Control of the finite-size corrections in exact diagonalization studies

Claudius Gros
Institut für Physik, Universität Dortmund, 44221 Dortmund, Germany
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The finite-size corrections in exact diagonalization studies of the one- and two-dimensional Hubbard model can be reduced systematically by a grand-canonical integration over boundary conditions. We present results for ground-state properties of the two-dimensional (2D) Hubbard model and an evaluation of the specific heat for the 1D and 2D Hubbard model. We find the reduction of the finite-size corrections to be substantial, especially in two dimensions.

I. INTRODUCTION

The exact diagonalization of the Hubbard model (or the *t-J* model) on finite clusters has become one of the prominent techniques in the study of correlated electron systems.[1] This technique has the advantage of treating the correlations on finite clusters without any approximation. Since the Hilbert space grows exponentially with cluster size one is limited, for the Hubbard model, to clusters with up $N_s=10$ sites. By *finite-size corrections* is meant the difference between the results obtained for the finite cluster and its (unknown) value in the thermodynamic limit, $N_s=\infty$.

The control of the finite-size corrections poses a great challenge to the exact diagonalization technique, especially in the case of two dimensions. In one dimension, it is a standard procedure to plot the results systematically as a function of chain length, $N_s=6,8,10,12,\ldots$ sites. In two dimensions, on the other hand, where most calculations have been done up to now with either periodic or antiperiodic boundary conditions, it is difficult to estimate the finite-size corrections by direct comparison of clusters of different sizes, for two reasons: (1) The finite-size corrections are often nonmonotonic as a function of N_s, due to strongly varying cluster geometries. (2) The nominal density of particles, $n=N_e/N_s$ normally does not coincide for clusters of different sizes as the allowed number of particles $N_e=1,2,3,\ldots$ is an integer. Both of these two difficulties can be circumvented by a method introduced recently,[2] the *integration over boundary conditions* (IBC). The IBC circumvents the first of the above difficulties by performing a grand-canonical integration over boundary conditions. It has been shown that this procedure removes all those finite-size corrections that are caused by the special geometry of the Fermi sea of the cluster.[3] The *grand-canonical* approach then leads to the possibility of directly comparing the results for different N_s with the *same* density n, solving also the second of the above difficulties.

In a previous publication[2] the IBC had been introduced and some results for the Hubbard model on very small clusters had been presented. Here we want to study in detail how the finite-size corrections can be estimated *systematically* within the IBC both at zero and at finite temperatures. For this purpose we will concentrate on the Hubbard model, the same study could be performed, in principle, for the *t-J* model or any other cluster Hamiltonian.

II. INTEGRATION OVER BOUNDARY CONDITIONS

We consider the Hubbard Hamiltonian on a cluster with N_s sites,

$$H=\sum_{\langle i,j\rangle,\sigma}\left(t_{i,j}c^{\dagger}_{i,\sigma}c_{j,\sigma}+t^{*}_{i,j}c^{\dagger}_{j,\sigma}c_{i,\sigma}\right)+U\sum_{i}\ n_{i,\uparrow}n_{i,\downarrow} \quad (1)$$

where the symbol $\langle i,j\rangle$ denotes pairs of nearest neighbors sites and where the $c^{\dagger}_{i,\sigma}$ and the $c_{i,\sigma}$ are the electron creation/destruction operators of spin $\sigma=\uparrow,\downarrow$, respectively. The hopping amplitudes,

$$t_{i,j}\equiv -t\ \exp[i\alpha_{i,j}], \quad (2)$$

depend, in general, on phases $\alpha_{i,j}$, related to the boundary condition. In the following all energies will be measured in unities of t. We will now give an account of the IBC for 1D, the generalization to two dimensions is then straightforward.

In one dimension we can choose the $\alpha_{i,j}=\alpha/N_s$, where $\alpha\in[0,2\pi[$ is the boundary condition. Periodic and antiperiodic boundary conditions correspond to $\alpha=0$ and $\alpha=\pi$, respectively. The IBC technique needs the exact diagonalization of the cluster for any particle number $N_e=0,1,2,\ldots,2N_s$ and any $\alpha\in[0,2\pi[$. For any given α one then calculates the free energy,

$$F_{\alpha}(\mu)=-Tk_B\ln\left(\sum_{N_e=0}^{2N_s}e^{\beta\mu N_e}\sum_{k=0}^{N_H-1}e^{-\beta E_k(\alpha,N_e)}\right), \quad (3)$$

where $\beta=1/(k_BT)$ is the inverse temperature, μ is the chemical potential, N_H is the dimension of the Hilbert space, and the $E_k(\alpha,N_e)$ are the eigenenergies. (N_H depends on both on N_s and N_e.) The total free energy of the cluster and the particle density $n\in[0,2]$ are then given by the average

$$F(\mu)=\int_0^{2\pi}\frac{d\alpha}{2\pi}F_{\alpha}(\mu) \quad (4)$$

and by $n=-(1/N_s)[\partial F(\mu)/\partial\mu]$. The free energy obtained in Eq. (4) with the IBC technique is constructed in such a way that the finite size corrections *vanish identically* in the limit $U=0$.[2] One can understand this result most easily in momentum space, noting that the Fermi sea, as obtained by the IBC, has no finite-size corrections for $U=0$. This prop-

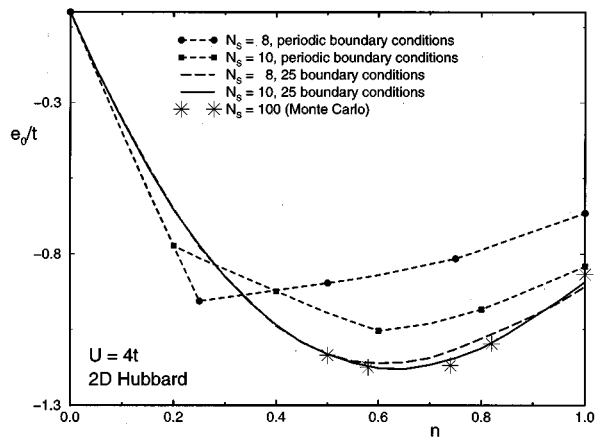

FIG. 1. The ground-state energy e_0 per site as a function of particle densitiy n. Plotted are the results for the 2D Hubbard model and $U=4t$. The filled circles and squares denote the results for clusters with periodic boundary conditions only, $N_\alpha=1$, for clusters with $N_s=8$ and $N_s=10$ sites, respectively. The long-dashed and the continuous line are the respective results for $N_\alpha=25$. Also shown (stars) are data obtained, by projection Monte Carlo for a 10×10 system, by Furukawa and Imada (Ref. 6).

erty of the IBC holds in any dimension and is especially important in two dimensions. The particle density n can, furthermore, be tuned to *any* value, by choosing an appropiate μ, allowing us to directly compare data from clusters with different N_s. These properties distingish the IBC technique from other exact diagonalization studies employing a range of boundary conditions.[4]

The integration over boundary conditions, appearing in Eq. (4), is replaced in actual calculations by a finite sum over N_α equidistant boundary conditions. Indeed, we will find here that only a few N_α are needed in order to already obtain most of the reduction in the finite-size corrections. Ground-state properties can be calculated, as usual, by the Lanczos technique. With $E_0(\alpha,N_e)$ being the ground-state energy for a given α and N_e one finds the estimate $e_0(\mu)$ for the grand-canonical ground-state energy per site to be

$$e_0(\mu)=\frac{1}{N_sN_\alpha}\sum_\alpha \inf_{N_e}[E_0(\alpha,N_e)-\mu N_e]. \tag{5}$$

A Legendre transformation then yields the canonical ground-state energy of the cluster, $e_0(n,N_s)$, as a function of density. In Fig. 1 we have plotted results obtained for the two-dimensional (2D) Hubbard model with $U=4t$. The results for $N_\alpha=1$, corresponding to periodic boundary conditions only, differ typically by $10\%-20\%$ in between clusters with $N_s=8$ and $N_s=10$ sites. Also shown in Fig. 1 are the data obtained for $N_\alpha=25$.[5] Here the data differ only by $1\%-2\%$ in between $N_s=8$ and $N_s=10$, an improvement by one order of magnitude. For comparision we have plotted also data obtained, by projection Monte Carlo for a 10×10 system with periodic boundary conditions, by Furukawa and Imada.[6]

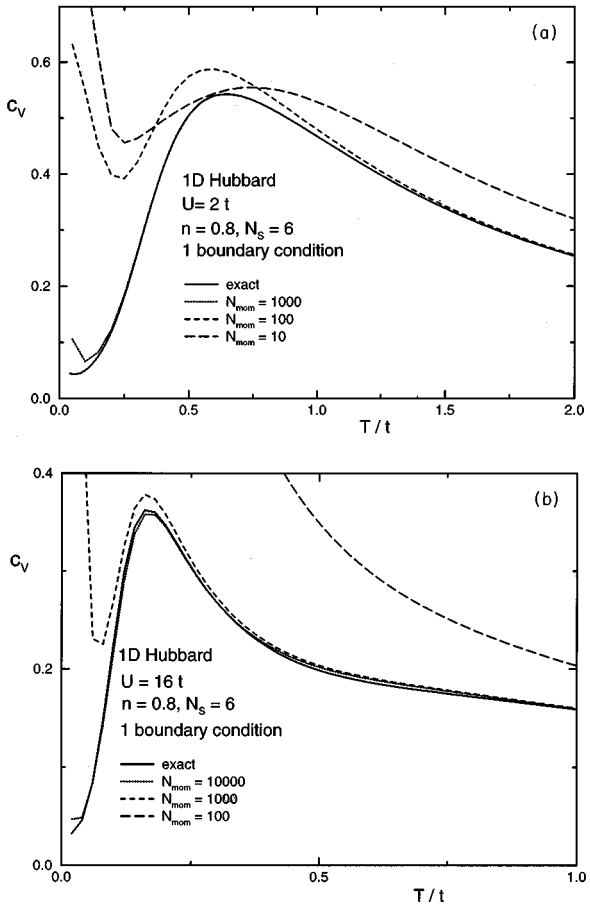

FIG. 2. The specific heat c_V per site, as a function of temperature, of a six-site chain with periodic boundary condition, $n=0.8$, and (a) $U=2t$ and (b) $U=16t$. Plotted are the exact results (solid line) and the results of the kernel polynomial approximation with (a) $N_{\mathrm{mom}}=10,100,1000$ and with (b) $N_{\mathrm{mom}}=100,1000,10\,000$.

III. SPECIFIC HEAT

Equation (3) for the free energy requires knowledge of all eigenstates and can therefore be used only for very small sytems, typically up to $N_s=6$ for the Hubbard model. Several approximative methods have been developed for the numerical evaluation of thermodynamic properties of systems with large Hilbert spaces.[7,8] Here we use the *kernel polynomial approximation* (KPA) developed by Silver and Roeder,[7] since it has a very good error control. One starts by scaling the Hamiltonian so that the magnitude of all eigenenergies is less than unity. The grand-canonical partition function, $Z_\alpha(\mu)=\exp[-\beta F_\alpha(\mu)]$, is then expressed as an integral over the density of states, $D_\alpha(\omega,N_e)=1/N_H\Sigma_{k=0}^{N_H-1}\delta[\omega-E_k(\alpha,N_e)]$,

$$Z_\alpha(\mu)=\sum_{N_e=0}^{2N_s} N_H e^{\beta\mu N_e}\int_{-1}^{1} d\omega D_\alpha(\omega,N_e)e^{-\beta\omega}. \tag{6}$$

The density of states can be expanded in a set of orthogonal polyomials; here we take Legendre polyomials $P_l(\omega)$:

$$D_\alpha(\omega,N_e)=\sum_{l=0}^{N_{\mathrm{mom}}} a_l(\alpha,N_e)P_l(\omega), \tag{7}$$

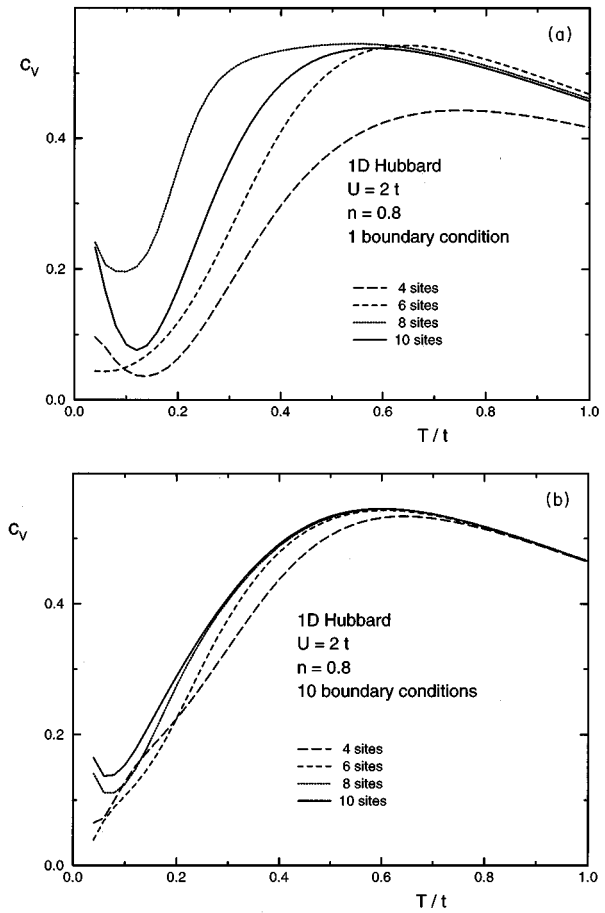

FIG. 3. The specific heat c_V per site as a function of temperature, for 1D chains with $N_s=4,6,8,10$, $U=2t$, $n=0.8$, and (a) $N_\alpha=1$ and (b) $N_\alpha=10$. For $N_s=4,6$ the data are exact, for $N_s=8,10$ the KPA has been used with $N_{\mathrm{mom}}=1000$ and $N_r=100,10$ for $N_s=8,10$, respectively.

with $N_{\mathrm{mom}}\to\infty$. Using the orthogonality relations for Legendre polynomials one can express the coefficients $a_l(\alpha,N_e)$ in term of the eigenstates of the Hamiltonian, $H|E_k(\alpha,N_e)\rangle=E_k(\alpha,N_e)|E_k(\alpha,N_e)\rangle$, via

$$a_l(\alpha,N_e)=\frac{2l+1}{2N_H}\sum_{k=0}^{N_H-1}\langle E_k(\alpha,N_e)|P_l(H)|E_k(\alpha,N_e)\rangle. \tag{8}$$

In practice one uses a finite $N_{\mathrm{mom}}<\infty$. A finite value of N_{mom} leads to the well-known Gibbs oscillations in $D_\alpha(\omega,N_e)$. The Gibbs oscillations can be smoothed out by the replacement $a_l\to a_l g_l(N_{\mathrm{mom}})$ in (7). The optimal functional form of the smoothing functions $g_l(N_{\mathrm{mom}})$, with $g_0(N_{\mathrm{mom}})=1$ and $g_{N_{\mathrm{mom}}+1}(N_{\mathrm{mom}})=0$, has been studied intensively in the literature.[7] We use $g_l(N_{\mathrm{mom}})=[\sin(z)/z]^3$, with $z=l\pi/(N_{\mathrm{mom}}+1)$.

The number N_{mom} of polynomials necessary for an accurate representation of the density of states in (7) increases with decreasing temperature T. We have evaluated the specific heat $c_V=\beta^2\langle(H-\langle H\rangle)^2\rangle/N_s$ per site for a six-site Hubbard chain with periodic boundary conditions exactly, via Eq. (3), and via the kernel polynomial approximation with various N_{mom}. We have plotted in Fig. 2 the results for (a)

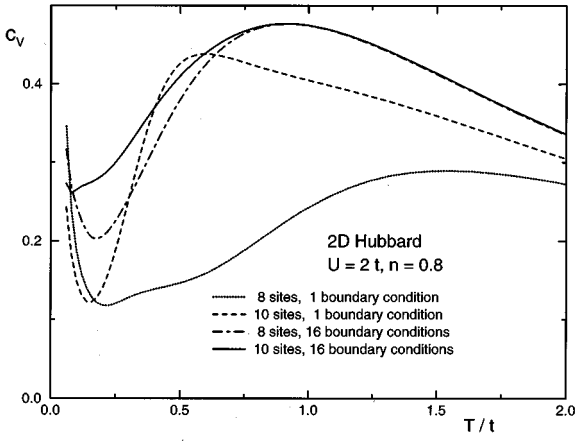

FIG. 4. The specific heat c_V per site as a function of temperature, for 2D clusters with $N_s=8,10$, $U=2t$, $n=0.8$. Plotted are the data for $N_\alpha=1$ (dotted/dashed line) and $N_\alpha=16$ (dashed-dotted/solid line). The KPA has been used with $N_{\mathrm{mom}}=1000$ and $N_r=10,8$ for $N_\alpha=1,16$, respectively.

$U=2$ and (b) $U=16$. The KPA becomes asymptotically exact for large temperatures and any values of N_{mom}. A numerically accurate approximation to the specific heat for temperatures down to $T\sim 0.25t$ may be obtained with $N_{\mathrm{mom}}\sim 10^3$ and $N_{\mathrm{mom}}\sim 10^4$, for $U=2$ and $U=16$, respectively. The large value, $N_{\mathrm{mom}}\sim 10^4$, needed for big U's, is the reason that all data presented in Sec. IV will be for $U=2$.

Formula (8) is clearly not useful for larger clusters. It has been observed[7] that one can *systematically* approximate the trace occuring in the right-hand side of (8) by sampling over N_r random states $|r\rangle$,

$$a_l(\alpha,N_e)\approx\frac{2l+1}{2N_r}\sum_{r=1}^{N_r}\langle r|P_l(H)|r\rangle. \tag{9}$$

It is possible to evaluate (9) recursively, by a procedure very similar to the Lanczos technique.[7] The errors introduced by random averaging vanish like $1/\sqrt{N_r}$.[7] We have performed extensive tests of the dependence of the data on N_r; we will present in Sec. IV only data that are unaffected by finite-N_r effects.

IV. RESULTS

In Fig. 3 we have plotted the results for the specific heat per site for various 1D chains of length $N_s=4,6,8,10$, both for the case of periodic boundary conditions only, $N_\alpha=1$, and for $N_\alpha=10$. Let us first note that the specific-heat curves for clusters of different sizes must eventually all coincide at large enough temperatures, due to the grand-canonical formulation. At large enough temperatures the leading terms contributing to the specific heat of a cluster of a given size are identical to the leading terms of high-temperature expansions. One can consequently define a $T^*(N_s,\epsilon)$ as the temperature above which the finite-size corrections to the specific heat are smaller than a given accuracy ϵ, say $\epsilon\sim 1\%$. As the specific heat for $N_s=\infty$ is generally not known, we took as a practical estimate for $T^*(N_s,\epsilon)$ the criterion that

$|c_v(T,N_s)-c_v(T,N_s-2)|<\epsilon$ for all $T>T^*(N_s,\epsilon)$. We found that $T^*(N_s,\epsilon)$ is roughly inversely proportional to N_s, for the 1D data presented in Fig. 3, and that the integration over boundary conditions reduces $T^*(N_s,\epsilon)$ by factors of 2–3, as is evident from a comparison of Figs. 3(a) and 3(b).

The IBC improves the cluster estimates of the specific heat in a second way, besides the reduction of $T^*(N_s,\epsilon)$. One finds empirically that the specific heat becomes *linear* at low temperatures in the limit $N_\alpha\to\infty$. This property of the low-T specific heat is present for all N_s and is a consequence of the absence of those finite-size corrections that are caused by the geometry of the Fermi surface of the cluster, within the IBC.[3] For finite N_α there will be in general an intermediate temperature range where the specific heat is roughly linear, as is the case for $N_\alpha=10$ in Fig. 3(b) for temperatures $0.1t\lesssim T\lesssim 0.3t$. This feature of the specific-heat data obtained with the IBC may be used, e.g., to estimate the inverse effective mass.

In Fig. 4 we present the specific heat per site, as a function of temperature, for 2D clusters with $N_s=8,10$, $U=2t$, $n=0.8$ and $N_\alpha=1$, and $N_\alpha=16$. The improvement obtained with the IBC is even more pronounced than in one dimension. The data for periodic boundary conditions are affected so much by finite-size errors that they do not allow for a reliable estimate of the specific heat for $T<2t$. For $N_\alpha=16$ the finite-size corrections are, on the other hand, practically absent for $T>T^*(N_s=10,\epsilon\sim 1\%)\sim 0.72t$.

In conclusion, we have shown that the IBC can be used to reduce substantially the finite-size corrections occuring in exact diagonalization studies. The data obtained by the IBC show, typically, a smooth behavior as a function of cluster size, even in two dimensions, where the cluster geometry may vary widely from cluster to cluster. This smooth behavior often allows for *quantitative* estimates of the finite-size corrections of the data obtained by the IBC, even in two dimensions. One obtains, furthermore, certain qualitative improvements with the IBC, such as a linear specific heat for the Hubbard model on one- and two-dimensional clusters.

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