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The moment sum rule and its consequences for ferromagnetism in the Hubbard model

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The sum rule for the moments of the spectral density is discussed for the single-band Hubbard model. It is shown that respecting the sum rule up to the order $m = 3$ is conceptually important for a qualitatively correct description of the quasi-particle band structure in the strong-correlation regime. Different analytical approximations for the self-energy are analyzed with respect to their compatibility with the moment sum rule. To estimate the practical usefulness of the sum rule, correlation functions and dynamical quantities are determined. The results obtained within the various approximation schemes of different complexity are compared with each other and also with essentially exact results available for infinite-dimensional lattices. It turns out that the $m = 3$ moment is rather unimportant for the paramagnetic phase on the hyper-cubic lattice. Contrary, it decisively influences the magnetic phase boundary as well as the critical temperature for the ferromagnetic phase on an fcc-type lattice.

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I. INTRODUCTION

The Hubbard model [1, 2, 3] plays a central role in the attempts to understand the physics of correlated electrons on a lattice. It is surely oversimplified when it comes to a description of real materials such as the 3d transition metals and their oxides, for example. Nevertheless, it can provide deep insight into the fundamental mechanisms that are responsible for various prominent correlation effects.

The Hubbard model sets up a notoriously difficult problem which now as before is not accessible to an exact solution in general. An exception is given for the one-dimensional case ($d = 1$) where a yet incomplete but very detailed understanding of the model properties in the whole parameter range has been achieved [4, 5, 6, 7, 8]. An important simplification of the model is also given in the opposite limit of high spatial dimensions $d = \infty$ [9, 10, 11, 12] which was recognized as a well-defined and non-trivial limiting case by Metzner and Vollhardt [9]. Here the electronic self-energy is $\mathbf{k}$ independent or site-diagonal [13], and thereby the model becomes equivalent to an effective impurity problem [14]. An exact solution is possible by self-consistent mapping [15, 16] onto the single-impurity Anderson model (SIAM) [17], for example, followed by the numerical treatment [18] within the Quantum-Monte-Carlo (QMC) approach [16, 19, 20, 21]. In dimensions $d = 3$ or $d = 2$, however, one still has to resort to approximate treatments.

Valuable information that helps to judge of the reliability of a particular method is provided by exact identities, sum rules, limiting cases etc. In any dimension d such rigorous results impose strong necessary conditions for the inevitable approximations. The purpose of the present paper is to focus on a particular sum rule: Exact expressions can be obtained for the (low-order) moments $\int E^m A_{\mathbf{k}\sigma}(E)\, dE$ of the spectral density $A_{\mathbf{k}\sigma}(E)$. We will argue that the first four moments ($m = 0 - 3$) yield valuable information on the quasi-particle band structure; they are especially important in the strong-coupling regime and also decisively influence the possibility and characteristics of spontaneous magnetic order. The moment sum rule has been considered not only within the context of the standard single-band Hubbard model in $d = \infty$ [22, 23, 24, 25], in $d = 3$ [26, 27, 28, 29, 30], $d = 2$ [31, 32, 33] and $d = 1$ [31], but also for the negative-U case [34] and for reduced translational symmetry [35, 36], for the SIAM [37], for the t-J [38] and for localized spin models [39, 40, 41] and

may thus be of general interest for the construction of analytical approaches.

There are several questions related to the moment sum rule which are not yet finally clarified. Firstly, we have to ask how to check to which order the sum rule is fulfilled for a particular (approximate) method. Secondly, a kind of recipe is required that shows up how a given method can be modified to respect the sum rule up to a certain desired order. Thirdly, it should be worked out what is the actual conceptual improvement that is thereby achieved. Finally and most important, we need to know what can be achieved in practice, i. e. whether the sum rule can help to come "closer" to the exact solution.

Especially the last question requires to compare with exact results. As has been mentioned above, these are available for the Hubbard model in infinite dimensions. In the recent years there has been extensive work for $d = \infty$ lattices concerning the Fermi-liquid phase at and off half-filling [21], the metal-insulator (Mott) transition [16, 19, 20, 21, 42, 43, 44], transport properties [45, 46] and antiferromagnetic [16, 21, 42, 43, 44, 47] and ferromagnetic ordering [21, 48, 49]. These QMC studies have been supplemented by the exact diagonalization method [50, 51] and by a number of approximate methods that are reliable in certain limits. Let us mention the non-crossing approximation (NCA) [45, 52, 53] as a strong-coupling approach, weak-coupling methods [54, 55, 56, 57], variational approaches [58, 59, 60] and others [61, 62, 63]. Moreover, the $d = \infty$ model is physically meaningful since the local approximation for the self-energy appears to be reasonable down to $d = 3$ [64] or even $d = 2$ [65]. The essential physical properties of the $d = \infty$ Hubbard model are thus expected to be comparable to those at $d = 3$ ($d = 2$). For the present study we therefore restrict ourselves to the $d = \infty$ case where we are able to judge of the reliability of a particular method on the firm basis that is provided by available QMC results. This should help us to come to conclusive results concerning the sum rule.

Our main idea is to elucidate the meaning and the usefulness of the moment sum rule by considering a number of standard approximations: (i) the simple Hubbard-I approximation (H-I) [2], (ii) Hubbard's alloy-analogy solution (AA) [66], (iii) the so-called Edwards-Hertz approach (EHA) [67] in its improved version by Wermbter and Czycholl [68], and finally (iv) the generalization [69] of the iterative perturbation theory [15] to arbitrary band-fillings as proposed by Kajueter and Kotliar (KK) [70]. It turns out that all approaches are inconsistent with the moment sum rule for $m = 3$ and yield the correct moments only up to $m = 2$.

The moments of the spectral density are intimately related to the coefficients in the high-energy expansion of the corresponding self-energy [71]. We will show that thereby a possibility is opened to improve upon a particular approximation analytically and to ensure that the moment sum rule is respected up to $m = 3$.

This program has been completed successfully for the four approaches mentioned above. The result is another set of methods, each evolving straightforwardly from its above counterpart: (i) the spectral-density approach (SDA) [27, 28, 22, 30], (ii) the modified alloy-analogy (MAA) [72, 73], (iii) the interpolating alloy-analogy-based approach (IAA) [24], and (iv) the modified perturbation theory (MPT) [23, 25].

Each of these new approaches can be considered as a conceptual improvement upon the original one: It can be shown that the additional inclusion of the fourth spectral moment does not affect their validity in different exactly solvable limiting cases. Furthermore, we will also show that significant improvement is achieved when comparing with the essentially exact QMC data of Refs. [21, 48, 49].

There is an interesting feature common to those four approaches that yield the correct moments up to $m = 3$: The analytical expression for the self-energy depends on a higher-order correlation function B_σ which can be shown to be responsible for a (possibly) spin-dependent shift of the centers of gravity of the lower and the upper Hubbard band in the strong-correlation regime $U \mapsto \infty$. On the other hand, the original approaches are obtained if B_σ is (ad hoc) replaced by its atomic-limit (H-I, AA) or by its Hartree-Fock value (EHA, KK), respectively. One may thus expect that the inclusion of the fourth spectral moment is especially important what concerns magnetic order.

After a general discussion of the moment sum rule and its conceptual importance in the next section, we briefly discuss each of the methods in sections III-VI. Section VII presents new results for the paramagnetic phase on the hyper-cubic and for the ferromagnetic phase on an fcc-type lattice. For the discussion a comparative opposition of the different methods against each other and against QMC results appears to be helpful. Our intention is to arrive at general conclusions

on the meaning and importance of the moment sum rule and of the correlation function B_σ in particular which may be helpful for future analytical work.

II. SPECTRAL MOMENTS AND $1/U$ PERTURBATION THEORY

Let us start by recalling some essential facts for the limiting case of strong interaction ($U \gg t$). This will be important for the later discussion and for a concise formulation of the different approaches mentioned above. We first introduce the model as well as the basic physical quantities of interest.

Using standard notations the Hubbard model reads:

$$H = \sum_{ij\sigma} (T_{ij} - \mu\delta_{ij})\, c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}\,. \quad (1)$$

The hopping integrals T_{ij} are assumed to be non-zero up to nearest-neighbor distances: $T_{\langle ij\rangle} = -t$. The on-site energy $T_{ii} \equiv T_0$ defines the energy zero. We consider an infinite-dimensional lattice with the usual scaling $d\,t^2 =$ const. for the hopping to retain the model non-trivial [9]. Restricting ourselves to homogeneous phases (para- and ferromagnetism), the one-electron Green function,

$$G_\sigma(E) = \langle\langle c_{i\sigma}; c^\dagger_{i\sigma}\rangle\rangle_E\,, \quad (2)$$

depends on the lattice geometry via the free Bloch density of states (BDOS) only and can be written in the form:

$$G_\sigma(E) = \int_{-\infty}^{\infty} \frac{\hbar\rho^{(\mathrm{B})}(z)}{E - (z-\mu) - \Sigma_\sigma(E)}\, dz\,, \quad (3)$$

where the BDOS

$$\rho^{(\mathrm{B})}(E) = \frac{1}{N}\sum_{\mathbf{k}} \delta(E - \epsilon(\mathbf{k})) \quad (4)$$

is given in terms of the tight-binding dispersion

$$\epsilon(\mathbf{k}) = \frac{1}{N}\sum_{ij} e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} T_{ij}\,. \quad (5)$$

The expression (3) for the Green function is based on the fact that the self-energy $\Sigma_\sigma(E)$ is $\mathbf{k}$ independent or site-diagonal for $d = \infty$ [9, 13]. Let us also introduce the $\mathbf{k}$-resolved spectral density,

$$A_{\mathbf{k}\sigma}(E) = -\frac{1}{\pi}\mathrm{Im}\frac{\hbar}{E + i0^+ - (\epsilon(\mathbf{k}) - \mu) - \Sigma_\sigma(E + i0^+)}\,, \quad (6)$$

and the on-site or $\mathbf{k}$-summed spectral density:

$$A_\sigma(E) = \frac{1}{N}\sum_{\mathbf{k}} A_{\mathbf{k}\sigma}(E)\,. \quad (7)$$

The atomic limit of vanishing hopping ($t = 0$) represents the zeroth-order result for the strong-coupling regime. We have:

$$\Sigma_\sigma(E) = U n_{-\sigma} + \frac{U^2 n_{-\sigma}(1 - n_{-\sigma})}{E + \mu - T_0 - U(1 - n_{-\sigma})}\,, \quad (8)$$

where $n_\sigma = \langle c^\dagger_{i\sigma} c_{i\sigma}\rangle$. Let us now consider the first non-trivial correction to the atomic solution (8) in the strong-coupling regime. For $U \mapsto \infty$ perturbational results can be derived by performing a canonical transformation of the Hubbard model [26, 74, 75, 76]. As has been shown first by Harris and Lange [26], the $1/U$ perturbation theory predicts the spectrum to be dominated by two charge-excitation peaks (Hubbard bands); the weight of additional satellites in the spectrum is of the order $(1/U)^4$ and can thus be neglected for strong interaction. Furthermore, at each $\mathbf{k}$ point in the Brillouin zone the center of gravity $T_{p\sigma}(\mathbf{k})$ as well as the spectral weight $\alpha_{p\sigma}(\mathbf{k})$ of the lower ($p = 1$) and of the upper ($p = 2$) Hubbard band can be calculated exactly. Specializing the results of Harris and Lange to the $d = \infty$ case, one obtains:

$$\begin{aligned}
T_{1\sigma}(\mathbf{k}) &= (1 - n_{-\sigma})\epsilon(\mathbf{k}) + n_{-\sigma} B_{-\sigma} + \mathcal{O}(1/U)\,,\\
T_{2\sigma}(\mathbf{k}) &= U + n_{-\sigma}\epsilon(\mathbf{k}) + (1 - n_{-\sigma}) B_{-\sigma} + \mathcal{O}(1/U)\,,\\
\alpha_{1\sigma}(\mathbf{k}) &= 1 - n_{-\sigma}\\
&\quad + \frac{2}{U} n_{-\sigma}(1 - n_{-\sigma})(B_{-\sigma} - \epsilon(\mathbf{k})) + \mathcal{O}(1/U)^2\,,\\
\alpha_{2\sigma}(\mathbf{k}) &= 1 - \alpha_{1\sigma}(\mathbf{k})\,, \quad (9)
\end{aligned}$$

where the $B_{-\sigma}$ is defined as:

$$B_\sigma = T_0 + \frac{1}{n_\sigma(1 - n_\sigma)}\sum_{j\neq i} T_{ij}\langle c^\dagger_{i\sigma} c_{j\sigma}(2n_{i-\sigma} - 1)\rangle\,. \quad (10)$$

Contrary to the finite-dimensional case [30, 31, 32], the $\mathbf{k}$ dependence of $T_{p\sigma}(\mathbf{k})$ and $\alpha_{p\sigma}(\mathbf{k})$ is exclusively due to the Bloch dispersion $\epsilon(\mathbf{k})$. For finite d an additional $\mathbf{k}$ dependence is introduced via $B_{-\sigma} \mapsto B_{\mathbf{k}-\sigma}$.

From the result (9) valuable "global" information on the quasi-particle band structure can be read off: Apart from the Hubbard splitting, electron correlations manifest themselves in a specific narrowing of the lower

and upper Hubbard band, in a redistribution of spectral weight among them and in a shift of their centers of gravity that is given by $n_{-\sigma}B_{-\sigma}$ and $(1-n_{-\sigma})B_{-\sigma}$, respectively. These (possibly spin-dependent) shifts, in particular, are expected to be important for ferromagnetic symmetry breaking: A spin-dependent shift of the band center of gravity may generate and stabilize ferromagnetic solutions.

Here the question arises how it can be ensured that a given analytical approach is consistent with the exact perturbational results of Harris and Lange for $U \mapsto \infty$. For this purpose we consider the moments of the spectral density which for $m = 0, 1, 2, \ldots$ are defined as:

$$M_{\mathbf{k}\sigma}^{(m)} = \frac{1}{\hbar} \int_{-\infty}^{\infty} E^m A_{\mathbf{k}\sigma}(E)\, dE \,. \tag{11}$$

There is an alternative but equivalent way to calculate the moments:

$$M_{\mathbf{k}\sigma}^{(m)} = \langle [\mathcal{L}^m c_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}^\dagger]_+ \rangle \,, \tag{12}$$

where $\mathcal{L}\mathcal{O} = [\mathcal{O}, H]_-$ denotes the commutator of an operator $\mathcal{O}$ with the Hamiltonian, and $[\cdots,\cdots]_+$ is the anticommutator. Eqs. (11) and (12) represent the moment sum rule for the spectral density. In practice the sum rule is useful for low m only. The limitation arises from the fact that with increasing m Eq. (12) involves equal-time correlation functions of higher and higher order which are usually unknown.

As has been shown in Ref. [33], the correctness of the moments up to $m = 2$ is a necessary condition for the evolution of the Hubbard bands as $U \mapsto \infty$. On the other hand, it is not sufficient as the following example shows: The self-consistent second-order perturbation theory in the interaction U for $d = \infty$ [54] predicts the correct moments up to $m = 2$ but does not yield the Hubbard splitting for large U [33, 54].

To be consistent with the results of $1/U$ perturbation theory, one has to check the existence of the Hubbard bands (which normally can be done easily). Then, it is sufficient to ensure that the moment sum rule is fulfilled for $m = 0-3$: For each $\mathbf{k}$ point of the Brillouin zone, the first four moments provide four pieces of information on the spectral density that (for $U \mapsto \infty$) unambiguously determine both, the centers of gravity and the weights, for the two Hubbard bands. Explicit expressions for the Hubbard model up to $m = 3$ can be found Refs. [28, 35], for example. The dispersions $T_{p\sigma}(\mathbf{k})$ and weights $\alpha_{p\sigma}(\mathbf{k})$ that result from the above reasoning are the same as found by Harris and Lange in Eq. (9).

In most analytical approaches one obtains an (approximate) expression for the self-energy. To make use of the sum rule, it becomes necessary to determine the spectral density from Eq. (6) and to calculate the moments by carrying out the integration in Eq. (11). Finally, the (approximate) result for the moments has to be compared with the exact one given by Eq. (12).

The inconvenient integration in (11) can be avoided when considering the high-energy expansion of the Green function and of the self-energy: In the spectral representation of the on-site Green function,

$$G_\sigma(E) = \int_{-\infty}^{\infty} \frac{A_\sigma(E')}{E - E'}\, dE' \,, \tag{13}$$

we expand the denominator in powers of $1/E$. With Eq. (11) we immediately get:

$$G_\sigma(E) = \hbar \sum_{m=0}^{\infty} \frac{M_\sigma^{(m)}}{E^{m+1}} \,. \tag{14}$$

The coefficients in the high-energy expansion of the Green function are given by the (on-site) moments: $M_\sigma^{(m)} = M_{ii\sigma}^{(m)} = N^{-1} \sum_{\mathbf{k}} M_{\mathbf{k}\sigma}^{(m)}$. Via Eq. (3) they also determine the high-energy expansion coefficients of the self-energy:

$$\Sigma_\sigma(E) = \sum_{m=0}^{\infty} \frac{C_\sigma^{(m)}}{E^m} \,. \tag{15}$$

Using the explicit expressions for the moments as obtained from Eq. (12) [28, 35], a straightforward calculation yields:

$$\begin{aligned} C_\sigma^{(0)} &= U n_{-\sigma} \,, \\ C_\sigma^{(1)} &= U^2 n_{-\sigma} (1 - n_{-\sigma}) \,, \\ C_\sigma^{(2)} &= U^2 n_{-\sigma} (1 - n_{-\sigma}) (B_{-\sigma} - \mu + U(1 - n_{-\sigma})) \,. \end{aligned} \tag{16}$$

Any analytical (approximate) expression for the self-energy can easily be checked against these rigorous results simply by expanding in powers of $1/E$. Provided that the coefficients $C_\sigma^{(m)}$ turn out to be correct up to $m = 2$, the moments of the resulting spectral density $M_{\mathbf{k}\sigma}^{(m)}$ will be correct up to $m = 3$. For $U \mapsto \infty$ this ensures complete consistency with the $1/U$ perturbational results of Harris and Lange.

Finally, we have to express the expectation values in Eq. (16) in terms of known quantities. For the (spin-dependent) average occupation number we have:

$$n_\sigma \equiv \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = \frac{1}{2} + \frac{2}{\hbar\beta} \,\mathrm{Re} \sum_{n=0}^{\infty} G_\sigma(iE_n) \,, \tag{17}$$

where $E_n = (2n+1)\pi/\beta$ and $\beta = 1/k_\mathrm{B}T$. We also define the band-filling $n = n_\uparrow + n_\downarrow$. Ferromagnetic order is indicated by an asymmetry $n_\uparrow \neq n_\downarrow$ in the spin-dependent occupation numbers. In this case the (dimensionless) spontaneous magnetization is given by $m = n_\uparrow - n_\downarrow$. We can also determine B_σ (see Refs. [24, 28, 29, 35], for example):

$$\begin{aligned} B_\sigma = T_0 \,+\, & \frac{1}{n_\sigma(1-n_\sigma)} \frac{2}{\hbar\beta} \,\mathrm{Re} \sum_{n=0}^{\infty} \left(\frac{2}{U} \Sigma_\sigma(iE_n) - 1 \right) \\ & \times \left[(iE_n - \Sigma_\sigma(iE_n) - T_0 + \mu)\, G_\sigma(iE_n) - \hbar \right] \,. \end{aligned} \tag{18}$$

Fortunately, it can be expressed in terms of the one-electron Green function and self-energy, despite the fact that the definition of B_σ (10) includes higher-order correlation functions.

III. TWO-POLE GREEN FUNCTION

In the following we consider four different standard approximations for the self-energy: The Hubbard-I solution (Sec. III), the alloy analogy solution (Sec. IV), the Edwards-Hertz approach (Sec. V) and the ansatz of Kajueter and Kotliar (Sec. VI). Carrying out the high-energy expansion, we can check to which order m the moment sum rule is fulfilled. Furthermore, we will show up how the respective approaches can be corrected (if necessary) such that the sum rule is obeyed up to $m = 3$.

A. Hubbard-I approximation (H-I)

The so-called Hubbard-I solution is the simplest approach that predicts a splitting of the non-interacting Bloch band into the two quasi-particle (Hubbard) subbands. In the original work [2] it is derived by decoupling the hierarchy of equations of motion at the second level, i. e. by assuming $\langle\langle c_{i\sigma} n_{i-\sigma}; c_{j\sigma}^\dagger \rangle\rangle \approx \langle n_{i-\sigma} \rangle \langle\langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle\rangle$. From the resulting approximate Green function and from the Dyson equation one obtains the Hubbard-I self-energy which is identical with the self-energy (8) of the atomic limit. The high-energy expansion is readily performed, the expansion coefficients read:

$$\begin{aligned} C_\sigma^{(0,\mathrm{H-I})} &= U n_{-\sigma} \,, \\ C_\sigma^{(1,\mathrm{H-I})} &= U^2 n_{-\sigma} \left(1 - n_{-\sigma}\right) \,, \\ C_\sigma^{(2,\mathrm{H-I})} &= U^2 n_{-\sigma} \left(1 - n_{-\sigma}\right) \left(T_0 - \mu + U(1 - n_{-\sigma})\right) \,. \end{aligned} \tag{19}$$

Comparing with (16), we notice that the $m = 2$ coefficient (and thereby the $m = 3$ moment) is incorrect.

B. Spectral-density approach (SDA)

It is easily seen from the expansion coefficients that the sum rule up to order $m = 3$ can be restored if the atomic level T_0 in the H-I self-energy (8) is replaced by $T_0 \mapsto B_{-\sigma}$. We obtain:

$$\Sigma_\sigma^{(\mathrm{SDA})}(E) = U n_{-\sigma} + \frac{U^2 n_{-\sigma}(1 - n_{-\sigma})}{E + \mu - B_{-\sigma} - U(1 - n_{-\sigma})} \,. \tag{20}$$

The Green function can be calculated from Dyson's equation, and from (18) we get $B_{-\sigma}$. We thus arrive at a conceptually simple improvement of the H-I solution that introduces an effective atomic level which is determined self-consistently.

It turns out that this is identical with the spectral-density approach (SDA) [28, 77, 35, 30] in infinite dimensions. The SDA is essentially equivalent to the Roth two-pole approximation for the Green function [78, 32]. Furthermore, the SDA self-energy can also be obtained by means of the Mori-Zwanzig projection technique [79, 80, 31].

IV. ALLOY ANALOGY

The main idea of an alloy-analogy solution for the Hubbard model is to consider the $-\sigma$ electrons to be "frozen" and to be randomly distributed over the sites of the lattice. The σ electrons then move through a fictitious two-component alloy that is characterized by two atomic levels $E_{1\sigma}$ and $E_{2\sigma}$ and the concentrations $x_{1\sigma}$ and $x_{2\sigma}$. The coherent potential approximation (CPA) [81] can be used to perform the configurational average

over the positions of the frozen $-\sigma$ electrons. The self-energy for the σ electrons is thus obtained via:

$$0 = \sum_{p=1}^{2} x_{p\sigma} \, \frac{E_{p\sigma} - \Sigma_\sigma(E) - T_0}{1 - \frac{1}{\hbar} G_\sigma(E) \left[E_{p\sigma} - \Sigma_\sigma(E) - T_0 \right]} \, . \quad (21)$$

A. Hubbard's alloy-analogy solution (AA)

Any two-component alloy analogy requires the specification of the two atomic levels $E_{p\sigma}$ and the concentrations $x_{p\sigma}$. Within the conventional alloy-analogy solution due to Hubbard [66] (AA) these are taken by referring to the atomic limit:

$$\begin{aligned} E_{1\sigma}^{(\mathrm{AA})} &= T_0 \, , \qquad E_{2\sigma}^{(\mathrm{AA})} = T_0 + U \, , \\ x_{1\sigma}^{(\mathrm{AA})} &= 1 - n_{-\sigma} \, , \qquad x_{2\sigma}^{(\mathrm{AA})} = n_{-\sigma} \, . \end{aligned} \quad (22)$$

Using this ansatz in the general CPA equation (21) and rearranging the terms, we arrive at:

$$\Sigma_\sigma^{(\mathrm{AA})}(E) = \frac{U n_{-\sigma}}{1 - \frac{1}{\hbar} G_\sigma(E) \left(U - \Sigma_\sigma^{(\mathrm{AA})}(E) \right)} \, . \quad (23)$$

This AA solution turns out to be exact for a special but non-trivial limiting case of the Hubbard model: Switching off the hopping of the $-\sigma$ electrons only ($T_{ij} \mapsto T_{ij\sigma}$, $T_{ij-\sigma} = \delta_{ij} T_0$), defines the Falicov-Kimball model (FKM) [82]. As has been shown by Brandt and Mielsch [83], in infinite dimensions the exact self-energy is given by Eq. (23).

To get the high-energy expansion coefficients of the AA self-energy, we insert the expansions (14) and (15) into the CPA equation (21) and sort the different terms in powers of $1/E$. Considering all terms up to order $1/E^2$ yields the following set of equations:

$$\begin{aligned} 1 &= \sum_p x_{p\sigma} \, , \\ 0 &= \sum_p x_{p\sigma} \left(E_{p\sigma} - T_0 - C_\sigma^{(0)} \right) , \\ 0 &= \sum_p x_{p\sigma} \left[(E_{p\sigma} - T_0 - C_\sigma^{(0)})^2 M_\sigma^{(0)} - C_\sigma^{(1)} \right] , \\ 0 &= \sum_p x_{p\sigma} \Big[(E_{p\sigma} - T_0 - C_\sigma^{(0)})^3 (M_\sigma^{(0)})^2 \\ &\quad + (E_{p\sigma} - T_0 - C_\sigma^{(0)})^2 M_\sigma^{(1)} \\ &\quad - 2 (E_{p\sigma} - T_0 - C_\sigma^{(0)}) C_\sigma^{(1)} M_\sigma^{(0)} - C_\sigma^{(2)} \Big] . \end{aligned} \quad (24)$$

Inserting the atomic levels and concentrations from (22) as well as the exact low-order moments $M_\sigma^{(0)} = 1$ and $M_\sigma^{(1)} = T_0 - \mu + U n_{-\sigma}$ and solving for $C_\sigma^{(m)}$ results in:

$$C_\sigma^{(\mathrm{m,AA})} = C_\sigma^{(m)} \Big|_{B_{-\sigma} \mapsto T_0} = C_\sigma^{(\mathrm{m,H-I})} \quad (25)$$

for $m = 0 - 2$. The high-energy expansion coefficients of the AA self-energy turn out to be identical to the coefficients within the H-I solution. Again the $m = 2$ coefficient is found to be incorrect.

B. Modified alloy-analogy (MAA)

Simply replacing $T_0 \mapsto B_{-\sigma}$ in the CPA equation (21) and in (22) does not yield the correct $m = 2$ coefficient since $B_{-\sigma}$ would cancel out again in Eqs. (24). Another idea, however, turns out to be successful: The choice (22) for the levels and concentrations is rather obvious. On the other hand, it is by no means predetermined. We therefore consider $E_{p\sigma}$ and $x_{p\sigma}$ ($p = 1, 2$) as free parameters to be fixed by the Eqs. (24) where $C_\sigma^{(m)}$ and $M_\sigma^{(m)}$ are taken to be the exact coefficients (16). This automatically ensures the correctness of the moments up to $m = 3$ and thereby provides an "optimized" alloy analogy. Solving Eqs. (24) for the parameters of the fictitious alloy yields:

$$\begin{aligned} E_{p\sigma}^{(\mathrm{MAA})} = \frac{1}{2} \left(T_0 + U + B_{-\sigma} \right) + (-1)^p \times \\ \sqrt{\frac{1}{4} \left(U + B_{-\sigma} - T_0 \right)^2 + U n_{-\sigma} \left(T_0 - B_{-\sigma} \right)} \end{aligned} \quad (26)$$

and

$$x_{1\sigma}^{(\mathrm{MAA})} = \frac{B_{-\sigma} + U(1 - n_{-\sigma}) - E_{1\sigma}^{(\mathrm{MAA})}}{E_{2\sigma}^{(\mathrm{MAA})} - E_{1\sigma}^{(\mathrm{MAA})}} = 1 - x_{2\sigma}^{(\mathrm{MAA})} \, . \quad (27)$$

It turns out that this result is identical to the result of the recently proposed modified alloy analogy (MAA) [72, 73] where it was derived by referring to the split-band regime [81] of the CPA.

Inserting the result into the CPA equation (21) yields the MAA self-energy:

$$\Sigma_\sigma^{(\mathrm{MAA})}(E) = \frac{U n_{-\sigma}}{1 \; - \; \frac{\frac{1}{\hbar} G_\sigma(E) \left(U - \Sigma_\sigma^{(\mathrm{MAA})}(E) \right)}{1 \; - \; \frac{1}{\hbar} G_\sigma(E) \left(B_{-\sigma} - T_0 \right)}} \, . \quad (28)$$

One recognizes that the MAA reduces to the AA if $B_{-\sigma}$ is replaced by T_0. As can be seen from Eq. (10) this is correct for the atomic limit and for the Falicov-Kimball model. Just as the AA, the MAA therefore remains exact within these two limits. It also reduces to the AA for a paramagnet at half-filling with symmetric BDOS where $B_{-\sigma} = T_0$ is required by particle-hole symmetry [84].

V. ALLOY-ANALOGY-BASED INTERPOLATION SCHEME

A severe drawback of the alloy-analogy solutions consists in the fact that they are unable to reproduce the weak-coupling limit. This defect can be eliminated if the CPA equation is considered as a mere starting point for a reasonable interpolation formula which is demanded to be exact for small U as well as in the atomic limit and in the case of the FKM.

Standard perturbation theory in the interaction U [85] provides us with the exact result for the self-energy in the weak-coupling regime. The first non-trivial perturbational result for the self-energy,

$$\Sigma_\sigma(E) = Un_{-\sigma} + \Sigma_\sigma^{(\mathrm{SOC})}(E)\,, \tag{29}$$

beyond the Hartee term $Un_{-\sigma}$ is given by the second-order contribution (SOC):

$$\Sigma_\sigma^{(\mathrm{SOC})}(E) = \frac{U^2}{\hbar^3}\iiint \frac{A_\sigma^{(1)}(x)A_{-\sigma}^{(1)}(y)A_{-\sigma}^{(1)}(z)}{E-x+y-z} \times (f(x)f(-y)f(z) + f(-x)f(y)f(-z))\,dx\,dy\,dz\,. \tag{30}$$

Here $f(x) = 1/(\exp(\beta x)+1)$ denotes the Fermi function, and $A_\sigma^{(1)}(E)$ is the free ($U = 0$) spectral density being shifted in energy by a (possibly spin-dependent) constant E_σ:

$$A_\sigma^{(1)}(E) = A_\sigma^{(0)}(E - E_\sigma)\,, \tag{31}$$

with $A_\sigma^{(0)}(E) = -\frac{1}{\pi}\mathrm{Im}\,G_\sigma(E+i0^+)|_{U=0}$. The plain or conventional second-order perturbation theory (SOPT) is recovered for $E_\sigma = 0$, and with $E_\sigma = Un_{-\sigma}$ one obtains the SOPT around the Hartree-Fock solution (SOPT-HF) [64, 86, 87]. To this end there is no need to specify the constant E_σ. The expression (30) is correct up to order U^2 for any function $E_\sigma = E_\sigma(U)$ with $E_\sigma(0) = 0$.

A. Edwards-Hertz approach (EHA)

An interpolation scheme that is based on the alloy-analogy idea but correctly accounts for the weak-coupling limit, has been suggested by Edwards and Hertz [67]. Within the Edwards-Hertz approximation (EHA) the self-energy has to be calculated from [67, 68]:

$$\Sigma_\sigma^{(\mathrm{EHA})}(E) = \frac{Un_{-\sigma}}{1 - \frac{1}{\hbar}\widetilde{G}_\sigma(E)\,(U - \Sigma_\sigma^{(\mathrm{EHA})}(E))}\,. \tag{32}$$

This differs from the conventional AA with respect to the propagator $\widetilde{G}_\sigma(E)$: The Green function $G_\sigma(E)$ in Eq. (23) is (ad hoc) replaced by

$$\widetilde{G}_\sigma(E) = \frac{\hbar}{U^2 n_{-\sigma}(1-n_{-\sigma})}\Sigma_\sigma^{(\mathrm{SOC})}(E - \Sigma_\sigma^{(\mathrm{EHA})}(E) + E_\sigma), \tag{33}$$

where $\Sigma_\sigma^{(\mathrm{SOC})}(E)$ is the second-order contribution to the SOPT self-energy introduced in Eq. (30). A simple calculation shows that the EHA reproduces the atomic and the FKM limit for arbitrary band-fillings provided that the shifts E_σ in the definition (31) of the spectral density $A_\sigma^{(1)}(E)$ and in Eq. (33) are determined self-consistently from the condition:

$$n_\sigma = \int_{-\infty}^{\infty} f(E)\,A_\sigma(E)\,dE = \int_{-\infty}^{\infty} f(E)\,A_\sigma^{(1)}(E)\,dE\,. \tag{34}$$

This improvement upon the original theory [67] has been introduced by Wermbter and Czycholl [68]. Expanding the EHA self-energy in powers of U up to order U^2, one recovers the exact weak-coupling result (29).

The high-energy expansion is performed straightforwardly. For the modified propagator one obtains:

$$\frac{1}{\hbar}\widetilde{G}_\sigma(E) = \frac{1}{E} + \left(B_{-\sigma}^{(\mathrm{HF})} - \mu + Un_{-\sigma}\right)\frac{1}{E^2} + \cdots\,, \tag{35}$$

where $B_\sigma^{(\mathrm{HF})}$ is the Hartree-Fock decoupled B_σ defined as:

$$B_\sigma^{(\mathrm{HF})} = T_0 + \frac{2n_{-\sigma}^{(1)} - 1}{n_\sigma^{(1)}(1-n_\sigma^{(1)})}\sum_{j\neq i} T_{ij}\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle^{(1)} \tag{36}$$

and $\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle^{(1)} = -\frac{1}{\hbar\pi}\int dE f(E)\ \mathrm{Im}\ G_{ij\sigma}(E + i0^+ - E_\sigma)|_{U=0}$. With this result at hand, the high-energy expansion coefficients are obtained from Eq. (32):

$$C_\sigma^{(\mathrm{m,EHA})} = C_\sigma^{(m)}\Big|_{B_{-\sigma}\mapsto B_{-\sigma}^{(\mathrm{HF})}}\,. \tag{37}$$

Again, the first two coefficients $C_\sigma^{(0)}$ and $C_\sigma^{(1)}$ are predicted correctly while the $m = 2$ coefficient turns out to be wrong. Only in the atomic and in the FKM limit as well as for the symmetric case $n = 1$ we have $B_{-\sigma} = B_{-\sigma}^{(\mathrm{HF})} = T_0$.

B. Interpolating alloy-analogy approach (IAA)

The EHA interpolation formula can be improved such that the moments up to $m = 3$ are reproduced correctly: The interpolating alloy-analogy approach (IAA) [24] starts from the CPA equation (21) with the Green function replaced by the modified propagator $\widetilde{G}_\sigma(E)$ which is given by Eq. (33):

$$0 = \sum_{p=1}^{2} x_{p\sigma}^{(\mathrm{IAA})} \, \frac{E_{p\sigma}^{(\mathrm{IAA})} - \Sigma_\sigma(E) - T_0}{1 - \frac{1}{\hbar}\widetilde{G}_\sigma(E)\,[E_{p\sigma}^{(\mathrm{IAA})} - \Sigma_\sigma(E) - T_0]} \,. \tag{38}$$

The high-energy expansion of this equation is then used to determine the (unknown) atomic levels and concentrations. The only difference with respect to the expansion (24) of the general CPA equation is that the coefficients $M_\sigma^{(m)}$ for $m = 0, 1$ have now to be interpreted as the moments of the modified propagator. For $m = 0, 1$ they can be read off from Eq. (35). Solving for the unknowns yields the following result:

$$\begin{aligned} E_{p\sigma}^{(\mathrm{IAA})} &= T_0 + \frac{1}{2}\left(U + B_{-\sigma} - B_{-\sigma}^{(\mathrm{HF})}\right) + (-1)^p \times \\ &\quad \sqrt{\frac{1}{4}\left(U + B_{-\sigma} - B_{-\sigma}^{(\mathrm{HF})}\right)^2 + U n_{-\sigma}\left(B_{-\sigma}^{(\mathrm{HF})} - B_{-\sigma}\right)} \,, \\ x_{1\sigma}^{(\mathrm{IAA})} &= \frac{B_{-\sigma} - B_{-\sigma}^{(\mathrm{HF})} + T_0 + U(1 - n_{-\sigma}) - E_{1\sigma}^{(\mathrm{IAA})}}{E_{2\sigma}^{(\mathrm{IAA})} - E_{1\sigma}^{(\mathrm{IAA})}} \\ &= 1 - x_{2\sigma}^{(\mathrm{IAA})} \,. \end{aligned} \tag{39}$$

Inserting into (38) results in:

$$\Sigma_\sigma^{(\mathrm{IAA})}(E) = \frac{U n_{-\sigma}}{1 \; - \; \dfrac{\frac{1}{\hbar}\widetilde{G}_\sigma(E)\left(U - \Sigma_\sigma^{(\mathrm{IAA})}(E)\right)}{1 \; - \; \frac{1}{\hbar}\widetilde{G}_\sigma(E)\left(B_{-\sigma} - B_{-\sigma}^{(1)}\right)}} \,. \tag{40}$$

This differs from the MAA self-energy with respect to the modified propagator; also T_0 is replaced by $B_{-\sigma}^{(\mathrm{HF})}$ in (40). By construction the moments of the spectral density are correct up to $m = 3$ in the IAA. Furthermore, the theory is exact up to order U^2 and in the atomic and FKM limit.

VI. ITERATIVE PERTURBATION THEORY

While for the alloy-analogy-based theories the correct weak-coupling behavior has to be enforced artificially, it can be automatically accounted for within a diagrammatic approach. Furthermore, a diagrammatic ansatz appears to be attractive since it allows to construct thermodynamically consistent theories which are conserving in the sense of Kadanoff and Baym [88] and thus respect Luttinger's sum rule [89]. The simplest conserving approximation is given by Hartree-Fock theory. It recovers the $m = 0$ and $m = 1$ moments only. One additional moment ($m = 2$) is correct within the self-consistent second-order perturbation theory (SC-SOPT) [54, 56]. No improvement, however, is achieved by higher-order conserving approximations: On the contrary, within the fluctuation-exchange approximation (FLEX) [90] and also for its analogue in $d = \infty$ [55], already the $1/E$ coefficient in the expansion of the self-energy and thus the $m = 2$ moment turns out to be incorrect.

The (non-conserving) SOPT around the Hartree-Fock solution (SOPT-HF) [64, 86, 87] yields the correct moments up to $m = 1$. For a paramagnet at half-filling, however, the moments are correct even up to $m = 3$ (in infinite dimensions). Furthermore, for $t = 0$ SOPT-HF recovers the atomic-limit solution (8) and may thus provide a reasonable interpolation between the weak- and the strong-coupling regime at $n = 1$.

In infinite dimensions the Hubbard model can be self-consistently mapped onto the single-impurity Anderson model (SIAM) [15, 16]:

$$\begin{aligned} H_{\mathrm{SIAM}} &= \sum_\sigma (\epsilon_d - \mu) c_\sigma^\dagger c_\sigma + \sum_{k\sigma} (\epsilon_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma} \\ &\quad + U n_\sigma n_{-\sigma} + \sum_{k\sigma} V_{k\sigma}\left(c_\sigma^\dagger a_{k\sigma} + a_{k\sigma}^\dagger c_\sigma\right) \,. \end{aligned} \tag{41}$$

The on-site Green function and the local self-energy of the $d = \infty$ Hubbard model are identical with the impurity Green function and self-energy provided that the conduction band dispersion $\epsilon_{k\sigma}$ and the hybridization strength $V_{k\sigma}$ in the SIAM are chosen such that the self-consistency condition,

$$\Delta_\sigma(E + \mu) = E - (\epsilon_d - \mu) - \Sigma_\sigma(E) - \hbar\left(G_\sigma(E)\right)^{-1} \,, \tag{42}$$

for the hybridization function $\Delta_\sigma(E) = \sum_k V_{k\sigma}^2/(E - \epsilon_{k\sigma})$ is fulfilled.

Within the context of the *symmetric* single-impurity Anderson model (SIAM), SOPT-HF has been recognized to be quite well behaved [91]. Furthermore, as for the Hubbard model, SOPT-HF respects the moment sum rule up to $m = 3$ and the atomic limit of vanishing hybridization. The so-called iterative perturbation theory (IPT) [15] makes use of these advantages by combining SOPT-HF for the SIAM with the self-consistent mapping of the $d = \infty$ Hubbard model onto the SIAM. Indeed, IPT yields convincing results as has been proven by comparison with QMC studies [42, 43, 44]. The advantageous properties of the IPT are lost, however, if one considers the non-symmetric case $n \neq 1$.

A. Kajueter-Kotliar approach (KK)

Kajueter and Kotliar [70] proposed an interpolating ansatz for the self-energy of the SIAM which for arbitrary fillings is correct in the weak-coupling and the atomic limit. For the symmetric case the Kajueter-Kotliar approach (KK) reduces to the usual IPT. The interpolative self-energy is given by:

$$\Sigma_\sigma(E) = U n_{-\sigma} + \frac{a_\sigma \Sigma_\sigma^{(\mathrm{SOC})}(E)}{1 - b_\sigma \Sigma_\sigma^{(\mathrm{SOC})}(E)} , \tag{43}$$

where $n_\sigma = \langle c_\sigma^\dagger c_\sigma \rangle$ is the average occupancy of the impurity site and $\Sigma_\sigma^{(\mathrm{SOC})}(E)$ the second-order contribution within SOPT-HF for the SIAM. The coefficients a_σ and b_σ as well as a fictitious chemical potential $\widetilde{\mu}_\sigma$ that appears in the definition of the Hartree-Fock spectral density [cf. Eq. (30)],

$$A_\sigma^{(1)}(E) = -\frac{1}{\pi} \mathrm{Im} \frac{\hbar}{E + \widetilde{\mu}_\sigma - \epsilon_d - \Delta_\sigma(E + \mu) - U n_{-\sigma}} , \tag{44}$$

are considered as free parameters. $\widetilde{\mu}_\sigma$ is fixed by requiring $\mu = \mu|_{U=0} + \Sigma(0)$, i. e. the Luttinger sum rule in $d = \infty$ [54]. For any choice of a_σ and b_σ the first two moments $m = 0$ and $m = 1$ are correct. Within the KK approach, the parameters a_σ and b_σ are determined from the moment sum rule for $m = 2$ and the exact atomic-limit solution [70]. This yields:

$$a_\sigma = \frac{n_{-\sigma}(1 - n_{-\sigma})}{n_{-\sigma}^{(1)}(1 - n_{-\sigma}^{(1)})} \tag{45}$$

and

$$b_\sigma = \frac{U(1 - 2n_{-\sigma}) + \widetilde{\mu}_\sigma - \mu}{U^2 n_{-\sigma}^{(1)}(1 - n_{-\sigma}^{(1)})} , \tag{46}$$

where $n_\sigma^{(1)} = \hbar^{-1} \int f(E) A_\sigma^{(1)}(E) dE$.

This procedure, however, leads to an incorrect result for the $m = 3$ moment. Inserting (45) and (46) into the ansatz (43), expanding in powers of $1/E$, and comparing with the exact result (16), we have

$$C_\sigma^{(\mathrm{m,KK})} = C_\sigma^{(m)} \Big|_{B_{-\sigma} \mapsto B_{-\sigma}^{(\mathrm{HF})}} \tag{47}$$

up to $m = 2$. Here, within the context of the SIAM we have introduced the following definitions:

$$B_\sigma = \epsilon_d + \frac{1}{n_\sigma(1 - n_\sigma)} \sum_k V_{k\sigma} \langle a_{k\sigma}^\dagger c_\sigma (2n_{-\sigma} - 1) \rangle \tag{48}$$

and

$$B_\sigma^{(\mathrm{HF})} = \epsilon_d + \frac{2n_{-\sigma}^{(1)} - 1}{n_\sigma^{(1)}(1 - n_\sigma^{(1)})} \sum_k V_{k\sigma} \langle a_{k\sigma}^\dagger c_\sigma \rangle^{(1)} \tag{49}$$

which are related to the corresponding definitions for the Hubbard model (10) and (36) by means of the self-consistent mapping. As for the EHA the moment sum rule for $m = 3$ is violated since generally $B_{-\sigma}^{(\mathrm{HF})} \neq B_{-\sigma}$.

B. Modified perturbation theory (MPT)

It is possible to improve the Kajueter-Kotliar approach such that the moments up to $m = 3$ are recovered correctly [23]. This constitutes the modified perturbation theory (MPT) [25]. We start from the same ansatz (43) for the self-energy of the SIAM. Contrary to the KK approach, however, the parameters are fitted to the $m = 2$ and the $m = 3$ moment. Using

$$\Sigma_{d\sigma}^{(\mathrm{SOC})}(E) = \frac{U^2 n_{-\sigma}^{(1)}(1 - n_{-\sigma}^{(1)})}{E} + \frac{U^2 n_{-\sigma}^{(1)}(1 - n_{-\sigma}^{(1)})(B_{-\sigma}^{(\mathrm{HF})} - \widetilde{\mu}_\sigma + U n_{-\sigma})}{E^2} + \cdots , \tag{50}$$

the high-energy expansion of the ansatz (43) is easily performed. Comparing with the exact result for the expansion coefficients in Eq. (16), we have to choose

$$b_\sigma = \frac{B_{-\sigma} - \mu - B_{-\sigma}^{(\mathrm{HF})} + \widetilde{\mu}_\sigma + U(1 - 2n_{-\sigma}))}{U^2 n_{-\sigma}^{(1)}(1 - n_{-\sigma}^{(1)})} \tag{51}$$

for the parameter b_σ to ensure the correctness of the moments. a_σ is still given by Eq. (45).

We also modify the condition that fixes the parameter $\widetilde{\mu}_\sigma$. Analogous to the condition (34) used in the EHA and IAA, we demand:

$$n_\sigma^{(1)} = n_\sigma \, . \tag{52}$$

Choosing $\widetilde{\mu}_\sigma$ to enforce the Luttinger theorem implies the theory to be intrinsically limited to zero temperature. The condition (52) is less problematic. It also allows to perform calculations at finite temperatures. Numerical results for $T = 0$ have shown [25] that a significant violation of the Luttinger sum rule occurs for fillings that considerably differ from half-filling only.

The MPT reduces to the KK approach for the symmetric case of a paramagnet at half-filling and symmetric BDOS: Here we have $B_\sigma^{(\mathrm{HF})} = B_\sigma = \epsilon_d$ due to particle-hole symmetry. For small U the MPT recovers the exact weak-coupling result up to order U^2. By construction the moment sum rule is obeyed up to $m = 3$ which ensures the theory to be consistent with the strong-coupling perturbational results of Harris and Lange and also implies the validity of the MPT in the atomic limit for arbitrary filling.

For the following discussion we refer to the KK approach as the original approach of Ref. [70] but with the Luttinger theorem replaced by Eq. (52) as the condition to fix $\widetilde{\mu}_\sigma$. This allows to compare the "KK" approach with the MPT also for $T \neq 0$.

VII. RESULTS AND DISCUSSION

Numerical calculations have been performed for all approaches that have been discussed in the preceding sections. To study the effect of B_σ and the meaning of the moment sum rule for the paramagnet, we consider the hyper-cubic (hc) lattice in infinite dimensions. The coordination number is $Z = 2d$. We take $T_{\langle ij \rangle} \equiv t = t^*/\sqrt{2Z}$ ($t^* = \mathrm{const.}$) for the scaling of the hopping as $d \mapsto \infty$ [9]. The non-interacting Bloch density of states (BDOS) is a Gaussian [9]:

$$\rho^{(\mathrm{B})}(E) = \frac{1}{t^*\sqrt{\pi}} e^{-(E/t^*)^2} \, . \tag{53}$$

$T_0 \equiv T_{ii} = 0$ has been chosen to fix the energy zero.

We also consider a generalization of the $d = 3$ fcc lattice to infinite dimensions [92] which favors ferromagnetic order [48, 49]. The hopping is scaled as $t = t^*/\sqrt{Z}$ where $Z = 2d(d-1)$, and the BDOS reads:

$$\rho^{(\mathrm{B})}(E) = \frac{e^{-(1+\sqrt{2}E/t^*)/2}}{t^*\sqrt{\pi(1+\sqrt{2}E/t^*)}} \, . \tag{54}$$

Energy units are chosen such that $t^* = 1$.

A. Paramagnet

Let us consider the hc lattice first. In a wide region of the U-n plane the system is a paramagnetic Fermi liquid. Near half-filling antiferromagnetic order is observed [16, 21, 42, 43, 44, 47]. Saturated ferromagnetism can be excluded completely [59] while non-saturated ferromagnetic order has been found recently for very strong interaction U [53]. We will restrict our investigation for the hc lattice to the paramagnetic phase only.

According to the results of Harris and Lange, the first non-trivial effect of $1/U$ perturbation theory beyond the atomic limit consists in a specific shift of the centers of gravity of the Hubbard bands. For the lower one it is given by $n_{-\sigma}B_{-\sigma}$. Fig. 1 shows this band shift as a function of the filling n for the hc lattice at finite inverse temperature $\beta = 7.2$ and at moderate coupling strength $U = 4$ (the U dependence will be discussed below). For each of the approaches that obey the moment sum rule up to $m = 3$, the correlation function $B_{-\sigma}$ (inset in Fig. 1) has been determined self-consistently via Eq. (18). Electron correlations are meaningless for filling $n = 0$; consequently, the band shift $n_{-\sigma}B_{-\sigma}$ vanishes. At half-filling $n = 1$ we have $n_{-\sigma}B_{-\sigma} = 0$ due to particle-hole symmetry. Inbetween the band shift acquires positive values with a maximum at $n \approx 0.5 - 0.75$ depending on the approximation scheme considered. The typical size of the shift ($n_{-\sigma}B_{-\sigma} \approx 0.2$) is significant compared with the variance $\Delta = 1/\sqrt{2}$ of the BDOS.

For the same set of parameters but with the filling fixed at $n = 0.79$, Fig. 2 shows the quasi-particle density of states (DOS) $A_\sigma(E)$. For the discussion of the effects of the band shift we concentrate on the result for the spectral-density approach (SDA) and the Hubbard-I solution (H-I) first. Within the two-pole approaches the DOS for $U \mapsto \infty$ can be written in terms of the BDOS as:

$$A_\sigma(E) = \rho^{(\mathrm{B})}\left(\frac{E + \mu - n_{-\sigma}B_{-\sigma}}{1 - n_{-\sigma}}\right)$$

$$+ \rho^{(\mathrm{B})} \left(\frac{E + \mu - U - (1 - n_{-\sigma}) B_{-\sigma}}{n_{-\sigma}} \right) , \quad (55)$$

where $B_{-\sigma} \mapsto T_0$ for the H-I solution. Comparing the SDA with the H-I solution, the shift $n_{-\sigma} B_{-\sigma}$ of the lower Hubbard band present in the SDA must be canceled exactly by a corresponding shift of the chemical potential μ for a fixed filling n. Thus the small differences between SDA and H-I seen in the lower Hubbard band exclusively result from the finite value for U and will disappear for $U \mapsto \infty$. On the other hand, the upper Hubbard band is significantly shifted to higher energies compared with the H-I solution. This effect persists also for $U \mapsto \infty$ where the energetic positions will differ by an amount $(1 - 2n_{-\sigma}) B_{-\sigma}$.

Comparing the other pairs of approximation schemes among each other, we notice similar qualitative effects. Generally, the inclusion of $B_{-\sigma}$ in the theory results in fairly small changes of the lower but in a significant shift of the upper Hubbard band to higher energies (for fixed n). For the MAA there is an additional change in the peak heights compared with the AA. For the IAA and the MPT the shift of the respective upper Hubbard band against the EHA and the KK result turns out to be much smaller when compared with the MAA/AA or

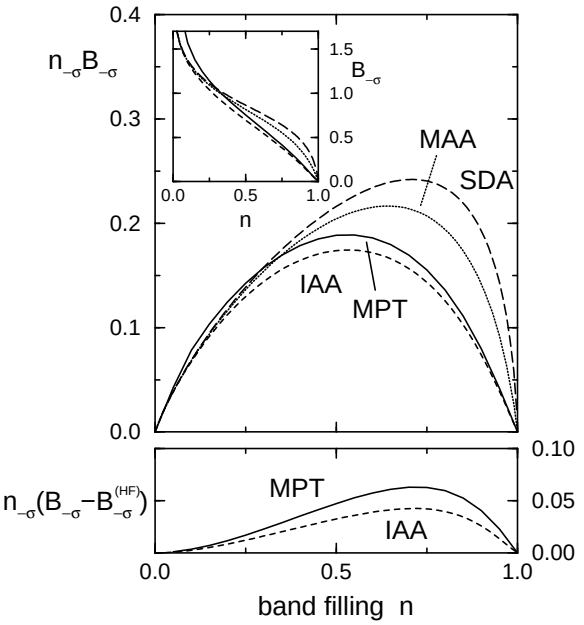

Fig. 1. Filling dependence of the shift $n_{-\sigma} B_{-\sigma}$ of the center of gravity of the lower Hubbard band as obtained self-consistently within the spectral-density approach (SDA), the modified alloy analogy (MAA), the interpolating alloy-analogy-based approach (IAA) and the modified perturbation theory (MPT). Inset: filling-dependence of $B_{-\sigma}$. Lower panel: difference $n_{-\sigma}(B_{-\sigma} - B_{-\sigma}^{(\mathrm{HF})})$ for the IAA and MPT. Calculations for the $d = \infty$ paramagnetic Hubbard model on the hc lattice at $U = 4$ and $\beta = 7.2$. The results are symmetric to the $n = 1$ axis (half-filling). Energy units are chosen such that $t^* = 1$.

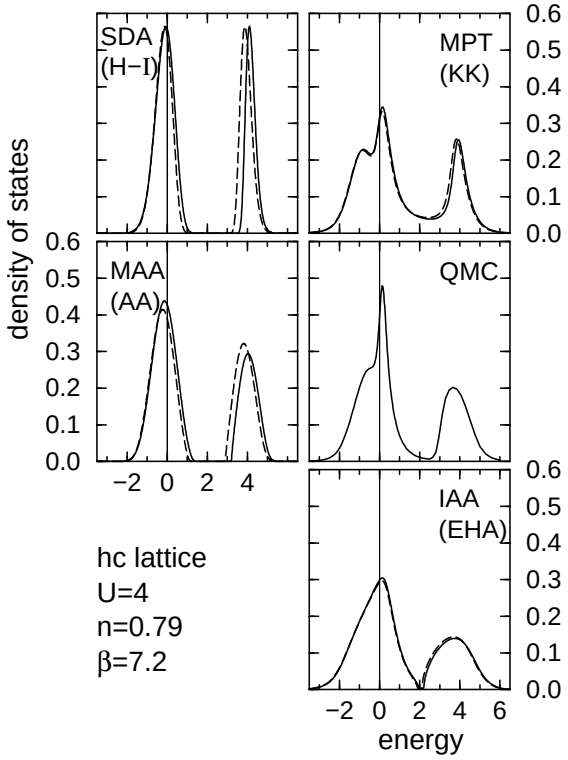

Fig. 2. Density of states $A_\sigma(E)$ as a function of energy for the hc lattice at $U = 4$, $n = 0.79$ and $\beta = 7.2$ as obtained within the Hubbard-I solution (H-I), the conventional alloy analogy (AA), the Kajueter-Kotliar approach (KK) and the Edwards-Hertz approach (EHA): dashed lines. Solid lines: resulting DOS within the improved theories: SDA, MAA, EHA and MPT. For comparison the numerically exact result obtained within the Quantum Monte Carlo method (QMC) by Jarrell and Pruschke [21] is shown.

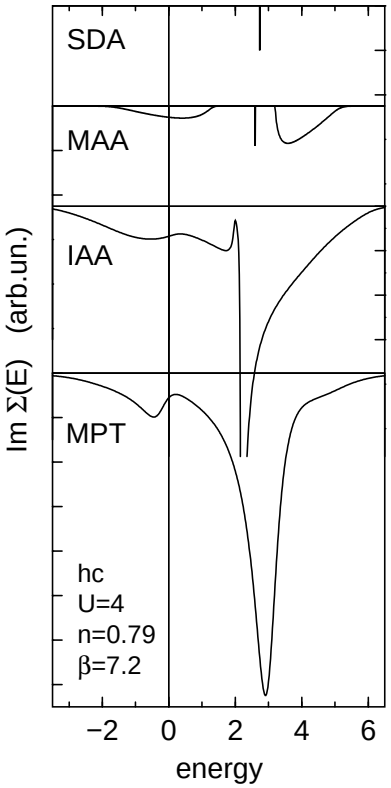

Fig. 3. Imaginary part of the self-energy as a function of energy for the hc lattice at $U = 4$, $n = 0.79$ and $\beta = 7.2$. Thin horizontal lines indicate $\mathrm{Im}\,\Sigma(E) = 0$. Within the SDA $\mathrm{Im}\,\Sigma(E)$ consists of a single delta peak only which is indicated by a vertical solid line at the calculated energetic position (also for the MAA). For the IAA $\mathrm{Im}\,\Sigma(E)$ is always finite, large (negative) values near $E = 2.2$ are not shown.

SDA/H-I. The reason is that within the EHA and the KK approach the band shift is not neglected completely (as for H-I and AA where $n_{-\sigma}B_{-\sigma} \mapsto n_{-\sigma}T_0$), but is taken into account on the Hartree-Fock level at least: $n_{-\sigma}B_{-\sigma} \mapsto n_{-\sigma}B_{-\sigma}^{(\mathrm{HF})}$. Indeed, as is shown in the second panel of Fig. 1, the difference $n_{-\sigma}(B_{-\sigma} - B_{-\sigma}^{(\mathrm{HF})})$ as calculated self-consistently within the IAA and the MPT is considerably smaller than the difference $n_{-\sigma}(B_{-\sigma} - T_0)$ relevant for the SDA and MAA.

Fig. 2 also shows the essentially exact result for the DOS as obtained by Jarrell and Pruschke [21] by means of the QMC method. One clearly recognizes the two Hubbard bands which are well separated from each other. The energetic difference is approximately given by U. Additionally, in the vicinity of $E = 0$ there is a rather sharp quasi-particle resonance which is reminiscent of the Kondo peak in the SIAM. All approximate methods reliably reproduce the energetic positions as well as the weights of the Hubbard bands. If at all, there is only a slight improvement with respect to positions and weights when taking into account the correlation function $B_{-\sigma}$ additionally. We can conclude that in this respect and in the case of the paramagnet the effects of $B_{-\sigma}$ are rather unimportant; considering the moment sum rule does not help much to improve the agreement with the QMC result.

Since quasi-particle damping is neglected completely within the SDA, the Hubbard peaks turn out to be too narrow. Furthermore, there is no additional structure at $E = 0$. Obviously, the Kondo-type resonance cannot evolve in a two-pole approach. Somewhat broader peaks are predicted by the MAA; compared with the QMC density of states, however, their width is still too small. The IAA yields a considerable improvement. Yet, the size of the Hubbard gap is underestimated, and only a small asymmetry in the shape of the lower Hubbard band hints towards the resonance. The MPT achieves a reasonable agreement with the exact result. The Kondo-type resonance is clearly visible but not as pronounced as in the QMC spectrum.

Additional insight is provided by the imaginary part of the retarded self-energy which is shown in Fig. 3. The pole of the SDA self-energy (20) at $E = B_{-\sigma} + U(1 - n_{-\sigma}) - \mu$ gives rise to a single delta peak in $\mathrm{Im}\,\Sigma(E)$, which, however, is meaningless since it falls into the Hubbard gap. Taking the imaginary part of the CPA equation (21) at an energy E where $\mathrm{Im}\,G(E) = 0$ (is exponentially small), we obtain:

$$0 = \mathrm{Im}\,\Sigma_\sigma(E) \sum_{p=1}^{2} \frac{x_{p\sigma}}{\left|1 - \frac{1}{\hbar} G_\sigma(E)(E_{p\sigma} - \Sigma_\sigma(E) - T_0)\right|^2} \,. \tag{56}$$

This implies that a finite imaginary part of the MAA self-energy can be found in those energy ranges with non-vanishing DOS only, except for the energy point at which there is a zero of the denominator in Eq. (56). Here we find a delta peak in $\mathrm{Im}\,\Sigma(E)$ again (vertical line in Fig. 3). The delta peak does not contribute to the damping of the DOS but acquires most of the weight. This explains why the broadening of the Hubbard bands is still underestimated by the MAA.

In the IAA $G_\sigma(E)$ is replaced by the modified propagator $\widetilde{G}_\sigma(E)$ which yields a considerably stronger quasiparticle damping. We also note a small dip in the imaginary part of the IAA self-energy at $E \approx 0$. This tends to reproduce the correct Fermi-liquid behavior $\mathrm{Im}\,\Sigma(E) \sim E^2$ for $T = 0$. A $T = 0$ calculation, however, shows $\mathrm{Im}\,\Sigma(0) \neq 0$ at $U = 4$ and $n = 0.79$. Similar to the EHA [67, 68], the IAA does not yield a Fermi surface in wide regions of the U-n plane. Contrary, the MPT self-energy always vanishes quadratically at $E = 0$ and $T = 0$. Fig. 3 also shows a more pronounced dip in $\mathrm{Im}\,\Sigma(E)$ at $E \approx 0$ in the finite-temperature MPT result. Compared with the IAA, the damping effect is of the same order of magnitude. In all cases the total weight $\int \mathrm{Im}\,\Sigma_\sigma(E)\,dE$ is given by $-\pi U^2 n_{-\sigma}(1 - n_{-\sigma})$. This follows directly from the high-energy asymptotics of the self-energy (16).

There is a strong dependence of the band shift on the interaction strength U. Fig. 4 shows $B_{-\sigma}$ as a function of U as resulting from the different approximation schemes for $n = 0.79$ and $\beta = 7.2$. For large U the correlation function $B_{-\sigma}$ becomes essentially independent of U. Within all approaches this asymptotic behavior is reached for $U \approx 4$; for $U > 4$ there is a very slight U dependence only. The asymptotic values predicted by the SDA and the MAA are considerably larger than those predicted by the IAA and MPT. Although the underlying physical concepts are quite different, there is a remarkable similarity between the results from the latter two approaches over the whole U range. For small U the results are nearly identical (up to $U \approx 2$). This had to be expected since the IAA as well as the MPT self-energies are correct up to order U^2. Via Eq. (18) this implies that $B_{-\sigma}(U)$ is exact in order U, i. e. at $U = 0$ $B_{-\sigma}(U)$ starts with the correct slope within the IAA and MPT. Of course, at $U = 0$ all approaches yield the same value for $B_{-\sigma}$.

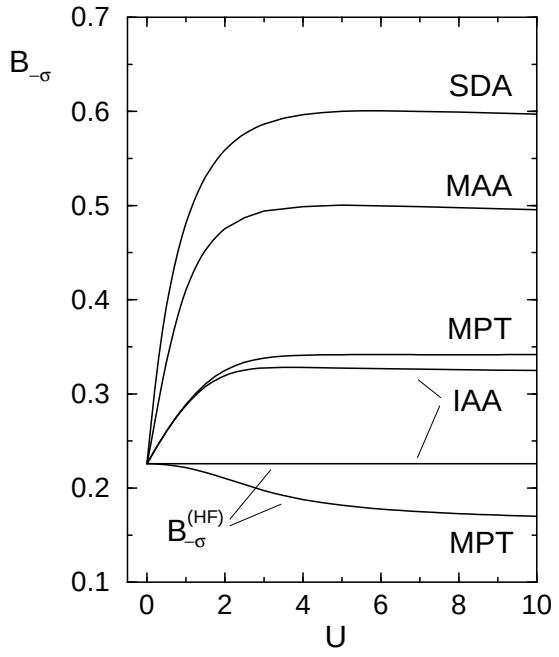

Fig. 4. U dependence of the correlation function $B_{-\sigma}$ (hc lattice, $n = 0.79$, $\beta = 7.2$). For the IAA and the MPT $B_{-\sigma}^{(\mathrm{HF})}$ is shown additionally.

For the IAA and the MPT Fig. 4 also shows the dependence of $B_{-\sigma}^{(\mathrm{HF})}$ on U. Within the IAA $B_{-\sigma}^{(\mathrm{HF})}$ is given by Eq. (36). The condition (34) that fixes the shifts E_σ can be written as $n_\sigma^{(1)} = n_\sigma$. It implies that $n_\sigma^{(1)}$ as well as $\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle^{(1)}$ are independent of U, and therefore $B_{-\sigma}^{(\mathrm{HF})}$ turns out to be a constant that depends of n and β only. Analogously, due to the condition (52) there is no U dependence of $n_\sigma^{(1)}$ in the MPT. The hybridization function Δ_σ, however, does depend on U due to the self-consistent mapping procedure. This leads to a U dependence of the second factor in Eq. (49) and thus of $B_{-\sigma}^{(\mathrm{HF})}$ as can be seen in Fig. 4.

For all approaches considered here we did not find ferromagnetic solutions on the hc lattice. We calculated the uniform static susceptibility by applying an infinitesimally small external field: $\chi = \partial m/\partial H$. The susceptibility never diverged for $U < 6$. This is consistent with the QMC results of Refs. [12, 65] and also with the complete instability of the Nagaoka state on the hc lattice [59]. Let us mention, however, that a partially polarized ferromagnetic state has been found recently for extremely strong interaction U [53].

B. Ferromagnetism

While the moment sum rule for $m = 3$ has turned out to be of marginal importance for the paramagnetic phase, it is much more decisive with respect to the possibility and the characteristics of ferromagnetic order. This shall be elucidated by the following arguments:

Firstly, ferromagnetism is a strong-coupling phenomenon. We thus have to account for the Hubbard splitting. It is a necessary condition for the evolution of the Hubbard bands as $U \mapsto \infty$, however, that the moment sum rule is obeyed up to $m = 2$ (see Ref. [33], for example). This is achieved e. g. by the H-I and the AA solution.

Secondly, within the H-I approach ferromagnetism turns out to be rather unlikely. Ferromagnetic order may be possible for small n only when there is a large BDOS at the Fermi energy away from the band center of gravity [2]. The AA solution is even more prohibitive with respect to ferromagnetic order [93, 94]. The *reason* [94] for this tendency to paramagnetism is that even in a (possible) ferromagnetic phase, the band centers of gravity $T_{p\sigma}(\mathbf{k})$ of the majority and of the minority electrons at each $\mathbf{k}$ point are *equal*: $T_{p\uparrow}(\mathbf{k}) = T_{p\downarrow}(\mathbf{k})$ for both, the lower ($p = 1$) and the upper ($p = 2$) Hubbard band. What is missing in the H-I and the AA approach to get a stable and extended ferromagnetic phase, is the possibility for a *spin-dependent* shift of the centers of gravity of the Hubbard bands.

Thirdly, the possibility for a spin-dependent band shift is not only required but in fact is predicted by the $1/U$ perturbational approach of Harris and Lange which is exact for $U \mapsto \infty$: As is seen from Eq. (9), the spin-dependent shifts of the lower and the upper σ band are $n_{-\sigma}B_{-\sigma}$ and $(1 - n_{-\sigma})B_{-\sigma}$, respectively. The higher-order correlation functions included in the definition (10) of $B_{-\sigma}$ open the channel for ferromagnetic solutions in the Hubbard model.

Finally, as has been discussed in Sec. 2, the perturbational results of Harris and Lange for the strong-coupling regime can only be recovered if the moment sum rule is respected up to $m = 3$.

It goes without saying that the $1/U$ perturbation theory merely determines the global features of the quasi-particle spectrum and abstracts from any internal structure of the Hubbard bands which may be due to damping effects or low-energy excitations, for example. Indeed, in the preceding section we have seen that different approximations yield rather different results even if all respect the sum rule up to $m = 3$. Thus it has to be expected that there is a dependence of the results on the approximation used also in the case of the ferromagnet.

Our intention here is twofold: Firstly, as has been noticed in the case of the paramagnet, conceptually improving the method (SDA $\mapsto$ MAA $\mapsto$ IAA, MPT) also yields a closer agreement with the QMC results. This will be checked for the ferromagnet, too. Secondly, comparing the results of different methods with each other (H-I $\leftrightarrow$ SDA, AA $\leftrightarrow$ MAA, EHA $\leftrightarrow$ IAA, KK $\leftrightarrow$ MPT), we are able to "switch on" and to "switch off" in a controlled way the possibility for a spin-dependent band shift that is given via $B_{-\sigma}$. This will clarify whether the concept of the spin-dependent band shift really helps to understand ferromagnetism, i. e. whether the system "uses" this possibility and "realizes" the spin-dependent shift of the bands.

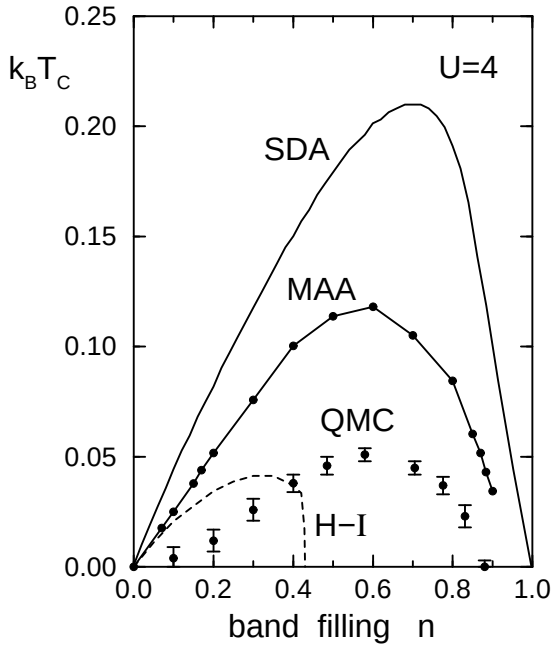

Fig. 5. Filling dependence of the Curie temperature T_C for the SDA (solid line) and H-I (dashed line) as well as for the MAA (circles) in comparison with the QMC results (error bars) by Ulmke [49] for the $d = \infty$ fcc-type lattice. (Within the AA there is no ferromagnetic instability at all).

For the infinite-dimensional fcc-type lattice with the BDOS given by Eq. (54), ferromagnetic order even occurs at a moderate coupling strength $U = 4$ and extends over a rather wide region in the n-T plane. This was proven numerically within the QMC method by Ulmke [49]. Due to the strong frustration of the fcc-type lattice antiferromagnetic order is not expected. The highly asymmetric BDOS (54) with its square-root singularity at the lower band edge $E_b = -1/\sqrt{2}$ favors ferromag-

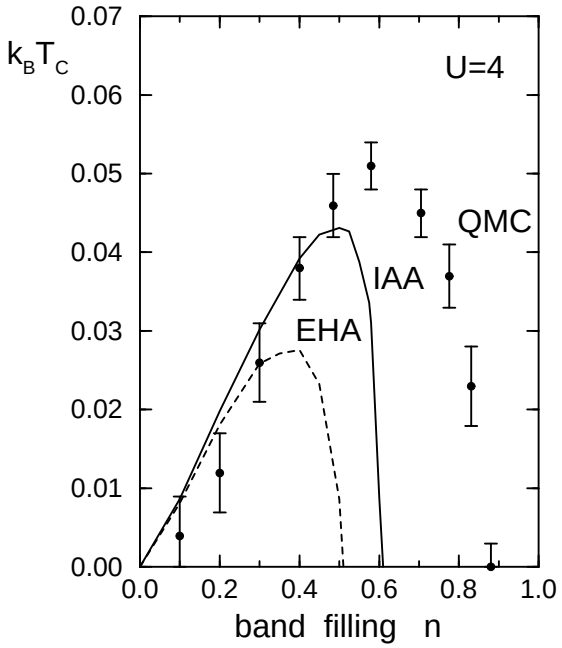

Fig. 6. $T_C(n)$ as obtained within the IAA (solid line) and the EHA (dashed line) compared with the QMC result [49].

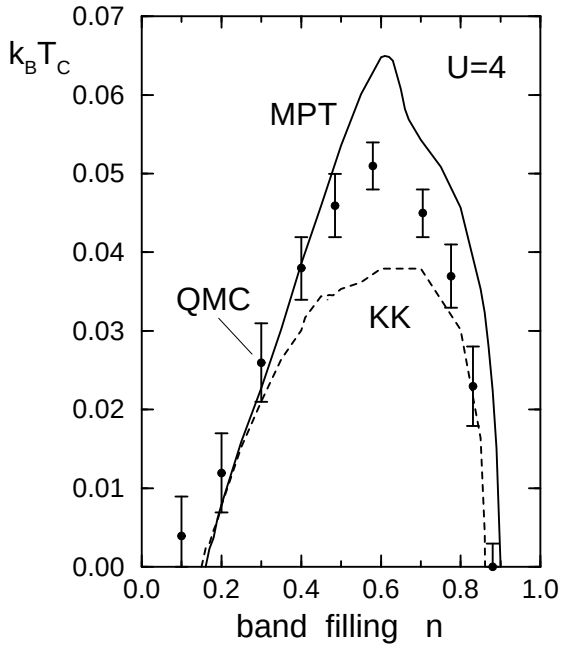

Fig. 7. $T_C(n)$ as obtained within the MPT (solid line) and KK (dashed line) compared with the QMC result [49].

netic order [48, 49, 95]. The QMC results of Ulmke [49] are shown in Fig. 5. The filling-dependence of the Curie temperature T_C has been obtained from the zero of χ^{-1} which shows a linear Curie-Weiss behavior.

The high density of states at the lower band edge is sufficient to produce stable ferromagnetism within the H-I solution. The resulting filling dependence of T_C is shown in Fig. 5. The ferromagnetic region in the n-T plane, however, is confined to very low densities only. As mentioned this is known to be typical for the H-I approach [2]. Contrary to the H-I solution, the SDA allows for a spin-dependent band shift. Fig. 5 shows that this leads to a considerable increase of the Curie temperature. Furthermore, ferromagnetic solutions are found for all fillings up to half-filling $n = 1$. These effects of $B_{-\sigma}$ are much stronger than those found for the paramagnetic phase.

At $n = 0.58$ and $T = 0$ the system is fully polarized ($m = n$). The spin splitting of the center of gravity of the lower Hubbard band amounts to $n_\uparrow B_\uparrow - n_\downarrow B_\downarrow = 0.73$. This has to be removed as T approaches the Curie temperature while the Hubbard gap still exists above T_C. The spin splitting is considerably smaller compared with the exchange splitting $Un_\uparrow - Un_\downarrow = 2.32$ within Hartree-Fock (Stoner) theory where correlation effects are neglected altogether. Consequently, the SDA yields a Curie temperature that is smaller by more than a factor 3: $k_B T_C^{(\mathrm{SDA})} = 0.19$ and $k_B T_C^{(\mathrm{Stoner})} = 0.74$ (at $n = 0.58$, $U = 4$). The difference becomes larger and larger with increasing U since as a function of U the Curie temperature is unbounded in the Stoner theory while it reaches saturation within the SDA [30]. The unrealistically high Stoner Curie temperature results from the necessity to bridge an exchange splitting of order U by the thermal energy $k_B T_C$.

A spin-dependent band shift is also realized within the MAA approach. Stable ferromagnetism is found for fillings $0 < n < 1$ (close to half filling we have not succeeded to obtain truely converged numerical solutions). Compared with the SDA, the Curie temperature is significantly lower for all fillings. While the mechanism leading to ferromagnetic symmetry breaking is the same in the SDA and MAA, ferromagnetism is destabilized to some extent by means of quasi-particle damping (see also Ref. [72]). The broadening of the respective

spin-dependent bands tends to enhance their overlap and leads to a (self-consistent) depression of the magnetization and thereby of T_C. The decisive meaning of the $m = 3$ sum rule becomes most apparent when we "switch off" the possibility of a spin-dependent band shift, i. e. if we compare the MAA results with those of the conventional AA. There is no ferromagnetic instability at all in the AA as has been proven in Ref. [93] and also tested numerically for the fcc-type lattice considered here. Therefore, ignoring the possible spin-dependent band shift $n_{-\sigma}B_{-\sigma}$, misses the most important route to ferromagnetic order.

Quasi-particle damping becomes stronger when turning from the MAA to the IAA. Again, we notice a considerable decrease of the Curie temperature for all fillings. Fig. 6 shows that the maximum T_C in the IAA is less than half of the maximum T_C predicted by the MAA. Moreover, the ferromagnetic region shrinks to $n < 0.61$. Comparing with the EHA, we again notice that the spin-dependent band shift induced by $B_{-\sigma}$ favors ferromagnetic order: Since $B_{-\sigma}$ is replaced by $B_{-\sigma}^{(\mathrm{HF})}$ in the EHA [cf. Eq. (37)], the EHA partially accounts for the band shift. However, we find the spin splitting of $B_{-\sigma}$ to be larger than that of $B_{-\sigma}^{(\mathrm{HF})}$. Consequently, T_C is enhanced in the IAA although the differences seen in Fig. 6 are moderate compared with the cases H-I/SDA and AA/MAA.

The same arguments hold for the MPT and the KK approach: The spin splitting of the center of gravity due to $B_{-\sigma}^{(\mathrm{HF})}$ is somewhat smaller than that due to $B_{-\sigma}$. This implies a higher T_C in the MPT compared with the KK approach [see Eq. (47)]. The filling dependence of T_C is shown in Fig. 7. The differences between the KK approach and the MPT are moderate again and comparable to the EHA/IAA case. Once more, this suggests a one-to-one correspondence between the critical temperature and the band shift due to $B_{-\sigma}$ in the $m = 3$ moment.

For comparison we included the essentially exact QMC result [49] for $T_C(n)$ in Figs. 5-7. While the Stoner theory yields a Curie temperature that is by more than one order of magnitude too high (see Ref. [95], for example), realistic values are found by the approximations discussed here. Even the simplest scheme consistent with the requirements of Harris and Lange, the SDA, considerably improves upon the Stoner result. A quantitative agreement with the essentially exact result, however, cannot be expected since damping effects are neglected completely. A further improvement towards the QMC result is achieved by the MAA which takes into account a finite quasi-particle life time. Yet, the Curie temperatures are systematically too high since damping effects are underestimated (cf. previous section and Fig. 9). The correct order of magnitude for T_C can only be expected if (i) the theory respects the $m = 3$ sum rule and (ii) realistically accounts for quasi-particle damping as is done by the IAA and the MPT.

Fig. 8 focuses on the temperature dependence of the magnetization at $n = 0.58$. The QMC data can be well fitted to an $S = 1/2$ Brillouin-function. Extrapolation to $T = 0$ yields $m = n$ [49]. A fully polarized ground state is also obtained by the SDA and MAA, the MPT predicts a slightly lower m. The filling $n = 0.58$ is near to the quantum-critical point $n_c^{(\mathrm{IAA})} = 0.61$ in the IAA (cf. Fig. 6). Since phase transitions have been found to be always of second order within the IAA, a partially polarized ground state near $n_c^{(\mathrm{IAA})}$ is plausible from the result in Fig. 6. The vicinity to $n_c^{(\mathrm{IAA})} = 0.61$ may also explain the non-Brillouin-function-like shape of the magnetization curve. Fig. 8 shows second-order transitions for the SDA, MAA and MPT at $n = 0.58$. Depending on the filling, however, all three methods may also predict first-order transitions to the paramagnetic phase. Non-continuous transitions are observed for fillings larger than $\sim n_{\max}$ where $n_{\max}$ is the filling at which T_C reaches its maximum. For the MPT the change of second-order into first-order transitions is marked by the kink in the $T_C(n)$ curve at $n = 0.67$ (Fig. 7). While magnetic first-order transitions may seem to be implausible, they cannot be ruled out by a rigorous argument. On the other hand, we cannot strictly exclude that they are artefacts of the approximations.

For the second-order transitions shown in Fig. 8 the homogeneous, static susceptibility $\chi = \partial m/\partial H|_{H=0}$ diverges at $T = T_C$. Within all approaches considered χ obeys the Curie-Weiss law for high temperatures. But also for temperatures close to T_C we observe an almost linear trend of χ^{-1}. This is consistent with the QMC result. Note that the different slopes in the plot result from the different Curie temperatures. From $\chi = C/(k_{\mathrm{B}}T - k_{\mathrm{B}}\Theta)$ we have calculated the (dimensionless) Curie constant C. For the paramagnetic Curie temperature we have assumed $\Theta = T_C$ except for the IAA where $k_{\mathrm{B}}\Theta = 0.057$ has been obtained by extrapolation of the linear trend of χ^{-1} at high temperatures. The QMC value $C = 0.47$ is to be compared

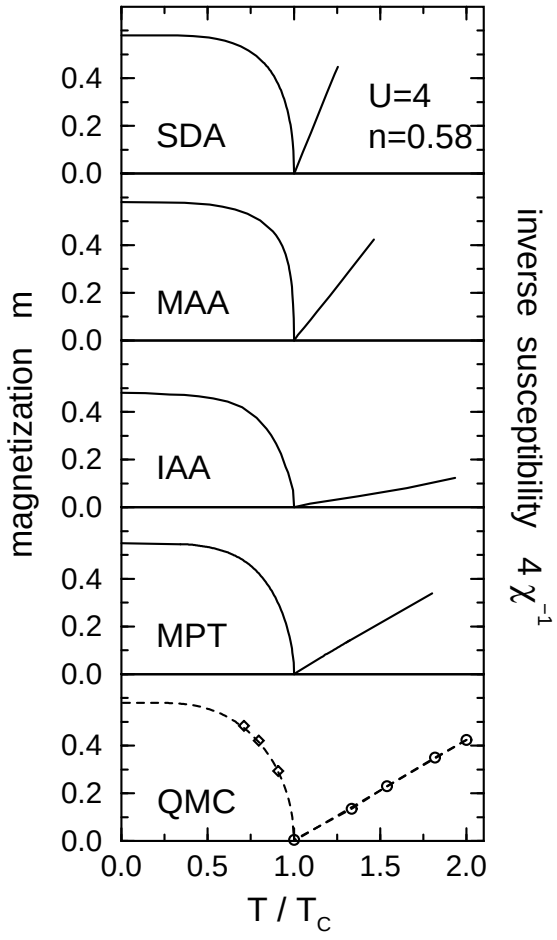

Fig. 8. Homogeneous magnetization m as a function of the reduced temperature T/T_C for the fcc-type lattice at $U = 4$ and $n = 0.58$ as obtained self-consistently within the SDA, MAA, IAA and the MPT (solid lines below $T/T_C = 1.0$). Bottom panel: QMC data from Ulmke [49] (diamonds). The dashed line below $T/T_C = 1.0$ is a Brillouin-function fit to the data. For $T/T_C > 1.0$ the inverse homogeneous static susceptibility χ^{-1} (multiplied by a factor 4) is shown. Circles: QMC data [49]. Dashed line: linear fit to the data.

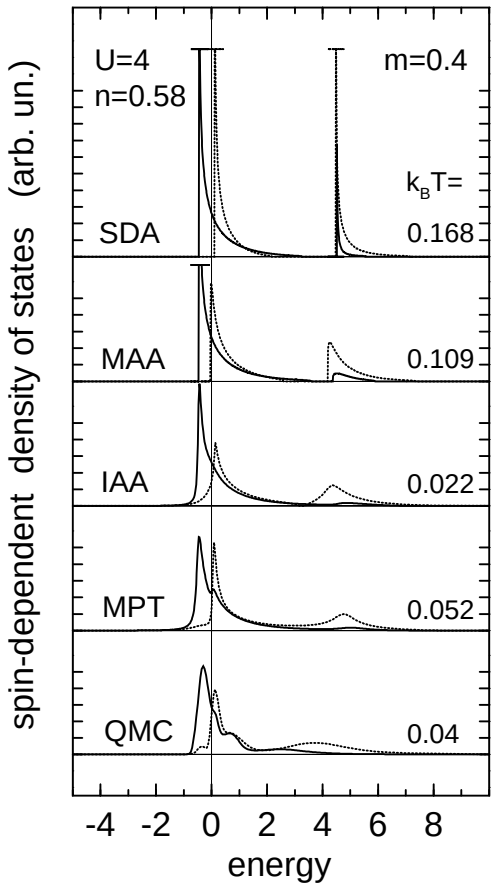

Fig. 9. Spin-dependent density of states $A_\sigma(E)$ as a function of energy (fcc lattice, $U = 4$, $n = 0.58$). Solid (dotted) lines: majority (minority) spin. QMC result from Ref. [49]. In each case (SDA, MAA, IAA, MPT) the respective temperature (given in the figure) has been chosen to yield a magnetization of $m = 0.4$.

with $C = 0.42, 0.52, 0.50, 0.57$ for the SDA, MAA, IAA and MPT, respectively.

Finally, we compare the spin-dependent spectral density as obtained by the approximate schemes with the essentially exact QMC result. Fig. 9 shows $A_\sigma(E)$ in the ferromagnetic phase for $\sigma =\uparrow$ (majority) and $\sigma =\downarrow$ (minority spin) at $U = 4$ and $n = 0.58$. For a meaningful comparison the respective temperature has been chosen to yield a magnetization of $m = 0.4$. In the SDA spectrum we recognize the large Hubbard splitting $\sim U$ and a much smaller additional spin splitting for each of the two Hubbard bands. Furthermore, a correlation-induced spin-dependent narrowing as well as a spin-dependent weight of the subbands is observed. All features agree qualitatively well with the predictions of Harris and Lange which are valid for $U \mapsto \infty$. A more quantitative estimate shows up discrepancies with respect to the positions and weights given by Eq. (9) which are due to the moderate value assumed for U.

The shape of the peaks only slightly deviates from the shape of the BDOS. This is an artefact resulting from the complete disregard of quasi-particle damping. Turning to the MAA spectrum, a broadening of the peaks is introduced. Damping effects are even more pronounced by the IAA and the MPT. This turns out to be quite realistic when comparing with the QMC spectrum which also shows up a considerable peak broadening. In all approximations the spin-dependent position and weight of the lower Hubbard band is well reproduced, the position of the upper Hubbard band, however, is shifted to higher energies compared with the QMC spectrum. This indicates that for $U = 4$ the interaction is not sufficiently strong to reproduce the position resulting from the $1/U$ perturbation theory. An additional peak in the $\sigma =\uparrow$ as well as in the $\sigma =\downarrow$ channel of the QMC spectrum shows up at $E \approx 0.8$ the physical origin of which is unclear. It is not reproduced by the approximate methods. At $E \approx 0$ there is also a weak shoulder in the $\sigma =\uparrow$ QMC spectrum. This is clearly reproduced by the MPT; but also in the IAA spectrum there is a (very weak) structure at $E \approx 0$. As for the paramagnet the peak is interpreted as a Kondo-like resonance. It cannot show up in the $\downarrow$ spectrum, since the filling of the $\downarrow$ band is too small.

VIII. CONCLUSIONS

The present paper has discussed the moment sum rule as a valuable source of a priori information on the physical properties of strongly interacting lattice fermion models. The analysis has been restricted to the single-band Hubbard model in infinite dimensions since this allows to compare with numerically exact solutions. Here the reliability of approximate approaches as well as the usefulness of the sum rule for practical improvements can be estimated safely. The general trends that show up for $d = \infty$ are expected to hold also for finite dimensions, where extensive use of the sum rule has been made in the past. Let us briefly list up the conclusions evolving from our analysis:

(i) The moment sum rule fixes the norm, the center of gravity, the variance, etc. of the interacting spectral density at each $\mathbf{k}$ point in the Brillouin zone. To some extent this determines the "global" single-particle excitation spectrum for arbitrary U. The sum rule is of special conceptual importance in the strong-coupling regime. We could argue that any approximation that predicts the Hubbard splitting for $U \mapsto \infty$ and that yields the correct moments up to $m = 3$ is fully consistent with the first non-trivial results of the perturbation theory in $1/U$ by Harris and Lange. This includes important correlation effects such as the U, filling and spin dependence of the centers of gravity, the widths and the weights of the two Hubbard bands.

(ii) The high-energy expansion of the Green function and of the self-energy provides a practicable way to check to which order m a particular approximation is consistent with the sum rule. The majority of analytical but approximate approaches commonly used turn out to be at variance with the sum rule for $m = 3$. We considered four methods in detail: The Hubbard-I and the Hubbard-III alloy-analogy solutions as well as the Edwards-Hertz and the Kajueter-Kotliar approaches. In each case the sum rule is fulfilled up to $m = 2$ only.

(iii) We have shown that the compatibility with the $m = 3$ moment sum rule can be restored by slight modifications of the original methods. Starting from the H-I and the conventional AA solution, this yields an optimized two-pole and an optimized alloy-analogy approach which turn out to be identical with the spectral-density approach and the so-called modified alloy-analogy solution, respectively. Analogously, the interpolating alloy-analogy-based approximation and the modified perturbation theory evolve straightforwardly from the EHA and the KK approach. We have checked that the applied modifications do not affect the validity of the orig-

inal methods in exactly solvable limiting cases of the Hubbard model.

(iv) All approximation schemes have been implemented for numerical evaluation. We have presented and discussed new results for correlation functions and dynamical quantities which are directly compared with essentially exact QMC results on the hyper-cubic and an fcc-type lattice in infinite dimensions. We observed that with increasing complexity (which is necessary to recover an increasing number of exact limits) the agreement with the QMC results is improved. This corroborates the usefulness of an interpolative analytical approach to the Hubbard model.

In particular, we found it necessary to account for damping effects in a realistic way: If most of the total weight of the imaginary part of the self-energy does not contribute to quasi-particle damping, as in the MAA and more extremely in the SDA, the peak widths that are obtained by QMC cannot be recovered. Comparing the results of the different methods we also found that quasi-particle damping has a destabilizing effect on ferromagnetism which manifests itself in an overall decrease of the Curie temperature.

(v) Out of all approximation schemes considered here, the modified perturbation theory turns out to be most reliable. In the paramagnetic phase it correctly recovers the Kondo-type resonance, shows up the expected Fermi-liquid properties and approximately fulfills the Luttinger sum rule. The MPT yields the qualitatively correct density of states in the weak- and intermediate-coupling regime as confirmed by comparison with the QMC results. At half filling the approach reduces to the iterative perturbation theory (IPT) which is known to yield a rather realistic description of the Mott transition. For the ferromagnetic phase the MPT is able to predict the Curie temperature within an accuracy of $\sim 30\%$. Thereby, the MPT turns out to be superior compared with the IAA. The main drawback of the latter surely consists in its inability to predict a Fermi surface in wide regions of the phase diagram. The same defect is found in the MAA. However, the straightforward and physically well motivated concept of an "optimized alloy-analogy" remains rather attractive. Finally, the SDA is surely too simple to compete with the more elaborate methods. On the other hand, its simplicity is advantageous when a quick though rough estimation of the magnetic phase diagram is required.

(vi) The comparative opposition of the different methods has particularly shown the importance of the $m = 3$ moment sum rule with respect to ferromagnetism. While the differences between the methods with and without regard of B_σ are unimportant or even negligibly small for the paramagnetic phase, the correlation function B_σ considerably affects the ferromagnetic/paramagnetic phase boundary as well as the Curie temperature. The effect is most striking when comparing the AA, where ferromagnetic instabilities are ruled out completely, with the MAA which yields a reasonable dependence $T_C(n)$ for the fcc-type lattice and even overestimates T_C. The reason is found in the term B_σ that appears first in the expression for the $m = 3$ moment. It opens the possibility for a *spin-dependent* shift of the centers of gravity of the Hubbard bands. In the AA and also in the H-I solution this is missing completely ($B_\sigma \mapsto T_0$). In the EHA and the KK approach it is only approximately accounted for ($B_\sigma \mapsto B_\sigma^{(\mathrm{HF})}$). Since $B_\sigma^{(\mathrm{HF})}$ is found to be too small in the EHA and the KK approach, both methods yield a lowered T_C.

From the recent QMC studies [21, 48, 49], in particular from Ref. [95], but also from variational results [58, 59, 60], the importance of the lattice structure for ferromagnetism well established. It is striking that all presently considered approximations that account for B_σ yield a ferromagnetic instability for the non-bipartite fcc-type lattice while (at least up to $U < 6$) the paramagnet is stable on the hc lattice. In Ref. [48] Vollhardt et al. argue that a strongly asymmetric BDOS with high spectral weight at the lower band edge favors ferromagnetism because this minimizes the kinetic energy of the fully polarized state. The shape of the non-interacting BDOS is relevant since the $\uparrow$ DOS is unrenormalized if $n_\uparrow = n < 1$. If it is assumed that details of the BDOS are not so relevant for the paramagnetic state where correlation effects dominate, the ferromagnetic state becomes energetically more favorable. Considering the moment sum rule or, equivalently, the Harris and Lange results, the argumentation can be refined: For the fully polarized state the expression (10) for the band shift reduces to $(1-n)nB_\uparrow = -\langle \sum T_{ij} c_{i\uparrow}^\dagger c_{j\uparrow} \rangle = -E_{\mathrm{kin}}$. This implies that a strong asymmetry of the BDOS not only minimizes the kinetic energy (at a given filling n) but also maximizes the shift $n_\uparrow B_\uparrow > 0$ of the center of gravity of the lower $\downarrow$ Hubbard band to higher energies. Therewith, the spin splitting $n_\uparrow B_\uparrow - n_\downarrow B_\downarrow = n_\uparrow B_\uparrow$ of the lower Hubbard band becomes maximal which enhances the stability (reduces the instability) of the fully polar-

ized state. This mechanism is already present within the simple SDA. While the approach overestimates the possibility for ferromagnetism, it predicts the correct trend when comparing different lattices [22].

As an intermediate to strong-coupling phenomenon, ferromagnetism in all its different aspects is hardly amenable to a simple explanation. We feel, however, that by considering the spin-dependent band shift appearing in $1/U$ perturbation theory and the $m = 3$ moment one is able to capture some of the essentials in a rather simple and physically intuitive way.

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