Thermodynamics of the Extended Hubbard Model in High Dimensions

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(Received 21 February 1991; revised manuscript received 10 May 1991)

The extended Hubbard model with on-site interaction U and nearest-neighbor interaction V/d is studied at half filling in high dimensions ($d \gg 1$). At small U and V the critical temperature and the order parameter are calculated including the $1/d$ corrections. The results differ from those obtained in the Hartree approximation by a factor of order *unity*. At $V/U = 1/2$ a transition is found from an antiferromagnetic to a charge-density-wave phase. A similar transition is found at large U and V, suggesting that the transition is present for all U and V satisfying $V/U = 1/2$.

PACS numbers: 71.10.+x, 71.45.Lr, 75.10.Lp, 75.30.Fv

Since its introduction in 1963 by Hubbard, Gutzwiller, and Kanamori [1], the Hubbard model has become an important standard model for correlated fermions on a lattice. To illustrate its importance, we merely note that it has been used to explain the metal-insulator transition [1,2], antiferromagnetism [3], ferromagnetism [4], paramagnetism at high temperatures [5], and, most recently, superconductivity in the less-than-half-filled band [6]. A well-known generalization of the Hubbard model is the so-called extended Hubbard model, which also takes into account the nearest-neighbor interaction. Until now, the extended Hubbard model has been treated mainly on the mean-field level [7,8]. In this Letter we will study the extended Hubbard model beyond the mean-field approximation on a hypercubical lattice in high dimensions.

The Hamiltonian of the extended Hubbard model has the form

$$H = H_t + H_U + H_V + H_\mu , \tag{1}$$

where

$$H_t = -\frac{t}{\sqrt{2d}} \sum_{\langle \mathbf{ij} \rangle, \sigma} (c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \text{H.c.}), \quad H_\mu = -\mu \sum_{\mathbf{i}} n_{\mathbf{i}} ,$$

$$H_U = U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}, \quad H_V = \frac{V}{d} \sum_{\langle \mathbf{ij} \rangle} n_{\mathbf{i}} n_{\mathbf{j}} .$$

Here $c^\dagger_{\mathbf{i}\sigma}$ ($c_{\mathbf{i}\sigma}$) creates (destroys) an electron with spin σ at site $\mathbf{i}$, $n_{\mathbf{i}\sigma} \equiv c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma}$, $n_{\mathbf{i}} \equiv n_{\mathbf{i}\downarrow} + n_{\mathbf{i}\uparrow}$, and d is the space dimension. The grand canonical Hamiltonian (1) describes hopping of electrons (H_t), interacting with each other through on-site (H_U) and nearest-neighbor (H_V) Coulomb repulsion. The prefactors in H_t and H_V are chosen such that a finite, nonvanishing energy contribution is obtained for $d \to \infty$ [9,10]. Below we choose $U > 0$ and $V > 0$, and $t = 1$ to fix the energy scale. The original Hubbard model corresponds to $V = 0$ in (1). The half-filled band corresponds to $\mu = \frac{1}{2} U + 2V$.

Two years ago the concept of high dimensions was introduced [9] as a new approach to correlated Fermi systems on a lattice. Since then, the study of high-dimensional Fermi systems has been very fruitful [10,11], and led, e.g., to the exact solution of the Falicov-Kimball model in $d = \infty$ [12] and to the recent study of mean-field theories that become exact in high dimensions [13]. Unfortunately one of the most interesting goals, the exact solution of the Hubbard (or extended Hubbard) model in $d = \infty$, has not yet been reached. In this Letter we will show that it is nevertheless possible to obtain valuable information about these models in certain limits.

The basic questions addressed in this Letter are as follows: What is the phase diagram of the extended Hubbard model at half filling? Mean-field theory predicts a phase transition at low temperatures for all U and V: Does it really occur? If so, what is the critical temperature? What is the temperature dependence of the order parameter? Is the transition first or second order? The strategy of this Letter is as follows. First, we study the model at small interaction strengths U and V (which is the more difficult case). Next we consider the opposite limit, $U \to \infty$ and $V \to \infty$. In taking these limits we will keep the ratio $v \equiv V/U$ fixed. Combination of these results then gives insight into the global phase diagram of the extended Hubbard model at half filling.

We start with the thermodynamical properties for $U, V \to 0$. The basic idea at small U and V is that the thermodynamics of the extended Hubbard model in high dimensions can be determined by applying perturbation theory. The small parameters are, first the interaction strengths U and V and, second, the inverse dimension $1/d$. However, the *standard* perturbation expansion (around the Hartree solution) leads to incorrect results. To see this we consider the Hartree approximation first [14].

The Hartree approximation is obtained by decoupling the interaction terms in H_U and H_V in (1):

$$n_{\mathbf{i}\sigma} n_{\mathbf{j}\sigma'} \to \langle n_{\mathbf{i}\sigma} \rangle n_{\mathbf{j}\sigma'} + n_{\mathbf{i}\sigma} \langle n_{\mathbf{j}\sigma'} \rangle - \langle n_{\mathbf{i}\sigma} \rangle \langle n_{\mathbf{j}\sigma'} \rangle .$$

Since we consider half filling, we make the usual assumption [15] that the average density $\langle n_{\mathbf{i}\sigma} \rangle$ is equal to $\frac{1}{2}(1 + \Delta_\sigma)$ on one sublattice (labeled by $+$), and equal to $\frac{1}{2}(1 - \Delta_\sigma)$ on the other (labeled by $-$). The symmetry between $\sigma = \uparrow, \downarrow$ then implies that either $\Delta_\uparrow = \Delta_\downarrow$ [which corresponds to a charge-density wave (CDW)], or $\Delta_\uparrow = -\Delta_\downarrow$ [which corresponds to antiferromagnetism (AFM)]. The order parameter $\Delta \equiv \Delta_\uparrow$ is denoted by Δ^H in the Hartree approximation, and can be calculated from

the consistency requirement $\langle n_{i\uparrow}\rangle_H = \frac{1}{2}(1 \pm \Delta^H)$ if $i \in (\pm)$. As usual there are two solutions: a trivial solution $\Delta^H = 0$ and a nontrivial solution $\Delta^H > 0$ that has a lower (Hartree) free energy. We focus on the nontrivial solution below. What does the Hartree approximation predict? The critical temperature T_c^H in d dimensions can be determined by putting $\Delta^H(T_c) = 0$ and solving for T_c as a function of U and V. The result is

$$k_B T_c^H \sim \exp\left[I_d - \frac{1}{2\alpha U \nu_d(0)} \right] \quad (U, V \to 0), \tag{2}$$

where the constant I_d is given by

$$I_d = \int_0^\infty dy \frac{1}{y}\left[\tanh y - 1 + \frac{\nu_d(y)}{\nu_d(0)} \right] - \ln 2 .$$

Here $\nu_d(y)$ is the density of states in d dimensions and $\alpha = 2v - \frac{1}{2}$ for the CDW or $\alpha = \frac{1}{2}$ in the antiferromagnetic (AFM) phase. Thus T_c^H is exponentially small if U is small. One can introduce a rescaled order parameter $\delta \equiv \frac{1}{2}\alpha U \Delta^H / k_B T_c^H$ and a rescaled temperature $\theta \equiv T/T_c^H$, which for $U \to 0$ are related by

$$0 = \int_0^\infty dy \left[\frac{\tanh[(y^2+\delta^2)^{1/2}/\theta]}{(y^2+\delta^2)^{1/2}} - \frac{\tanh y}{y} \right]. \tag{3}$$

The limiting behavior of $\delta(\theta)$ for $\theta \downarrow 0$ and $\theta \uparrow 1$ can be calculated analytically. For $\theta \downarrow 0$ one finds that $\delta(\theta)$ approaches the limiting value $\delta(0) = \frac{1}{2}\pi e^{-\gamma}$ exponentially, where $\gamma = 0.577\ldots$ is Euler's constant. For $\theta \uparrow 1$ one obtains mean-field critical behavior, $\delta(\theta) \sim A(1-\theta)^{1/2}$ with $A \simeq 1.53$. Since $\delta(\theta) = \mathcal{O}(1)$, the order parameter Δ^H is of order $k_B T_c^H / U$, which is exponentially small if U is small. The gain in free energy Ω_S^H due to symmetry breaking can also be calculated:

$$\Omega_S^H(T) \sim -\alpha^2 U^2 (\Delta^H)^2 \nu_d(0) \Phi(\theta) \quad (U \downarrow 0), \tag{4}$$

where

$$\Phi(\theta) \equiv \int_0^\infty dy \left[\frac{2\theta}{\delta^2} \ln\left[\frac{\cosh[(y^2+\delta^2)^{1/2}\theta]}{\cosh(y/\theta)} \right] - \frac{\tanh y}{y} \right].$$

Note that the *lowest* free energy is obtained for the state with the *largest* value of α. Hence the system is in the CDW phase for $v > \frac{1}{2}$ and AFM for $v < \frac{1}{2}$, at least in the Hartree approximation [7].

The fact that the prefactor of $(\Delta^H)^2$ in (4) is small, of order U^2 for $U \downarrow 0$, shows that one *cannot* use standard perturbation theory around the Hartree solution to study the fluctuations. The reason is that the contribution of the second-order diagrams to the free energy gain is of the *same* order of magnitude as Ω_S^H in (4). Hence the thermodynamics at small U and V is determined by the Hartree contribution and the fluctuations together—the Hartree approximation alone leads to incorrect results. Indeed, we will see below that the actual critical temperature and order parameter differ from the Hartree predictions by factors of the order of *unity*. To study the fluctuations we use a method proposed very recently by Georges and Yedidia [16]. The basic idea is to calculate the free energy $\Omega(U,\Delta)$ in perturbation theory at an arbitrary but *fixed* value of the order parameter Δ:

$$\Omega(U,\Delta) = \Omega_0(\Delta) + U\Omega_1(\Delta) + U^2\Omega_2(\Delta) + \cdots . \tag{5}$$

The various terms in (5) depend implicitly on v and T. The equilibrium value of Δ is then determined by minimization of $\Omega(U,\Delta)$ with respect to Δ. In order to keep the order parameter in (5) fixed one introduces a Lagrange parameter $h(U)$, which couples linearly to the staggered magnetization (in the AFM case) or to the staggered charge density (in the CDW case). The value of $h(U)$ is tuned such that Δ is fixed, at least up to the desired order in perturbation theory.

The various diagrams that have to be calculated (up to order $1/d$) in this approach are listed in Fig. 1. A vertex H_U is represented by a broken line, and a vertex H_V by a wiggly line. The Green functions have the form of Hartree Green functions, with the usual energy gap replaced by the Lagrange parameter $h_0 \equiv h(0)$. The basic simplification occurring in high dimensions is that the Green functions $\langle T_\tau c_{j+s,\sigma}(\tau) c_{j\sigma}^\dagger(0)\rangle$ in position space fall off very rapidly with distance ($\propto d^{-|s|/2}$ as $d \to \infty$). Hence only the Green functions for $|s| = 0, 1$ are needed to calculate the free energy as a function of h_0 for $U \downarrow 0$ up to order $1/d$. These matrix elements can readily be calculated in general dimensions d.

Minimization of $\Omega(U,\Delta)$ in (5) up to second order in U yields the following results. The critical temperature and the order parameter can be expressed in terms of a scaling factor $q(v) \equiv \exp(-C_0 - C_1 d^{-1})$, with

$$C_0 = \frac{1}{2\sqrt{2}\alpha^2} \ln \tan\left(\frac{3\pi}{8}\right),$$
$$C_1 = \frac{(\alpha-1)v}{2\alpha^2} - \frac{1}{64\alpha^2} + C_0\left(\frac{3}{32} + v + 4v^2\right). \tag{6}$$

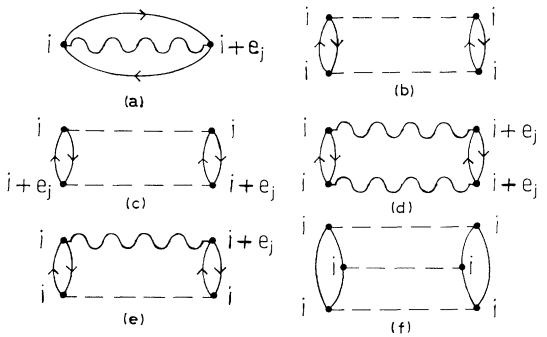

FIG. 1. Some diagrams describing the fluctuations due to H_U [graphs (b), (c), and (f)], H_V [graphs (a) and (d)], or both [graph (e)]. The site index $\mathbf{i}$ and the lattice vector $\mathbf{e}_j$ in the j direction are summed over.

The constants C_0 and C_1 are strictly positive, so that $q(v) < 1$ for all $v \geq 0$. From the minimization procedure to second order in perturbation theory one finds that the actual critical temperature is reduced by a factor q relative to the Hartree prediction T_c^H:

$$T_c \sim q T_c^H \quad (U,V \downarrow 0). \tag{7}$$

Similarly the order parameter is reduced by a factor q relative to $\Delta^H(T)$,

$$\Delta(T) \sim q \Delta^H(T/q) \quad (U,V \downarrow 0), \tag{8}$$

and the free-energy gain due to symmetry breaking is

$$\Omega_S(T) \sim q^2 \Omega_S^H(T/q) \quad (U,V \downarrow 0). \tag{9}$$

Equations (7) and (8) show that, if we redefine $\theta \equiv T/T_c$ and $\delta \equiv \frac{1}{2} \alpha U \Delta / k_B T_c$, the relation between δ and θ is precisely the same as in Eq. (3) for the Hartree approximation. Combination of (4) and (9) further shows that $\Omega_S < 0$, i.e., that symmetry breaking is stable also if fluctuations are taken into account. Another important point is that the constants C_0 and C_1 are smallest (so that T_c and $|\Omega_S|$ are largest) if one chooses $\alpha = \max\{\frac{1}{2}, 2v - \frac{1}{2}\}$. This shows that the first-order transition between the AFM and CDW phases, occurring at $v = \frac{1}{2}$ at the Hartree level, is robust against the inclusion of fluctuations and $1/d$ corrections.

We comment briefly on the calculation of $q(v)$. The leading contribution C_0 in (6) is solely due to graph (b) in Fig. 1. The $1/d$ corrections represented by C_1 come from diagrams (a), (d), and (e), and from the $1/d$ terms in diagram (b). The contribution of graph (c) is negligibly small (of relative order U) [17]. An important point is that the higher-order graphs due to H_U yield vanishingly small contributions as $U \downarrow 0$. In particular, the contribution due to the third-order diagram [graph (f)] is of relative order U compared to graph (b), yielding only a correction of order U to $q(v)$.

Next consider the thermodynamics at large U and V. The important point here is that the same transition from an AFM to a CDW phase, that was found above for small U and V, is also found for $U,V \rightarrow \infty$. Just as for $U,V \downarrow 0$, the transition between these two types of symmetry breaking occurs at $v = \frac{1}{2}$.

The CDW phase is obtained for $v > \frac{1}{2}$. In this case the kinetic energy is negligible (of relative order U^{-1}) compared to the remaining terms in (1), so that the Hamiltonian can be approximated by $H_U + H_V + H_\mu$. In $d = \infty$, H_V can be treated in Hartree approximation [10], and the free energy can readily be calculated as a sum of one-site contributions. As above, we parametrize the density by Δ_σ, where now $\Delta_\uparrow = \Delta_\downarrow > 0$. The order parameter $\Delta(T)$ can be obtained as the value of $\Delta_\uparrow$ for which the free energy is minimal. The result is

$$\Delta = \frac{\sinh(2\beta V \Delta)}{e^{\beta U/2} + \cosh(2\beta V \Delta)}, \tag{10}$$

where $\beta \equiv 1/k_B T$. For $v \rightarrow \infty$, (10) reduces to the well-known Curie-Weiss form, with a critical temperature $T_c = V/k_B$. In general, (10) implies that the phase transition is *second* order if $v > 3/(4 \ln 2)$, or, numerically, $v > 1.0820$. For $\frac{1}{2} < v < 1.0820$ the transition is *first* order, with a transition temperature that vanishes as $v \downarrow \frac{1}{2}$: If $V = \frac{1}{2} U + \epsilon$, then $k_B T_c \sim \epsilon / \ln 2 \rightarrow 0$ as $\epsilon \downarrow 0$. No (nonmagnetic) broken symmetry phase exists for $\epsilon < 0$, or $v < \frac{1}{2}$.

For $v < \frac{1}{2}$ the low-temperature phase has AFM order. One can carry out a canonical transformation to new fermionic variables in a subspace without double occupancy [18]. As a result one finds [8] that (1) reduces for general d to an effective AFM Heisenberg Hamiltonian with coupling constant $J = -2/(dU - V)$. For $d \rightarrow \infty$ this implies that one has AFM order with a critical temperature $T_c \sim 1/k_B U$. The order parameter satisfies the Curie-Weiss relation $\Delta = \tanh(\Delta/\theta)$, with $\theta \equiv T/T_c$.

The transition from the AFM to the CDW phase can easily be understood by considering the ground state. For the CDW ground state ($v > \frac{1}{2}$) the energy per site is $\frac{1}{2}$U, and for the Néel state it is $V - \mathcal{O}(U^{-1})$. Hence the transition occurs at $v = \frac{1}{2}$, at least if U and V are large.

Combination of the results for $U,V \downarrow 0$ and $U,V \rightarrow \infty$ leads to several interesting observations. The behavior of the model for $v < \frac{1}{2}$ is qualitatively the same as that for the pure Hubbard model ($V = 0$): One finds antiferromagnetism both at small and at large interaction, with T_c exponentially small for $U,V \downarrow 0$ and $k_B T_c \sim U^{-1}$ for $U,V \rightarrow \infty$. For $v > \frac{1}{2}$ the low-temperature phase is a CDW, but now T_c *increases* proportionally to U or V as $U,V \rightarrow \infty$. Another interesting feature is the occurrence of a change in the nature of the phase transition as one passes from small to large U and V: For $\frac{1}{2} < v < 1.0820$ the transition is second order for small U and V, but first order for $U,V \rightarrow \infty$. The crossover between these two regimes must occur at some finite value of U and V. Combination of the results at small and large U and V further leads to the following conjecture. Since the transition from the AFM to the CDW phase occurs at $v = \frac{1}{2}$, both for $U,V \downarrow 0$ and $U,V \rightarrow \infty$, it seems plausible that $v = \frac{1}{2}$ marks the boundary between both phases also at *finite* values of U and V. Moreover, since the transition survives if one takes into account the $1/d$ corrections, it seems likely that the transition is present in sufficiently high, and possibly also in lower ($d = 2,3$), dimensions. It would be extremely interesting if this conjecture could be verified.

In summary, we considered the extended Hubbard model in high dimensions for small and for large values of the interaction parameters U and V. For small U and V we showed that the critical temperature and the temperature dependence of the order parameter, including the $1/d$ corrections, can be calculated from a recently proposed perturbation expansion—the standard perturbation expansion around the Hartree solution leads to incorrect

results. We found that the actual order-parameter curve has the same shape as in the Hartree approximation, but both the amplitude of the order parameter and the temperature scale are reduced by factors of the order of *unity*. For both small and large U and V one finds a transition from antiferromagnetism to a charge-density-wave state at $V/U=1/2$. The conjecture, based on the $1/d$ expansion, is that this transition is also present in finite and physically relevant dimensions ($d=2,3$).

I am very grateful to Dr. A. Georges (Princeton) for drawing my attention to Ref. [16]. I further acknowledge valuable discussions with Professor D. Vollhardt (Rheinisch-Westfälische Techische Hochschule, Aachen), Professor P. A. Lee and Professor B. Altshuler (MIT), and Dr. F. Gebhard (Rutgers University). This work is financially supported by the Deutsche Forschungsgemeinschaft (DFG).

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