

Temperature-dependent electronic structure and ferromagnetism in the $d=\infty$ Hubbard model studied by a modified perturbation theory

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(Received 3 September 1997)

The infinite-dimensional Hubbard model is studied by means of a modified perturbation theory. The approach reduces to the iterative perturbation theory for weak coupling. It is exact in the atomic limit and correctly reproduces the dispersions and the weights of the Hubbard bands in the strong-coupling regime for arbitrary fillings. Results are presented for the hypercubic and an fcc-type lattice. For the latter we find ferromagnetic solutions. The filling-dependent Curie temperature is compared with the results of a recent quantum Monte Carlo study. [S0163-1829(98)04111-3]

Correlations among itinerant electrons are responsible for various interesting phenomena like spontaneous magnetic order, the metal-insulator (Mott) transition, and high-temperature superconductivity. One of the simplest but nontrivial models describing correlated electrons on a lattice is the Hubbard model.¹ Studying the Hubbard model in the limit of infinite spatial dimensions^{2,3} d is of special importance for the construction of a dynamical mean-field theory.³ For $d=\infty$ the Hubbard model is considerably simplified but nevertheless remains nontrivial: It becomes equivalent to an effective impurity problem and can be mapped^{4,5} onto the single-impurity Anderson model (SIAM), for example. For the latter, numerically exact solutions can be obtained by quantum Monte Carlo (QMC) calculations. On the other hand, it may be helpful to have an analytical (but approximative) expression for the self-energy at one's disposal, which recovers the exact QMC results as reliable as possible. This allows a direct calculation of dynamic quantities on the real energy axis for finite temperatures as well as for $T=0$. Furthermore, valuable hints for the approximative solution of more complicated lattice models not accessible to QMC may be obtained.

For the symmetric case the iterative perturbation theory^{4,6} (IPT) is known to give a rather realistic description of the Mott transition. The IPT employs the self-consistent mapping onto the SIAM, which is solved by means of second-order perturbation theory around the Hartree-Fock solution (SOPT-HF). To extend the IPT to nonsymmetric cases, Kajueter and Kotliar⁷ proposed an interpolating expression for the self-energy, which for arbitrary band fillings reproduces the atomic as well as the weak-coupling limit.

For the study of ferromagnetism special attention has to be paid to the strong-coupling regime. Fortunately, the $1/U$ perturbation theory of Harris and Lange⁸ provides rigorous results for $U\rightarrow\infty$: In the first nontrivial order beyond the atomic limit, the average dispersions as well as the weights of the two dominating Hubbard bands are known exactly.⁸ One possibility to account for these strong-coupling results in the construction of an analytical expression for the self-energy is to ensure that the moments

$$M_{\mathbf{k}\sigma}^{(n)} = \frac{1}{\hbar} \int dE E^n A_{\mathbf{k}\sigma}(E) \quad (1)$$

of the resulting spectral density $A_{\mathbf{k}\sigma}(E)$ are correct up to $n=3$. These moments can be calculated exactly by $M_{\mathbf{k}\sigma}^{(n)} = \langle [\mathcal{L}^n c_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}^\dagger]_+ \rangle$, where $\mathcal{L} = [\cdot, \mathcal{H}]_-$. At each \mathbf{k} point of the Brillouin zone the first four moments $n=0, \dots, 3$ provide four pieces of information that in the strong-coupling regime determine the dispersions and the weights of the two Hubbard bands. This moment approach has been successfully employed beforehand to improve upon the Hubbard-I solution.⁹

The approach of Kajueter and Kotliar⁷ reproduces the correct moments up to $n=2$. The $n=3$ moment, however, may be of particular importance in the context of ferromagnetism since it involves a higher-order correlation function ("band shift"),

$$B_\sigma = T_{ii} + \sum_{j \neq i} T_{ij} \frac{\langle c_{i\sigma}^\dagger c_{j\sigma} (2n_{i-\sigma} - 1) \rangle}{\langle n_{i\sigma} \rangle (1 - \langle n_{i\sigma} \rangle)}, \quad (2)$$

the (possible) spin dependence of which is known to favor magnetic order and thereby decisively influences the magnetic phase diagram.⁹

Based on these considerations the present authors have proposed an improvement of the Kajueter-Kotliar approach recently¹⁰ which is correct up to $n=3$ [hereafter referred to as "modified perturbation theory" (MPT)]. The main purpose of this paper is to study the effects of the band shift B_σ in the paramagnetic as well as in the ferromagnetic phase. We compare our results with corresponding findings of previous QMC studies.

Let us briefly recall the essentials of the theory. Details can be found in Ref. 10. In the $d=\infty$ Hubbard model the self-energy is a local quantity.^{2,3} Via the mapping onto the effective impurity problem, it can be regarded as the self-energy of the SIAM provided that the hybridization function of the SIAM is suitably chosen. According to Kajueter and Kotliar,⁷ we consider the following ansatz for the self-energy of the SIAM:

$$\Sigma_\sigma(E) = Un_{-\sigma} + \frac{a_\sigma \Sigma_\sigma^{(\text{SOC})}(E)}{1 - b_\sigma \Sigma_\sigma^{(\text{SOC})}(E)}, \quad (3)$$

where $\Sigma_{\sigma}^{(\text{SOC})}(E)$ is the second-order (U^2) contribution (SOC) to the self-energy within the SOPT-HF, while a_{σ} and b_{σ} are free parameters that will be chosen such that the moments (1) are correct up to $n=3$. This requires a_{σ} and b_{σ} to be¹⁰

$$a_{\sigma} = \frac{n_{-\sigma}(1-n_{-\sigma})}{n_{-\sigma}^{(\text{HF})}(1-n_{-\sigma}^{(\text{HF})})}, \quad (4)$$

$$b_{\sigma} = \frac{B_{-\sigma} - B_{-\sigma}^{(\text{HF})} - (\mu - \tilde{\mu}_{\sigma}) + U(1-2n_{-\sigma})}{U^2 n_{-\sigma}^{(\text{HF})}(1-n_{-\sigma}^{(\text{HF})})}, \quad (5)$$

where n_{σ} denotes the occupancy of the impurity level, $n_{\sigma}^{(\text{HF})}$ is its Hartree-Fock value, and $\tilde{\mu}_{\sigma}$ is a fictitious chemical potential that appears in the definition of the Hartree-Fock Green's function. The parameter $\tilde{\mu}_{\sigma}$ is fixed by imposing the condition $n_{\sigma}^{(\text{HF})} = n_{\sigma}$ (for further discussions on this point see Ref. 10). Finally, $B_{\sigma}^{(\text{HF})}$ is the Hartree-Fock value of the band shift B_{σ} . All expectation values in the theory can be expressed in terms of the spectral density and thus can be determined self-consistently.¹⁰

The MPT reduces to the IPT for small U and is exact in the atomic limit. By construction it is fully consistent with the rigorous results of Harris and Lange for $U \rightarrow \infty$ and yields the correct moments of the spectral density up to $n=3$ for arbitrary U . The approach of Kajueter and Kotliar⁷ is recovered if B_{σ} and $B_{\sigma}^{(\text{HF})}$ are set to their atomic limit values (i.e., $B_{\sigma} = B_{\sigma}^{(\text{HF})} = T_{ii} \equiv 0$). Note, however, that in Ref. 7 the fictitious chemical potential $\tilde{\mu}_{\sigma}$ has been used to enforce the Luttinger theorem. This implies that the theory is intrinsically limited to $T=0$ (see Ref. 10). The more unproblematic condition $n_{\sigma}^{(\text{HF})} = n_{\sigma}$ that is chosen here to fix $\tilde{\mu}_{\sigma}$ has to be preferred since it allows us to perform finite-temperature calculations, too. The results for $T=0$ and near half-filling show that this choice is still consistent with the Luttinger theorem (see below).

Let us first consider the paramagnetic Hubbard model on the hypercubic lattice away from half-filling ($n < 1$). The Bloch density of states (BDOS) is given by Ref. 2, $\rho_0(E) = \exp(-E^2)/\sqrt{\pi}$. Figure 1 shows the density of states (DOS) for $U=4$, $k_B T=0.138$ and different bandfillings obtained within the MPT. The comparison with the QMC results of Jarrell and Pruschke¹¹ shows that the MPT qualitatively yields the correct results as concerns the shifts as well as the changes in height and width of the high-energy charge-excitation peaks in the spectrum with varying filling. Even for temperatures $T \neq 0$ the Kondo-type resonance shows up at $E \approx \mu$. This low-energy feature is more pronounced in the QMC spectra compared with the MPT. We then investigated the effect of taking into account the $n=3$ moment: For any filling considered, it turns out that there are only minor changes in the spectra (which would hardly be visible on the scale in Fig. 1) when setting $B_{\sigma} = B_{\sigma}^{(\text{HF})}$. For the paramagnet we conclude that the effects introduced by the band shift are rather unimportant.

Figure 2 shows the MPT spectra for $U=4$, $n=0.94$ and different temperatures. We have also calculated the uniform static susceptibility in the paramagnetic phase by applying an

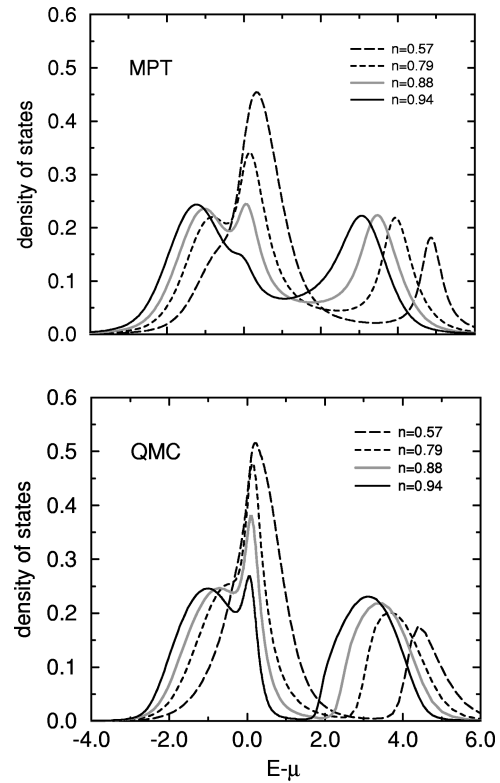


FIG. 1. Densities of states for $U=4$, $k_B T=0.138$, and different fillings on the hypercubic lattice. Results of the modified perturbation theory (MPT) in comparison with QMC results from Jarrell and Pruschke (Ref. 11).

infinitesimally small field: $\chi = (\partial/\partial H)(n_{\uparrow} - n_{\downarrow})|_{H \rightarrow 0}$. As can be seen in Fig. 2 the Kondo peak starts growing when the susceptibility differs from the Curie law. The local effective magnetic moment [$\mu_{\text{eff}}^2 \propto T\chi(T)$] is quenched as $T \rightarrow 0$. This effect has been termed ‘‘collective single-band Kondo-effect’’.¹² Furthermore, one can see in Fig. 2 by comparing the $T=0$ spectrum with the free ($U=0$) spectrum that the DOS is unrenormalised at the Fermi edge, $\rho_{\sigma}(\mu) = \rho_0(\mu_0)$, which is an equivalent formulation of the Luttinger theorem in infinite dimensions.¹³ Let us stress once more that, contrary to Ref. 7, this has not been enforced via

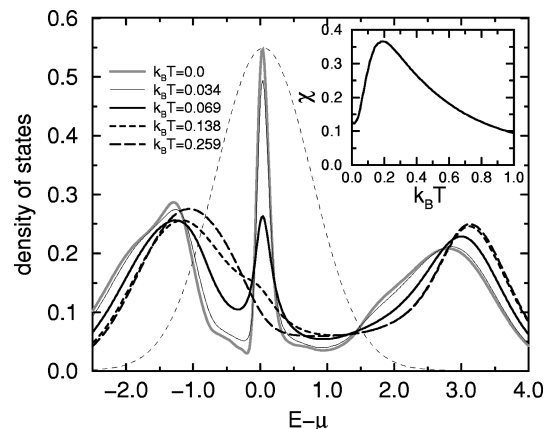


FIG. 2. Densities of states for $U=4$, $n=0.94$, and different temperatures. Thin dashed line: $U=0$. Inset: uniform static susceptibility χ vs temperature.

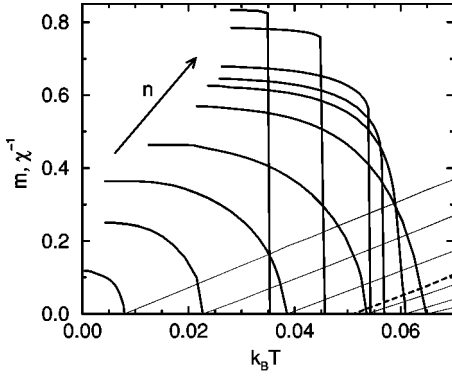


FIG. 3. Thick lines: magnetization for the fcc lattice, $U=4$ and $n=0.2, 0.3, 0.4, 0.5, 0.6, 0.65, 0.67, 0.7, 0.8, 0.85$ vs temperature. Thin lines: corresponding inverse static susceptibility χ^{-1} for $n=0.2, \dots, 0.65$. Dashed line: $n=0.67$.

the choice for the parameter $\tilde{\mu}_\sigma$. For fillings well below half-filling $\rho_\sigma(\mu)$ is found to be slightly lower than $\rho_0(\mu_0)$. We did not find ferromagnetic solutions on the hypercubic lattice. The susceptibility never diverged for $U \leq 6$. This is in agreement with the results in Ref. 11. For $U = \infty$, however, a region of nonvanishing ferromagnetic polarization is obtained within the noncrossing approximation¹⁴.

On an fcc-type lattice ferromagnetism has been found recently within QMC by Ulmke¹⁵. The high weight in the BDOS (Ref. 15) $\rho_0(E) = \exp[-(1 + \sqrt{2}E)/2] / \sqrt{\pi(1 + \sqrt{2}E)}$ at the lower band edge favors ferromagnetic order.¹⁶ Stable ferromagnetic solutions are likewise predicted by the MPT in a wide region of the phase diagram. Figure 3 shows the magnetisation $m = n_\uparrow - n_\downarrow$ for $U=4$ as a function of temperature for different band-fillings. For $n < 0.67$ we observe second-order phase transitions. The magnetization curves are continuous and terminate at the respective Curie temperature T_C . The inverse static susceptibility obeys a Curie-Weiss law for high temperatures. For lower temperatures with $T > T_C$ a slight curvature ($\partial^2 \chi^{-1} / \partial T^2 > 0$) is observed (not visible in Fig. 3). χ^{-1} vanishes at $T = T_C$. The critical exponent of the susceptibility turns out to be $\gamma \approx 1$ as expected. We encountered numerical difficulties to obtain an accurate value for γ .

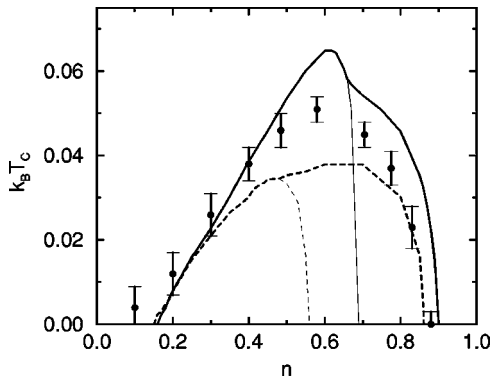


FIG. 4. Filling dependence of the Curie temperature T_C (T_2 for $n \geq 0.67$) for $U=4$ on the fcc lattice. Solid lines: MPT. Dashed lines: MPT results with $B_\sigma = B_\sigma^{(\text{HF})} = 0$. Thin (solid and dashed) lines: T_1 (zeros of χ^{-1}). Points with error bars: QMC results (zeros of χ^{-1}) by Ulmke (Ref. 15).

For $n \geq 0.67$ the phase transitions are of first order. A finite magnetisation is still found for temperatures above the zero T_1 of χ^{-1} (see Fig. 3 for $n=0.67$). At a temperature $T = T_2 > T_1$ the magnetization noncontinuously drops to zero. Between T_1 and T_2 there is a second ferromagnetic solution with a magnetization (not shown) that vanishes at T_1 and that coalesces with the plotted magnetization curve of the first solution at T_2 . Decreasing n also results in a stronger curvature of χ^{-1} near T_1 while at high temperatures we still have Curie-Weiss behavior. Finally, for $n \geq 0.69$, χ^{-1} remains positive for all temperatures. This scenario is well known from previous studies of the Hubbard model in conserving¹⁷ as well as nonconserving approximations¹⁸. For $n \geq 0.67$ the true Curie temperature T_C (with $T_1 < T_C < T_2$) can be found, e.g., by means of the Maxwell construction considering the H - m isotherms at different temperatures. On the other hand, we cannot exclude the fact that the first-order transition is an artefact of our approximation.

The filling dependence of T_C (for $n \geq 0.67$: T_1) can be compared with the available numerically exact QMC results from Ref. 15 where the Curie temperature has been obtained

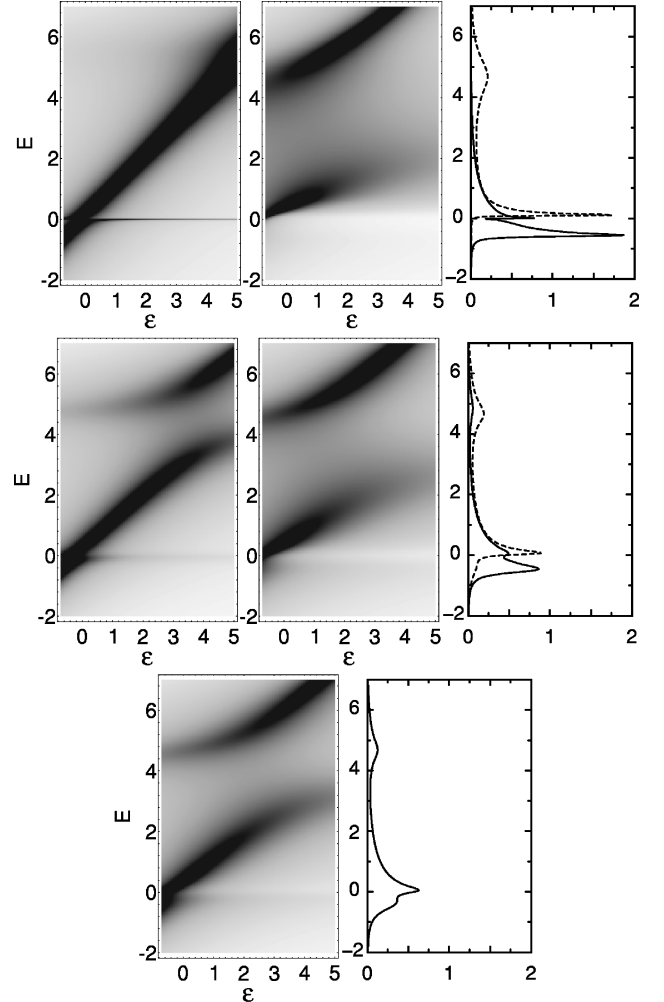


FIG. 5. Density plots of the spectral density: energy on the y axis, Bloch dispersion $\epsilon(\mathbf{k})$ on the x axis. $U=4$, $n=0.6$, and the fcc lattice. First row: \uparrow -spectral density, \downarrow -spectral density, and density of states $\rho_\sigma(E - \mu)$ (solid line \uparrow , dashed line: \downarrow) at $k_B T = 0.022$ (magnetization $m = 0.57$). Second row: $k_B T = 0.058$, $m = 0.32$. Third row: $k_B T = k_B T_C = 0.065$.

by linear extrapolation of the inverse susceptibility. As can be seen in Fig. 4, the MPT result reasonably agrees with the QMC data. In particular, there is remarkable agreement with respect to the maximum T_C and the corresponding filling. Contrary to the paramagnetic phase, there is a strong effect of the (spin-dependent) band shift B_σ for the ferromagnet. Both, the range of existing ferromagnetic solutions as well as the values for T_1 and T_C , are strongly affected if we set $B_\sigma = B_\sigma^{(\text{HF})}$. We find that taking into account correctly the $n=3$ moment tends to improve the agreement with the QMC results (see Fig. 4).

There are no hints for non-Fermi-liquid behavior in all our calculations. The imaginary part of the self-energy vanishes quadratically at $E = \mu$ in the paramagnetic as well as in the ferromagnetic solutions for $T=0$, even at the quantum-critical point $n_c \approx 0.16$ (for $U=4$).

The evolution of the spin-dependent spectral density with increasing temperature is shown in Fig. 5 for $n=0.6$. Since the self-energy is \mathbf{k} independent, the spectral density depends on \mathbf{k} via the Bloch dispersion $\epsilon(\mathbf{k})$ only. For the calculation of the density of states which is also shown in Fig. 5, the spectral density has to be weighted with the BDOS:

$$\rho_\sigma(E) = \frac{1}{\hbar} \int d\epsilon(\mathbf{k}) \rho_0(\epsilon(\mathbf{k})) A_{\epsilon(\mathbf{k})\sigma}(E - \mu). \quad (6)$$

At the temperature $k_B T = 0.022$, where the system is nearly fully polarized ($m=0.57$), the upper Hubbard band in the \uparrow spectrum is missing because there are not enough interaction partners. The same spectrum without the narrow Kondo-type

resonance (at $E \approx 0$) is expected in the noninteracting case. The \downarrow spectrum shows the lower as well as the upper Hubbard band. When increasing the temperature (second row, $k_B T = 0.058$, $m=0.32$) the upper Hubbard band in the \uparrow spectrum comes into existence. The resonance smears out and starts growing in the \downarrow spectrum. At $k_B T = k_B T_C = 0.065$ (third row) where \uparrow and \downarrow spectra coincide, it is still visible. Finally, we notice that there is a strong transfer of spectral weight between the Hubbard bands with increasing temperature. In the \uparrow channel the upper one gains weight at the cost of the lower, in the \downarrow channel the situation is reversed.

In conclusion, ensuring the correctness of the moments of the spectral density up to $n=3$ is a necessary condition to be consistent with the rigorous results of Harris and Lange for the strong-coupling regime. In this respect the modified perturbation theory not only represents a conceptual improvement upon the approach of Kajueter and Kotliar, but also yields closer agreement with QMC data. The (possible) spin dependence of the higher-order correlation functions (B_σ) that appear in the $n=3$ moment is important for ferromagnetic order and has been shown to affect critical fillings and temperatures considerably. On the contrary, there are only minor effects of B_σ for the paramagnet. Improvement upon the IPT can also be expected for the antiferromagnet at half-filling.

This work has been supported by the Deutsche Forschungsgemeinschaft (SFB 290).

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