Large-U expansions for the Hubbard model at $T=0$

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We report results for the ground-state energy of the Hubbard model in the form of perturbation expansions in t/U, i.e., expansions about the strong-coupling or "atomic" limit. Expansions to order $(t/U)^{40}$ are obtained for finite cells with number of sites ≤ 10, for the half-filled case, for both the linear chain and two-dimensional (2D) square lattice. Analysis of the series by Padé approximant methods yields, in the 1D case, results consistent with the known exact results. For the largest cell, $N=10$, on the square lattice there is an indication of a singularity on the real t axis, which may indicate a phase transition at $U/t \simeq 4$.

The single-band Hubbard model is the simplest model system for describing the physics of strongly correlated electrons on a lattice. As such it is of relevance for theories of high-temperature superconductivity,[1] even though no definitive theory for this intriguing phenomenon has yet appeared.

The Hubbard Hamiltonian is

$$H=-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where the first term represents noninteracting electrons hopping between Wannier states on neighboring sites and the second term is a Coulomb repulsion for electrons on the same site. The phase diagram is then described in terms of the two parameters U/t and n, the number of electrons per site. The half-filled band corresponds to $n=1$. Despite the simplicity of the Hamiltonian the number or rigorous (or even generally accepted) results is small.[2,3] It is known, for example, that in one dimension the ground state for $n=1$ is an antiferromagnetic insulator for all $U\neq 0$ and is metallic at $U=0$. For non-half-filling the model is a paramagnetic metal for all U. Thus, in a sense, the one-dimensional Hubbard model has a Mott transition at $U=0$. In higher dimensions even the form of the phase diagram at $T=0$ is not known with any degree of confidence. Mean-field approximations[4] give extended regions of ferromagnetic and antiferromagnetic ordering for sufficiently large U/t. For $n=1$ the antiferromagnetic region extends to $U/t=0$, but is asymptotically of zero width. It seems likely that this behavior is qualitatively correct in three-dimensions but may well be wrong in two dimensions where quantum fluctuations are stronger.

In this paper we report studies of the ground state of the one- and two-dimensional Hubbard models for the half-filled case $n=1$. In particular we seek to obtain expansions for the ground-state energy in the form

$$\varepsilon_0=E_0/N=-\sum_{r=2}^{\infty}a_r t^r\ , \tag{2}$$

where, without loss of generality, we take $U=1$ hereafter. This is an expansion about the "atomic limit" $t=0$ (or $U=\infty$) where the Hamiltonian is diagonal and trivial, albeit with a highly degenerate ground state. If there is a phase transition in the model at some finite U/t then, in principle, this might be evident as a singularity in the expansion (2) which could be detected by Padé approximant or other methods.

Perturbation expansions about the atomic limit for the Hubbard model have a long history, going back at least to Anderson's demonstration[5] that, to second order in t, the full Hamiltonian (1) is equivalent to the Heisenberg antiferromagnet

$$H_{\text{eff}}=\frac{4t^2}{U}\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})\ . \tag{3}$$

Subsequent workers[6] have extended this to the t^6 term, all the odd terms vanishing for the half-filled case. This work has all been at the Hamiltonian level so that to determine the coefficients in the expansion (2) there is a further task, namely, to determine the ground-state energy of the effective Hamiltonian. This is already an impossible task at second order for dimensionality $d>1$. Furthermore the effective Hamiltonian becomes so complicated with increasing order that it would be barely feasible to go beyond the t^8 terms and the resulting series would be too short for one to have any confidence in a Padé analysis.

For these reasons we have sought to work not at the level of effective Hamiltonians but rather with the ground-state energy directly. This is, of course, also a very difficult problem for the infinite lattice since the unperturbed ground state is already infinitely degenerate. However for finite systems the state space is finite dimensional and it is not difficult to develop the perturbation expansion to arbitrarily high order, as we do below. The problem then is to extrapolate to the $N=\infty$ limit. Fortunately the coefficients in the energy expansion can be obtained exactly[7] for the one-dimensional case for $n=\infty$ from the Bethe ansatz results of Lieb and Wu.[3] For $n=1$ the result

TABLE I. Coefficients in the perturbation expansion for the ground-state energy of the one-dimensional Hubbard model. Coefficients up to a_{40} inclusive have been obtained and can be supplied on request.

N	2	4	6	8	10	∞
a_2	8.0	3.0	2.8685	2.8255	2.8062	2.7726
a_4	−128.0	−30.0	−11.3061	−11.0852	−10.9869	−10.8185
a_6	4096.0	624.0	249.5302	79.3675	78.7335	77.7696
a_8	−163 840.0	−16 392.0	−8267.693	−2700.723	−696.655	−694.816
a_{10}	7 340 032.0	484 032.0	224 790.03	126 167.19	33 630.39	7042.6

$$\varepsilon_0=-(4\ln 2)t^2+\sum_{r=2}^{\infty}(-1)^{r-1}\left[\frac{(2r-1)!!}{(2r)!!}\right]^2\frac{\zeta(2r-1)}{2r-1}2^{4r}\left[1-\frac{1}{2^{2r-2}}\right]t^{2r} . \tag{4}$$

This provides an important check for our finite lattice results and extrapolation procedures.

We consider then the Hamiltonian

$$H=\sum_i n_{i\uparrow}n_{i\downarrow}-t\sum_{\substack{\langle i,j\rangle\\ \sigma}}(c_{i\sigma}^{\dagger}c_{j\sigma}+\mathrm{H.c.})$$
$$=H_0-tV ,$$

where the second term is taken as a perturbation and we treat lattices of N sites, with periodic boundary conditions. We take as our basis set the usual occupation number states, eigenstates of H_0, which are conveniently represented in terms of $2N$ bits of a single computer word. Since we are considering the half-filled case $n=1$ and since it is known[2] that the ground state has $S=0$ the size of the basis is reduced from 4^N to the following dimensions for $N=2$, 4, 6, 8, 10, respectively: 4, 36, 400, 4900, 63 504. Matrix elements of V can be easily computed with the aid of logical bit operations, and only nonzero elements of V are stored. The unperturbed ground state is highly degenerate, lying in the subspace with all sites singly occupied—the dimensionality of this subspace being 2, 6, 20, 70, 252 for the above values of N. The degeneracy is not lifted in first order, but is lifted completely in second order. According to standard degenerate state perturbation theory the second-order energy change [the coefficient a_2 is (2)] is given by the largest eigenvalue of the matrix W with elements

$$W_{ij}=\sum_{k=m_0+1}^{m}\frac{\langle i|V|k\rangle\langle k|V|j\rangle}{\varepsilon_0-\varepsilon_k} ,$$

where m_0,m are the dimensionalities of the unperturbed ground-state subspace and total space and ε_k are the unperturbed energies. W is itself of dimension m_0. The corresponding eigenvector of W gives, as usual, the correct linear combination of basis states for the zeroth-order wave function. Once this has been obtained the perturbation equations can be solved iteratively to obtain values of the successive a_r coefficients.

In Table I we give values of these coefficients for the linear chain for $N=2$, 4, 6, 8, 10 and, for comparison, the values for $N=\infty$ obtained from (4). By inspection it is apparent that the $a_r(N)$ coefficients are converging to the known $a_r(\infty)$ values, and for $r\le 8$ the $N=10$ results are within a fraction of a percent of the $N=\infty$ values. However for $r>8$ larger lattices are needed. For the one-dimensional Hubbard model the asymptotic form of the finite-size correction to the ground-state energy per site is known[8] to be

$$\varepsilon_0^{(N)}-\varepsilon_0^{(\infty)}=-\frac{1}{N^2}\left[\frac{\pi t}{3}\frac{I_1(2\pi t)}{I_0(2\pi t)}\right]+\dots$$
$$=-\frac{1}{N^2}\left[\frac{\pi^2}{3}t^2-\frac{\pi^4}{6}t^4+\frac{\pi^6}{9}t^6-\dots\right]$$

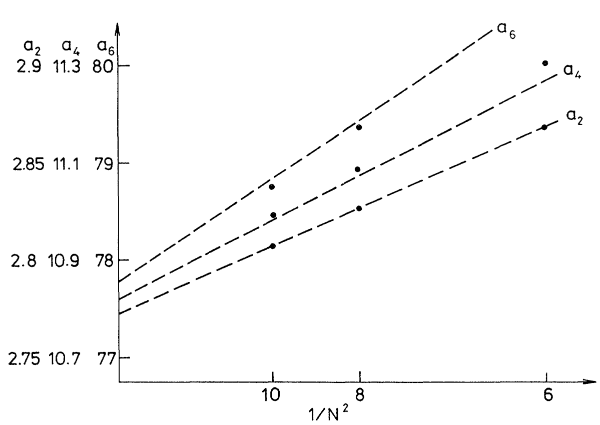

FIG. 1. Coefficients a_2,a_4,a_6 of the ground-state energy of the one-dimensional Hubbard model versus $1/N^2$. The lines represent the known asymptotic finite-size correction limits, Eq. (5).

TABLE II. Coefficients in the perturbation expansion for the ground-state energy of the two-dimensional Hubbard model. Coefficients to a_{40} to 12 significant figures can be obtained on request. $xEy = x\times 10^y$.

N	4	8	10
a_2	0.12E2	0.5E1	0.492 0E1
a_4	0.48E3	−0.14E3	−0.993 0E2
a_6	0.399 4E5	0.832 E4	0.570 9E4
a_8	−0.419 6E7	−0.631 4E6	−0.411 2E6
a_{10}	0.495 6E9	0.541 4E8	0.334 9E8
a_{12}	−0.628 2E11	−0.499 5E10	−0.292 8E10
a_{14}	0.834 9E13	0.483 9E12	0.268 7E12
a_{16}	−0.114 8E16	−0.485 3E14	−0.255 5E14
a_{18}	0.161 9E18	0.499 6E16	0.249 4E16
a_{20}	−0.233 0E20	−0.525 0E18	−0.248 4E18

and hence

$$a_r^{(N)} - a_r^{(\infty)} \simeq C_r/N^2 \quad (5)$$

with $C_2=\pi^2/3$, $C_4=\pi^4/6$, $C_6=\pi^6/9, \ldots$. In Fig. 1 we show a plot of these coefficients versus $1/N^2$, together with the known asymptotic behavior.

Another method for extrapolating from the finite lattice results to the infinite lattice is to consider the expansion (2) as a power series for E_0 in the (complex) variable t and to use Padé approximants to investigate the positions and nature of the singularities. In this way one can investigate the way in which the singularities change as N increases and infer something about the nature of the singularities for the infinite lattice. We first consider the one-dimensional case. For $N=2$ the ground-state energy is obtainable in closed form as

$$\varepsilon_0 = -\tfrac{1}{4}[(1+64t^2)^{1/2}-1]$$

and thus has square-root singularities on the imaginary axis at $\pm 0.125i$. For $N=4$ Villet and Steeb[9] have obtained a closed expression of ε_0 which can be written in the form

$$\varepsilon_0 = 1-(1+16t^2)^{1/2}\left[\sin\theta + \frac{1}{\sqrt{3}}\cos\theta\right],$$

where

$$\tan 3\theta = -\frac{1}{12\sqrt{3}\,t^2}(1+48t^2+336t^4+4096t^6)^{1/2}.$$

TABLE III. Poles and residues (in parentheses) from Padé approximants to $(d/dx)\ln E_0(x)$ $(x=t^2)$ for a finite cell with $N=10$ on the square lattice. Note that the negative poles correspond to poles on the imaginary axis in the t plane, whereas positive poles correspond to poles on the real axis in the t plane.

$[N,D]$	Poles and residues		
[7,11]	−0.008 62	−0.009 54	0.0678
	(0.053)	(0.055)	(−0.030)
[8,10]	−0.008 65	−0.009 83	0.0926
	(0.060)	(0.060)	(−0.072)
[9,9]	−0.008 64	−0.009 74	—
	(0.058)	(0.058)	
[10,8]	−0.008 63	−0.009 76	—
	(0.057)	(0.059)	
[11,7]	−0.008 63	−0.009 66	0.0585
	(0.056)	(0.056)	(0.053)
[6,11]	−0.008 63	−0.009 62	0.0845
	(0.055)	(0.056)	(−0.020)
[7,10]	−0.008 63	−0.009 63	0.0651
	(0.056)	(0.056)	(−0.027)
[6,10]	−0.008 62	−0.009 58	0.0680
	(0.054)	(0.055)	(−0.030)
[5,10]	−0.008 63	−0.009 61	0.0589
	(0.055)	(0.056)	(−0.015)

This result provides a check on our perturbation procedure. There are square-root singularities at $t=\pm 0.25i$, $t=\pm 0.1536i$, $t=\pm 0.185\pm 0.252i$, and these are consistently detected by a Padé analysis of the series. In practice the most consistent results are obtained by analyzing the series for the derivatives or logarithmic derivative. The series for $N=6$, 8, 10 have been analyzed in a similar way. In all cases the singularities lie either on or clustered around the imaginary axis, with the magnitudes of the real parts of complex singularities decreasing with increasing N. From this we might conjecture that for $N=\infty$ the singularities in ε_0 lie entirely on the imaginary axis. This is indeed correct as Takahashi has shown[7] that for $N=\infty$ ε_0 has logarithmic singularities at $t=\pm in/4$, $n=1,2,\ldots$.

Finally we turn to the two-dimensional case, where we consider periodic cells with $N=4$, 8, 10 on the square lattice. In Table II we give the values of the perturbation coefficients. It is clear that, except perhaps for the lowest coefficient a_2, there is insufficient data for any reasonable estimate of the infinite lattice coefficients to be made by extrapolation. Padé approximant analysis of the finite-lattice series, which have been computed to order t^{40}, yields interesting results. For $N=8$ we find a sequence of singularities on the imaginary axis at $t=\pm 0.090i$, $t=\pm 0.092i$, $t=\pm 0.097i,\ldots$, with no indication of any singularities on the real axis. This is very similar to the one-dimensional lattice and suggests the same kind of analytic structure. For $N=10$ we again find singularities predominantly on the imaginary axis at $t=\pm 0.093i$, $t=\pm 0.098i$. However there is also a consistent singularity on the real axis. Some typical results are shown in Table III. The singularity on the real axis at $t\pm 0.25(\pm 0.05)$ lies well outside the radius of convergence of the series, which is determined by the closest singularity to the origin. We have to admit the possibility that it is spurious, and does not represent a true physical singularity in ε_0. Yet is occurs in at least half of the high-order Padé approximants and it is tempting to conjecture that it represents a real phase transition, presumably a metal-insulator transition, at $U/t\simeq 4$. Although we do not expect such a finite-U transition at precisely $n=1$ an infinitesimal departure from half-filling could give rise to a finite U_c and the singularity we observe might be indicating this. This result, if confirmed, would suggest that the phase diagram of the two-dimensional Hubbard model is significantly different from the one-dimensional case. Further work is in progress.

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