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Re-entrant antiferromagnetism within a weak-coupling treatment of the Hubbard model

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Abstract. We study the infinite-dimensional Hubbard model within the self-consistent second-order U-perturbation treatment (SOPT), which is a conserving approximation and the simplest systematic improvement of the Hartree approximation (HA). For half filling we find antiferromagnetic solutions, but even for small Coulomb repulsion U the critical temperature is substantially reduced compared to that obtained in the HA. We construct the phase diagram as a function of doping and find regions of re-entrant behaviour in the temperature dependence of the staggered magnetization away from half filling. The stability of the ordered solutions is investigated by calculation of the grand canonical potential and the filling fraction dependence of the chemical potential; for small values of U the antiferromagnetic phase transition is continuous (as usual), but for larger U the SOPT yields a first-order phase transition. For low temperatures and away from half filling there may be a region of phase coexistence between the antiferromagnetic and homogeneous phases.

1. Introduction

Since its introduction the Hubbard model (HM) [1] has acquired a position as the generic model for correlated electron systems. It incorporates essential features of these systems such as the itinerant character of the electrons and local (screened Coulomb) repulsion. Though the model is stripped down to the bare essentials of a correlated electron system, it has proven very hard to treat in a controlled manner in dimensions $d > 1$. The discovery of the limit of infinite dimensions as a well defined and non-trivial limiting case [2] has proven very fruitful in this respect [3, 4]. This limit allows a mapping onto an atomic problem in the presence of two auxiliary, time-dependent (Kadanoff–Baym) fields [5] or, equivalently, onto the single-impurity Anderson model (SIAM) with a band-electron Green function to be determined self-consistently [6]. Unfortunately, in general the effective atomic or single-impurity problem cannot be solved exactly, but efficient numerical treatments are possible. The alternatives are time discretization of the auxiliary fields [7], or for the effective SIAM quantum Monte Carlo (QMC) calculations, finite-cluster diagonalizations or established approximations (second-order U-perturbation theory, SOPT, in the symmetric case or non-crossing approximation, NCA) [8, 9, 10, 11, 12]. By means of these recent treatments 'essentially exact' results are available for the $d = \infty$ HM, and antiferromagnetism of this model has been studied recently by means of the time-discretization treatment [7], the QMC and SOPT treatments of the SIAM [8, 11] and the NCA for the SIAM [13]. For strongly repulsive U these determinations of the antiferromagnetic (AF) phase at half-filled

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band confirm the Heisenberg limit of the model which should give a critical temperature (the Néel temperature) $T_c \sim 1/U$. At weak Coulomb repulsion it is consistent with the U-perturbation-theory results, which give exponentially small critical temperature for $U \to 0$, and there is a maximum in $T_c = T_c(U)$ for intermediate coupling. Away from half filling the tendency to antiferromagnetic ordering is suppressed and exists between some finite lower and upper values of U at low enough temperature and for a certain (small) regime in the filling fraction (near half filling).

In spite of these 'essentially exact' results it is still necessary and justified to investigate the antiferromagnetism of the $d = \infty$ HM within systematic (and controlled) approximations. The methods mentioned above rely either on approximations of the SIAM (SOPT or NCA) or on QMC data, which are available along the (discretized) imaginary time axis so that additional procedures ('maximum entropy method') are necessary to obtain results for real frequency. Furthermore, these methods are still numerically very expensive and therefore the range of parameters (temperature, Coulomb repulsion) and the number of data available for various physical quantities are limited. Finally, as they rely on the mapping onto the single-impurity problem, these methods cannot be extended to real finite dimension $d = 1, 2, 3$. Therefore, other methods applicable for finite as well as for infinite d are still very valuable, and an application to the $d = \infty$ HM allows for a comparison with the exact results and thus for a judgement of the quality of this method.

It is the purpose of this paper to study the AF phase diagram of the HM within a weak-coupling treatment in infinite dimensions. As shown by van Dongen [14] the free-energy gain due to symmetry breaking in the Hartree approximation is already of order U^2, so fluctuations cannot be neglected, but have to be included on an equal footing, at least to second order, giving a reduction of the critical temperature and order parameter by a factor ≈ 0.3. He used perturbation theory for the half-filled band at fixed staggered magnetization according to [15]. We will employ selfconsistent second-order perturbation theory (SOPT) for general filling fractions n. This is a conserving approximation in the sense of Kadanoff and Baym [16, 17], and hence it will be thermodynamically equivalent to a self-consistent treatment at fixed staggered magnetization by a Legendre transform with respect to the staggered external field h. We have applied the SOPT to the half-filled HM and find an antiferromagnetic solution even for very small Coulomb correlation U. Calculating the temperature dependence of the order parameter (staggered magnetization) we obtain the standard (mean-field-like) behaviour characteristic for a second-order phase transition for small U, but an unusual behaviour (with two magnetic solutions) for larger values of U; a calculation of the grand canonical potential (GCP) shows that the latter behaviour characterizes a first-order transition, i.e. one of the two formal AF solutions obtained turns out to be thermodynamically unstable. A comparison with the results obtained for T_c in SOPT and in the Hartree approximation (HA) shows that the SOPT yields a substantial reduction in complete agreement with the result obtained already by van Dongen [14]. Away from half filling, where the AF phase diagram of the HM seems to be only moderately well explored, we have calculated T_c as a function of the filling fraction n for different U. Here we obtain a clear indication of re-entrant behaviour, i.e. for fixed filling $n \neq 1$ we obtain a homogeneous phase at low and high temperatures and an AF phase between some lower critical temperature T_{c1} and some upper critical temperature T_{c2}. This feature is also present in the HA, but the region of the phase diagram in which AF solutions are obtained is substantially reduced within the SOPT compared to the HA. Somewhat closer to $n = 1$ there is still re-entrant behaviour, but m only decreases to a finite value as $T \to 0$. The AF solution turns out to be unstable towards phase separation upon decreasing temperature.

In the following section we will establish our notation and explain our method. In section

3 we will present and discuss our results. We first consider the half-filled band which will serve also as a benchmark for the approach. Then we consider the phase diagram in the temperature–density plane. Section 4 closes the paper with some concluding remarks. We set $\hbar$ and k_B equal to unity throughout this paper.

2. Formalism and numerical method

In our notation the Hubbard Hamiltonian reads

$$H = -\frac{t}{\sqrt{2d}} \sum_{\langle r,r' \rangle,\sigma} c^\dagger_{r,\sigma} c_{r',\sigma} + U \sum_r c^\dagger_{r,\uparrow} c_{r,\uparrow} c^\dagger_{r,\downarrow} c_{r,\downarrow} \tag{1}$$

where c_r ($c^\dagger_r$) annihilates (creates) an electron at site r of the d-dimensional hypercubic lattice, $t/\sqrt{2d}$ is the hopping-matrix element and U is the Coulomb repulsion. The scaling of the hopping-matrix element assures a non-trivial limit when $d \to \infty$. In this limit the self-energy becomes site diagonal [2]:

$$\Sigma_{r,r'} = \delta_{r,r'} \Sigma_{r,r} \tag{2}$$

but it may depend on the site r.

Here we search for an antiferromagnetically ordered state in a hypercubic lattice. The self-energy will then depend on the sublattice (here arbitrarily named A and B), and we have the symmetry

$$\Sigma_{A\sigma} = \Sigma_{B-\sigma}. \tag{3}$$

The site-diagonal matrix elements of the Green function for one sublattice (say A) read

$$G_\sigma(i\omega_n) = \sqrt{\frac{Z_{n-\sigma}}{Z_{n\sigma}}} G_0(\sqrt{Z_{n\uparrow} Z_{n\downarrow}}). \tag{4}$$

Here $\omega_n = (2n+1)\pi T$ denotes the Matsubara frequencies (T is temperature) and G_0 is the *unperturbed on-site Green function*

$$G_0(z) = -i\sqrt{\frac{\pi}{2t^2}} \operatorname{sgn}(\operatorname{Im} z) \exp\left(-\frac{z^2}{2t^2}\right) \operatorname{erfc}\left(-i\frac{\operatorname{sgn}(\operatorname{Im} z) z}{\sqrt{2t^2}}\right) \tag{5}$$

which corresponds to a Gaussian DOS, and

$$Z_{n\sigma} = i\omega_n + \mu - n\frac{U}{2} + \sigma m U - \Sigma^c_\sigma(i\omega_n). \tag{6}$$

Here

$$n = T \sum_n \left(G_\uparrow(i\omega_n) + G_\downarrow(i\omega_n)\right) \tag{7}$$

is the particle number per site, i.e. $n/2$ is the filling fraction, and the average magnetic moment per site, m, on this sublattice is

$$m = \frac{T}{2} \sum_n \left(G_\uparrow(i\omega_n) - G_\downarrow(i\omega_n)\right). \tag{8}$$

We approximate the self-energy by fully self-consistent second-order perturbation theory (SOPT). This is a Φ-derivable approximation [16] resulting from the approximate Φ potential shown in figure 1 by functional differentiation $\Sigma = \delta\Phi/\delta G$. Apart from the Hartree term we then have a correlation contribution to the self-energy:

$$\Sigma^c_\sigma(\tau) = -U^2 G_\sigma(\tau) G_{-\sigma}(\tau) G_{-\sigma}(-\tau). \tag{9}$$

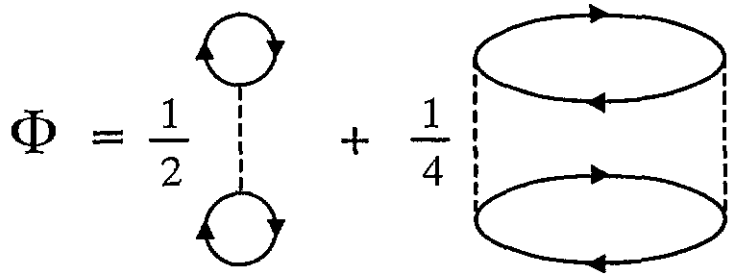

Figure 1. The Φ potential in the SOPT approximation.

Here (as usual) τ denotes the 'imaginary time' ($0 < \tau < \beta = 1/T$) and the standard relation between functions $F(\tau)$ and their Fourier components $F(\mathrm{i}\omega_n)$ defined at the discrete Matsubara frequencies $\mathrm{i}\omega_n$,

$$F(\tau) = T\sum_n \mathrm{e}^{-\mathrm{i}\omega_n\tau}F(\mathrm{i}\omega_n) \qquad F(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{e}^{\mathrm{i}\omega_n\tau}F(\tau)\,\mathrm{d}\tau \tag{10}$$

holds. This approach also allows for a consistent calculation of the grand canonical potential (GCP) Ω [16, 17] through

$$\beta\Omega = \Phi - \mathrm{Tr}\,\Sigma G + \mathrm{Tr}\,\ln G. \tag{11}$$

Here Tr means the sum over all Matsubara frequencies and the trace over all one-particle states; because of the site-diagonality of the self-energy the latter can be performed in site representation for $\mathrm{Tr}\,\Sigma G$ whereas it is more easily done in the k-space representation for $\mathrm{Tr}\,\ln G$. The temperature where the antiferromagnetic susceptibility diverges in the homogeneous phase is found by searching for the temperature which fulfils

$$1 = T\sum_n g(\mathrm{i}\omega_n) \tag{12}$$

where

$$g(\mathrm{i}\omega_n) = \lim_{m\to 0}\frac{G_\uparrow(\mathrm{i}\omega_n) - G_\downarrow(\mathrm{i}\omega_n)}{2m}. \tag{13}$$

The above equations (4)–(9) constitute a closed set of non-linear equations. For a given set of external parameters (i.e. temperature T, chemical potential μ, U) there might be several solutions. Then the solution which minimizes the thermodynamic potential being consistent with the approximation is chosen.

We use the Matsubara-frequency or imaginary-time representation in all the numerical calculations. The Green functions and self-energies for all positive Matsubara frequencies up to some cut-off are stored in tables. Self-energies are calculated from (9) by first transforming the Green functions to imaginary time, taking the product and transforming back to frequency. The high-frequency tails are approximated by their leading asymptotic behaviour by subtracting the asymptotic formula before the Fourier transform is performed (by FFT) and adding back the Fourier transform of the asymptotic part afterwards. Equations (4)–(9) are iterated until the maximum relative discrepancy between two successive iterations is less than about 10^{-7}.

The calculation of $\beta\Omega$ is done in two parts. The first one, $\Phi - \mathrm{Tr}\,\Sigma G$, is simply given by the diagrams in figure 1 but with different prefactors:

$$\Phi - \mathrm{Tr}\,\Sigma G = -\beta UN\left(\frac{1}{4}n^2 - m^2\right) - \frac{3}{4}N\sum_{n,\sigma}\Sigma_\sigma^{\mathrm{c}}(\mathrm{i}\omega_n)G_\sigma(\mathrm{i}\omega_n). \tag{14}$$

Here the first term on the right-hand side stems from the Hartree contribution to the self-energy. The second part Tr ln G is calculated by splitting off an analytically tractable and asymptotically correct part before the frequency summation is performed. The important point is to choose the asymptotic part such that the frequency summation can be done exactly. Explicitly we use the Hartree form, but with parameters (m, n) from the selfconsistent calculation.

$$\operatorname{Tr}\ln G = -2N\int_0^\infty \mathrm{d}\epsilon\,\rho_0(\epsilon)\sum_n \ln\left(1+\frac{Z_{n\uparrow}Z_{n\downarrow}-Z^0_{n\uparrow}Z^0_{n\downarrow}}{Z^0_{n\uparrow}Z^0_{n\downarrow}-\epsilon^2}\right)$$
$$-2N\int_0^\infty \mathrm{d}\epsilon\,\rho_0(\epsilon)\ln\left(1+e^{2\beta\mu'}+2e^{\beta\mu'}\cosh\left(\beta\sqrt{m^2U^2+\epsilon^2}\right)\right) \tag{15}$$

where

$$Z^0_{n\sigma} = \mathrm{i}\omega_n + \mu' + \sigma m U \qquad \mu' = \mu - \tfrac{1}{2}nU \tag{16}$$

and

$$\rho_0(\omega) = -\frac{1}{\pi}\operatorname{Im} G_0(\omega + \mathrm{i}0^+). \tag{17}$$

The essential numerical aspect is that the frequency summations in equations (14) and (15) are absolutely convergent.

3. Results and discussion

We have solved numerically the equations (4)–(9) as described in the previous section. There is always a homogeneous solution, and at half filling we always find antiferromagnetic phases at low enough temperature. The staggered magnetization found for a half-filled band for $U/t = 1.0, 1.25, 1.5, 2.0$ is shown as a function of temperature in figure 2. The curves for $U/t = 1.5, 2.0$ are typical for $U > U_c$, $U_c \approx 1.4t$ in that they show two solutions for the staggered magnetization in some temperature range. The other two curves are representative for all $U < U_c$ in giving a unique antiferromagnetic phase (counting only $m > 0$). In order to choose the correct phase in the two situations, we have plotted the grand canonical potential per site versus temperature for $U/t = 1.0$ and $U/t = 2.0$, see figures 3 and 4 respectively. For small U both the homogeneous and AF phases are locally stable as indicated by the curvature of $\Omega(T)$ in figure 3. At the point c corresponding to the temperature T_c the GCP for the AF phase coincides with that for the homogeneous phase. This is the temperature where the antiferromagnetic susceptibility diverges in the homogeneous phase. The AF solution always has the smaller GCP so we have a continuous phase transition at the temperature T_c as expected. This is the Néel temperature $T_N = T_c$. For larger U we have the situation in figure 4. At the point b at $T = T_b$ the two AF solutions coalesce, and at a ($T = T_a$) the homogeneous solution crosses the lower of the two AF solutions. The curve given by the solid line extending leftwards from a and the dashed line extending rightwards from a is the minimum of our solutions and it is concave, therefore it is the proper GCP for the system. The branch (a, b, c) corresponds to unphysical (thermodynamically unstable) solutions. T_c is the transition temperature one would obtain from (12) (temperature at which the order parameter vanishes), T_b is the largest temperature for which AF solutions are formally obtained, but the true thermodynamic phase transition temperature T_a lies in between, $T_c < T_a < T_b$. Thus the system undergoes a first-order phase transition at $T = T_a$. See the $U/t = 2.0$ results in figure 2 for an example of this.

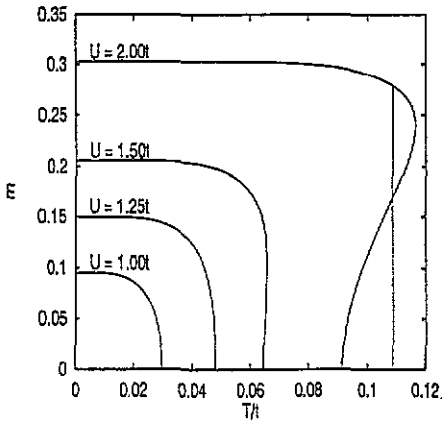

Figure 2. Solutions for the staggered magnetization as a function of temperature for different values of U at half filling. The dotted line indicates the first-order transition for $U/t = 2.00$.

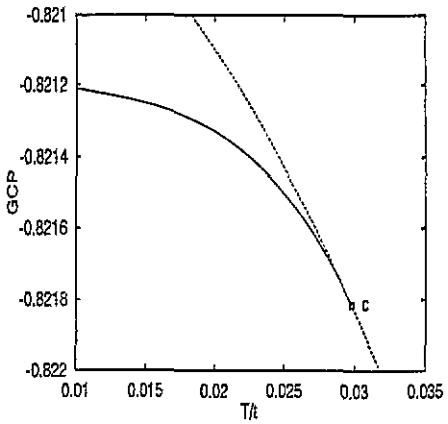

Figure 3. Grand canonical potential per site versus temperature T at $U/t = 1.0$ for the AF (solid line) and homogeneous (dashed line) phases as given by $\beta\Omega = \Phi - \mathrm{Tr}\,\Sigma G + \mathrm{Tr}\,\ln G$.

The phase transition can also be determined by looking at the h–m isotherms obtained from the Maxwell construction, which is well known from classical text-book treatments of first-order phase transitions, for instance for the van der Waals gas. One can then see that for $U > U_c$ $(T = T_a(U), h = 0, U)$ is a line of triple points and that $(T_c(U_c) = T_a(U_c), h = 0, U_c)$ is a tricritical point. Some examples are shown in figure 5 for $U = 2.0t$. A Maxwell equal-area construction on these gives one phase for $T/t = 0.15$, three phases for $T/t = 0.14, 0.13, 0.12, 0.11$ and two phases for $T/t = 0.10, 0.8$. For some temperature close to $T/t = 0.14$ there are two critical points at finite fields. The triple point is at $h = 0$ and T slightly less than $0.11t$.

In figure 6 we have plotted T_c as a function of U and compared it to the Hartree approximation. When $U \to 0$ we have $T_c \sim b\exp(-a/U)$ in both cases, but in the SOPT the constant b is smaller by a factor of about 0.3 in agreement with [14]. At larger values of U the SOPT result (in figure 6) has a slight negative curvature in contrast to the HA. This is in the regime where the SOPT actually predicts a first-order transition instead of a continuous one, so the plotted temperature T_c is not the transition temperature $T_a > T_c$ for these values of U.

The equations for the Hubbard model within our approach are very similar to those for the spinless-fermion model (SFM) in a self-consistent $1/d$ scheme [18]. The staggered magnetic moment in the SOPT for the Hubbard model translates into the charge order parameter of the SFM in the $1/d$ approach, but no first-order transition is predicted for the SFM at large interactions. The major difference is that the Fock term is absent for the Hubbard model. This tends to increase the band width thus effectively pushing the system towards the weak-coupling regime. Therefore the SOPT can (and does) give a different qualitative behaviour for stronger interaction in the HM compared to the SFM.

It is well established that the AF phase transitions are continuous (i.e. of second order) at small and large U. Therefore, a first-order transition as obtained here within the SOPT can exist only for some range of intermediate interaction. In the actual calculation a first-order transition will only be visible in the results for the order parameter or free energy in the ordered phase, but there are very few results on these quantities in the QMC literature.

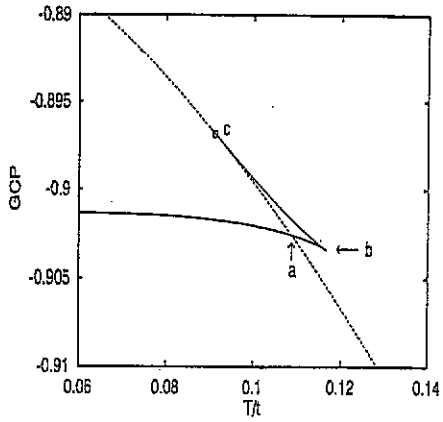

Figure 4. Same as figure 3, but for $U/t = 2.0$.

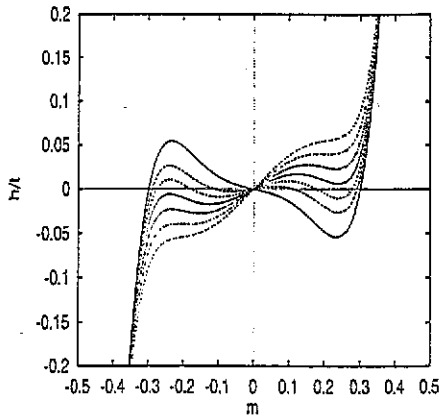

Figure 5. Solutions for the staggered external field h as a function of staggered magnetic moment m for $U = 2.0t$ and temperatures $T/t = 0.08, 0.10, 0.11, 0.12, 0.13, 0.14, 0.15$ (reading from above on the left-hand side of the figure).

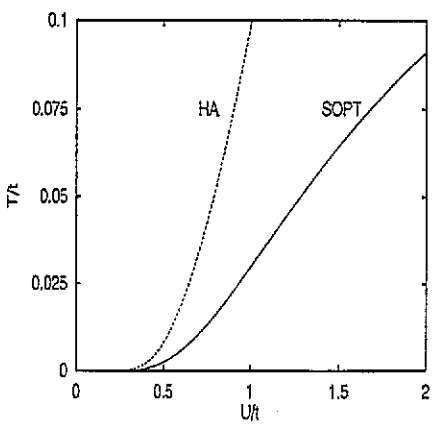

Figure 6. Temperature T_c at which the antiferromagnetic susceptibility diverges in the homogeneous phase as a function of interaction at $n = 1$. Solid line: SOPT, dashed line: Hartree approximation.

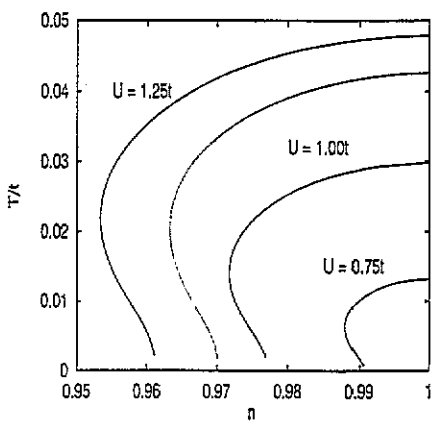

Figure 7. Phase diagrams in the T–n plane for various values of U. The lines denote the border between AF and homogeneous phases. The system is in the AF state close enough to half filling and for low enough temperature T. Solid lines: SOPT, dotted line: HA for $U/t = 0.75$.

The calculation by Georges and Krauth [11] for $U/t = 3.53$ (in our scaling) does not support such a behaviour, however. Therefore, it cannot be excluded that the first-order transition is an artifact of the approximation, which is a weak-coupling approximation using the interaction as the small parameter. Then the occurrence of the first-order transition could be an indication that the approximation actually breaks down at this value of the interaction strength. We therefore focus attention on $U < U_c$ where it does not appear and our approximation is increasingly accurate.

As one moves away from half filling the Néel temperature decreases, but there are intervals of n in which there is re-entrant behaviour in the temperature dependence, see figure 7. If not masked by some other phase transition, the system may be in the homogeneous phase at low temperature, then enter the AF state upon increasing the temperature, and finally become homogeneous again at sufficiently high temperature. This feature is present for all values of U that we have calculated. It is also present in the Hartree approximation, but the values of T_c and the ranges of densities in which AF is found are then much larger. Actually this type of re-entrant behaviour is present only in a very narrow range of filling fraction, because it is preceded by a phase separation at low temperature for most filling fractions. This is seen from figure 8 which shows the chemical potential versus filling fraction for temperatures $T/t = 0.01, 0.015, 0.02$. For $T/t = 0.01$ there is an interval where $\partial\mu/\partial n < 0$ indicating an instability of the phase. A Maxwell construction must be performed to determine the region of coexistence between the AF and homogeneous phases. Figure 9 shows the order parameter m versus filling fraction for various temperatures. The crossing of the curves for $T/t = 0.01$ and $T/t = 0.015$ shows that re-entrant behaviour is still present at least as close to the half-filled band as $n \approx 0.992$. In this case the solution for the AF phase does not disappear at low temperature (see also figure 7).

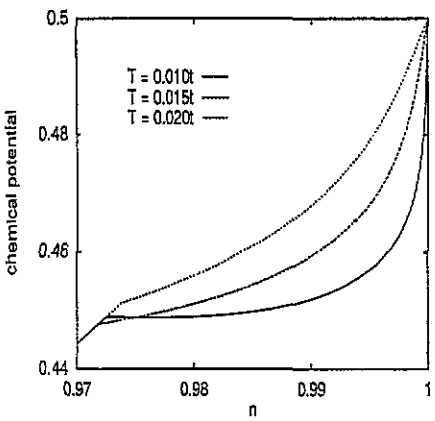

Figure 8. Chemical potential μ/t versus filling fraction n for $U = 1.0t$.

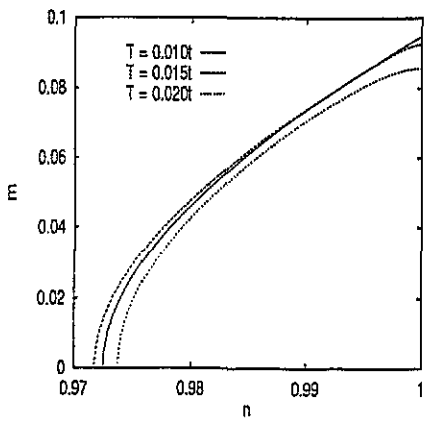

Figure 9. Staggered magnetization versus filling fraction at various temperatures for $U = 1.0t$.

It is instructive to compare our result to that of Uhrig and Vlaming for the spinless-fermion model in infinite dimensions [19]. The re-entrant behaviour of the order parameter and the appearance of phase separation in their calculation is of the same kind as ours for the Hubbard model when $U \to 0$. For the SFM a divergence of the density–density correlation function for incommensurate wave vectors was found.

4. Concluding remarks

We have investigated the Hubbard model in infinite dimensions with self-consistent second-order perturbation theory, which is a conserving approximation, and looked for the existence and stability of antiferromagnetic solutions. For half filling antiferromagnetism exists even for small interaction U, but the present approach yields a substantial correction for the critical (Néel) temperature compared to the corresponding result obtained within the

Hartree approximation. For small U the antiferromagnetic phase transition is continuous, as expected, but when increasing U it becomes first order. This can be true only for intermediate coupling U and may be an artifact of the approximation, which becomes increasingly crude with increasing U. Away from half filling antiferromagnetism is suppressed and exists only in a narrow region of the electron density n around half filling; the region in the T–n plane in which antiferromagnetic solutions are obtained (for fixed interaction U) is strongly reduced within the present approach compared to the corresponding Hartree result. For small interactions there is re-entrant behaviour in the temperature dependence of the staggered magnetization in some ranges of densities, and there is also a region of phase separation for low temperature.

Acknowledgments

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Note added in proof. After this work was completed, we learned about two other related works. Freericks and Jarrell [20] study the magnetic phase diagram of the HM using the QMC simulations [8] and find at a critical filling (away from half filling) a transition from a commensurate (AF) to an incommensurate phase. A recent weak-coupling study of the HM extended by nearest-neighbour interaction terms by van Dongen [21] shows that away from half filling and at zero temperature, phase separation may be more stable than incommensurate phases; this is consistent with our finding of phase separation at low temperature.

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