Exact Diagonalization Approach for the $D = \infty$ Hubbard Model

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We present a powerful method for calculating the thermodynamic properties of the Hubbard model in infinite dimensions, using an exact diagonalization of an Anderson model with a finite number of sites. At finite temperatures, the explicit diagonalization of the Anderson Hamiltonian allows the calculation of Green's functions with a resolution far superior to that of Quantum Monte Carlo calculations. At zero temperature, the Lanczòs method is used and yields the essentially exact zero-temperature solution of the model, except in a region of very small frequencies. Numerical results for the half-filled case in the paramagnetic phase (quasi-particle weight, self-energy, and also real-frequency spectral densities) are presented.

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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 non-trivial 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], [4], [5] have relied on the Hirsch-Fye Quantum Monte Carlo (QMC) algorithm [6]. A major limitation of this scheme is the difficulty of accessing the low-temperature regime, where statistical and finite time-step discretization errors of the QMC algorithm become very important.

In this paper, we present a powerful method for solving these mean-field equations, which leads to an essentially exact solution in the imaginary frequency domain. As an example, we consider the Hubbard model on a lattice of infinite connectivity $z \to \infty$ which, after proper rescaling of the kinetic energy, is written as

$$H = -\sum_{<ij>\sigma} \frac{1}{\sqrt{2z}} c_i^+ c_j + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

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 $G(\omega)$ of the Hubbard model and of a bath Green's function $G_0(\omega)$, which describes the interaction on the single site with the external environment. $G(\omega)$ and $G_0(\omega)$ are related by a self-consistency condition which, on the Bethe lattice, reads:

$$G_0^{-1}(\omega) = \omega + \mu - \frac{1}{2} G(\omega) \tag{2}$$

It is for simplicity only that we restrict our attention in this paper to the $z \to \infty$ Bethe lattice.

As is well known [7] [8], the on-site Green's function of the Hubbard model may be interpreted as the Green's function of an Anderson model

$$H_{And} = \epsilon_d \sum_\sigma d_\sigma^+ d_\sigma + \sum_{\sigma,k=2}^{n_s} \epsilon_k a_{k\sigma}^+ a_{k\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\sigma,k=2}^{n_s} (V_k a_{k\sigma}^+ d_\sigma + h.c.) \tag{3}$$

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

$$G_0(i\omega_n) = G_0^{And}(i\omega_n) = [i\omega_n - \epsilon_d - \mu - \sum_{k=2}^{n_s} \frac{V_k^2}{i\omega_n - \epsilon_k}]^{-1} \tag{4}$$

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 $n_s = \infty$. The main result of the present paper is that a systematic approximation of $G_0(i\omega)$ with a finite-n_s Anderson model gives extremely good results. We stress from the beginning that we are interested in an approximation of the imaginary-frequency Green's functions only.

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

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

where n_{max} is chosen sufficiently large ($\omega_{nmax} >> max_k(\epsilon_k)$) [9]. We search for the parameters ϵ_k and V_k minimizing the χ^2 in eq. (5) with a standard conjugate gradient method [10].

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 eq. (3). The procedure

$$G_0^{-1}(i\omega_n) \stackrel{eq.\ (5)}{\longrightarrow} G_0^{-1\ And}(i\omega_n) \stackrel{eq.\ (3)}{\longrightarrow} G(i\omega_n) \stackrel{eq.\ (2)}{\longrightarrow} G_0^{-1}(i\omega_n) \tag{6}$$

is then iterated to convergence.

The following observations are made:

1) We notice in general very small differences between $G_0^{-1}(i\omega)$ and $G_0^{-1\ And}(i\omega)$ 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.

2) The extensive comparisons with QMC results [5] which we have undertaken indicate that exact diagonalization is by far the superior method for this problem. As an example, we show in fig. 1 QMC and exact diagonalization data for the half-filled Hubbard model at $\beta = 32$ and $U = 3$. The Monte Carlo data are shown for a imaginary-time discretization of $\Delta\tau = 1, .5$, and $.25$ (*cf, e. g.* [5]), and the exact diagonalization data for $n_s = 3, 5$. It may be worthy of notice that the diagonalization calculations can be obtained in a few minutes on a work station, while for the QMC data acquisition (at $\Delta\tau = 0.5$) several hours were needed (several days for $\Delta\tau = 0.25$).

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 Lanczòs algorithm [11], which allows us to easily calculate $G(i\omega)$ and $G_0(i\omega)$ up to $n_s \sim 10$ on a workstation [12]. 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 β ($\omega_n = (2n+1)\pi/\beta$). β introduces a low-frequency cutoff in an obvious way. In fig. 2 we display the functions $G_0^{-1}(i\omega)$ and $G_0^{-1\ And}(i\omega)$ for $U = 2$ and $U = 4.8$. At the scale of the figure the two curves can hardly be distinguished, and an essentially perfect fit (*i.e.* perfect self-consistency) is obtained in the whole range of frequencies. The inset in the figure shows a blow-up of the small frequency regime as the number of sites is increased. Notice the *systematic* amelioration of the fit. Furthermore, the 'physical' Green's function G_0^{-1} 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 $n_s = 6, 8$, and 10.

For the data at $U = 4.8$, the quality of the fit is excellent even with a small number of sites. This is easily explained by the existence of a physical cutoff in frequency, which results from the Mott gap.

We now pass to the calculation of other physical quantities and present in fig. 3 some results for the quasi-particle spectral weight Z calculated from the slope of the self-energy $\Sigma = G_0^{-1} - G^{-1}$. In the inset of fig. 3 we present the raw data of $Im\Sigma(i\omega)$ at small frequencies from which the spectral weight is extracted ($Im\Sigma(i\omega) \sim (1 - 1/Z)\omega + \ldots$). To get a truly

stabilized slope of Σ we have found it to be necessary to reach very low temperatures. The main plot compares the results at $n_s = 10$ with the "iterated perturbation theory" (IPT) result. This method is based essentially on the use of a weak coupling calculation to second-order in U of Σ and has shown to give a satisfactory interpolation between the small and large U limits (exclusively at half filling and in the paramagnetic phase) [8], [13], [14]. On a few points we give in addition the results of the exact diagonalization 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 [13], the IPT approximation leads to a first-order Mott-Hubbard transition (*cf* fig. 3), and the quasi-particle 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 $\beta = 120$, we find a coexistence region within a very small interval of U: $4.45 \leq U \leq 4.60$ [15]. 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 a abrupt transition anywhere close to $U = 3.6$.

Finally, we show some data concerning the one-particle spectral densities $\rho(\omega) = -ImG(\omega+i\epsilon)/\pi$ as obtained from the Lanczòs calculation together with IPT-approximation solutions [13]. Fig. 4 shows the spectral density (n_s=10) for different values of U. In the Fermi-liquid regime the spectrum of our finite-size Anderson model consists of a large number of peaks, while in the insulating phase we systematically observe a simpler structure made of only a few peaks. As U is increased we see that $\rho(\omega)$ develops three well-separated structures: a central quasi-particle feature and two broad high-energy satellite features corresponding to the formation of the upper Hubbard band. At $U = 4.8$ a gap is observed in good agreement with the approximate IPT solution. In the insets of Fig. 4 we also present the integrated single particle density of states corresponding to Lanczòs and IPT solutions. The agreement between both curves is seen to be very good, provided we average over a frequency interval of $\omega \sim 0.5$. This indicates that the calculated spectral density contains coarse-grained information about the exact solution, as it should be. Due to the discrete nature of the Anderson model used, the fine details of the spectrum are poorly reproduced.

A remark is in order here: As is well known, the continuation of numerical data from the imaginary axis onto the real-frequency domain is a very difficult problem and constitutes for example one of the major limitations of the QMC method. Here we encountered the analytic continuation problem in the 'easy' direction. Indeed, in the present work very precise imaginary frequency data (*cf* fig, 1, fig. 2) can be obtained with a representation in ω , which very cleary has its limits (*cf* fig. 4). It is crucial in this context that we only attempt to satisfy the self-consistency condition on the imaginary axis.

In conclusion, we have presented a powerful numerical method for simulating the $D = \infty$ models for strongly correlated fermions based on a self-consistent single-impurity model treated by exact diagonalization. At the temperatures reachable by quantum Monte Carlo calculations we get essentially the exact solution of the model. At lower temperatures unreachable by QMC, we get also an amazingly good solution, except in the region of very small frequencies where some difficulties appear due to the finite degrees of freedom in the representation of the free propagator ($G_0^{-1\,And}$) of the impurity.

Elsewhere [16] we present a study of the instability of the normal phase with respect to superconductivity of an infinite-D two-band Hubbard model [17]. That work and additional calculations on the Hubbard model away from half-filling clearly show that the exact diagonalization method presented in this work is in no way limited to the particle-hole symmetric point of the Hubbard model. Broken-symmetry phases, magnetic fields, *etc*, as well as the calculation of susceptibilities [18] can be easily handled within this approach, which we expect to rapidly become a standard tool for the investigation of $D = \infty$ systems.

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[1] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62** 324 (1989)
[2] For a recent review and references, see *e.g.* D.Vollhardt, to appear in 'Correlated Electron Systems', proceedings of the Jerusalem Winter School of Theoretical Physics, V. J. Emery ed. (World Scientific). (preprint RWTH/ITP-C 6/92)
[3] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)
[4] M. Rozenberg, X. Y. Zhang and G. Kotliar, *Phys. Rev. Lett.* **69**, 1236 (1992)
[5] A. Georges and W. Krauth, *Phys. Rev. Lett.* **69**, 1240 (1992)
[6] J. E. Hirsch and R. M. Fye, *Phys. Rev. Lett.* **56** 2521 (1986)
[7] P. van Dongen and D. Vollhardt, *Phys. Rev. Lett.* **65** 1663 (1990)
[8] A. Georges and G. Kotliar *Phys. Rev. B* **45** 6479 (1992)
[9] The precise form of the function which is minimized plays no role, as it should be. Practically the same results can be obtained by fitting G_0 and G_0^{And} instead of their inverses *cf* [16], or by putting in ω-dependent factors.
[10] In order to force the particle-hole symmetry a symmetric distribution of the ϵ_l's around zero with one energy kept fixed at zero has been chosen ($n_s - 1$ independent parameters) in most of our simulations.
[11] R. Haydock, V. Heine, and M. J. Kelly J. Phys. C **8**, 2591 (1975)
[12] Higher n_s (say, up to $n_s \sim 16$) could be handled on a supercomputer using efficiently designed algorithms (that was not the purpose of this work). In any case, this would not change quantitatively our well-converged results (see below).
[13] A. Georges and W. Krauth, LPTENS preprint 92/24 (1992) to appear in *Phys. Rev. B* (Sept. 1993)
[14] X. Y. Zhang, M. Rosenberg and G. Kotliar, Preprint
[15] Convergence is very slow in the transition region. There it may take several hundred iterations to destroy an apparently stable Fermi-liquid or Mott insulating phase. However, we always end up with a fully stabilized solution. Such a situation is almost impossible to handle correctly in expensive QMC calculations at low temperatures.
[16] W. Krauth and M. Caffarel, LPSENS preprint 93/17 (1993)
[17] A. Georges, G. Kotliar, and W. Krauth, LPTENS preprint 93/10, to appear in Z. Phys. (1993)
[18] work in progress, in collaboration with A. Georges.

Figure Captions

1. Comparison of $G(\tau)$ for $U = 3$, and $\beta = 32$ between exact diagonalization ($n_s = 3, 5$ (bottom solid lines) the results cannot be distinguished on the scale plotted) and Quantum Monte Carlo (solid: $\Delta\tau = 1$, dashed: $\Delta\tau = 0.5$). Inset: $G(\tau = 4)$ *vs.* $\Delta\tau^2$ (the QMC algorithm converges roughly in $\Delta\tau^2$). At $\Delta\tau = 0.$ exact diagonalization results for $n_s = 3, 5$.

2. Plot of $G_0^{-1}(i\omega)$ and of $G_0^{-1\,And}$ for two values of the interaction, $U = 2$ (Fermi liquid-regime) and $U = 4.8$ (Mott insulator regime) at $n_s = 10$. The inset gives $G_0(i\omega)^{-1}$ and $G_0^{-1\,And}$ at small frequency for $n_s = 6, 8, 10$. Note the systematic improvement of the solution. The misfit between the two functions is the only source of error of the exact diagonalization approach.

3. Quasi-particle 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 $Im\Sigma(i\omega)$ for $n_s = 6, 8, 10$ from which the quasi-particle weight is calculated. Note the excellent convergence with n_s.

4. Density of states $\rho(\omega)$ for different values of U (a value of $\epsilon = 0.01$ is used). We compare with the IPT density of states [13]. Insets: Comparison of the integrated densities of states between exact diagonalization and IPT.