution [15] is presented in Fig. 3(a). Here, $\text{Re}[G_{d0}(i\omega)]$ and $\text{Re}[G_{d0}^{\text{And}}(i\omega)]$ are displayed. The "fictitious" temperature is $\tilde{\beta} = 250$, $U_d = 8$, $\epsilon_p - \epsilon_d = 4$, $\mu = 3.5$, and the density corresponds to the lightly doped regime of the two-band model ($n \sim 1.3$). We now consider the stability analysis of the normal state solution. A possible way of studying this stability is to calculate the pairing susceptibility. An alternative way used here is to establish the stability properties of the solution by introducing small superconducting terms in the Anderson Hamiltonian, and following the evolution under subsequent iterations [7]. Under such conditions, the normal state solutions very quickly acquire nonzero values of $F(\omega)$, which indicate a superconducting instability. More rigorously, and in order to study quantitatively the effects of increasing n_s , we may calculate the largest eigenvalue, and the corresponding eigenvector of the matrix $\partial F(i\omega)^{n+1} / \partial F(i\omega)^n$ close to the normal state, where the

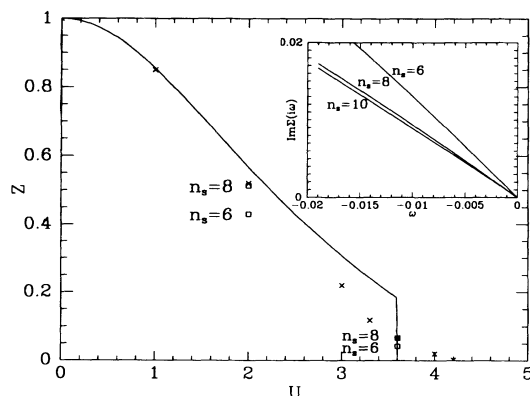


FIG. 2. Quasiparticle weight Z as a function of U for the half-filled Hubbard model. The curve gives the IPT approximation, which predicts a first-order transition. The crosses give the results for $n_s = 10$, with the corresponding results for $n_s = 6, 8$ at two points. The inset shows the small- ω behavior of $\text{Im}\Sigma(i\omega)$ for $n_s = 6, 8, 10$ from which the quasiparticle weight is calculated. Note the excellent convergence with n_s .

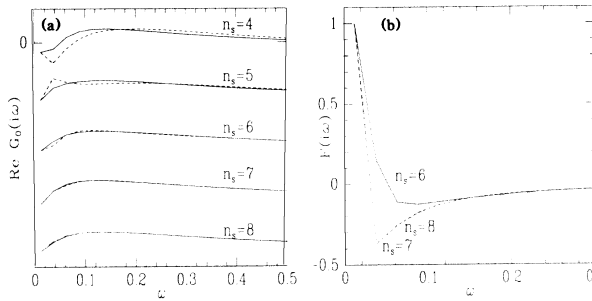


FIG. 3. (a) Real part of $G_d^{\text{And}}(i\omega)$ and $G_{d0}(i\omega)$ for $n_s = 4, \dots, 8$ (two-band model: $U_d = 8, \mu = 3.5, \epsilon_p - \epsilon_d = 4$). (b) Largest eigenvector of the matrix $\partial F(i\omega)^{n+1}/\partial F(i\omega)^n$ close to the normal state solution for $n_s = 6, 7$, and 8 (singlet sector). The corresponding eigenvalues are $\lambda_{\text{max}} \sim 2$ in all three cases.

superscripts on the F 's indicate two subsequent iterations of the self-consistency loop. We have done such calculations, which correspond to the well-known procedure of extracting the largest eigenvalue and eigenvector of a matrix with the "power method." We are able to identify a linear regime at small $F(i\omega)$, with the largest eigenvalue always of the order $\lambda_{\text{max}} \sim 2$. The corresponding (rescaled) eigenvectors for $n_s = 6, 7, 8$ are plotted in Fig. 3(b). Clearly, the agreement between these completely independent curves is excellent. We have checked this result in a variety of ways [by changing $\tilde{\beta}$, the precise form of the function used in Eq. (5), and the doping]. This leads us to the conviction that the normal state solution of the $d = \infty$ model at small doping is indeed unstable with respect to singlet superconductivity. We have performed a completely analogous stability analysis for the lightly doped ($n \sim 1.2$ and $n \sim 1.4$) regime of the corresponding one-band Hubbard model for a number of values of the interaction ($U = 2, 4, 6, 8$). In sharp contrast to the two-band Hubbard model, we have found no indication of a superconducting instability in that case.

We have also studied the point investigated previously [7], i.e., values of the physical parameters corresponding to a total density of $n \sim 2$, where the Hubbard interaction is just large enough to create a large overlap between the upper Hubbard band of the d -level and the p -level band. There our evidence for singlet superconductivity is very limited (at least for frequencies larger than $\sim 1/200$). However, we have on that point found very clear evidence for superconductivity in the triplet sector. Following the procedure outlined above (at $T = 0$), we find consistently that any small superconducting term, in addition to the normal state solution, blows up at a rate which corresponds to a largest eigenvalue of ~ 1.8 of the matrix $\partial F(i\omega)^{n+1}/\partial F(i\omega)^n$ [16] (typical values of parameters are $U_d = 4.5, \mu = \epsilon_p - \epsilon_d = 4, \tilde{\beta} = 200$). Superconducting order of this kind has been first proposed by Berezinskii [17] in the context of ^3He , and, very recently by Coleman, Miranda, and Tsvelik [18] for heavy-

fermion superconductors.

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