Proper weak-coupling approach to the periodic s-$d(f)$ exchange model

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The periodic s-$d(f)$ exchange model is characterized by a wide variety of interesting applications, a simple mathematical structure, and a limited number of reliable approximations which take care of the quantum nature of the participating spins. We suggest the use of a projection-operator method for getting information perturbationally, which are not accessible via diagrammatic approaches. In this paper we present, in particular, results beyond perturbation theory, which are obtained such that almost all exactly known limiting cases are incorporated correctly. We discuss a variety of possible methods and evaluate their consequences for one-particle properties. These considerations serve as a guideline for a more effective approach to the model.

I. INTENTION

The interplay of localized magnetic moments (of d- or f-type) with itinerant s electrons of a partially filled conduction band is of indisputable importance for the explanation of many effects in condensed-matter physics.[1,2] In recent years and in the context of diluted magnetic semiconductors it even became a driving mechanism for electronic applications (spintronics).[3,4] For a theoretical description the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{sf} = \sum_{i,j} \sum_{\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} - J \sum_i \boldsymbol{\sigma}_i \cdot \mathbf{S}_i \qquad (1)$$

is probably the simplest choice possible. The localized magnetic moments are represented by quantum-mechanical spin operators $\mathbf{S}_i$ and interact with the spin of the conduction electrons $\boldsymbol{\sigma}_i$ via an exchange interaction J. The dispersion $\varepsilon_\mathbf{k}$ of the latter is determined by the hopping integrals T_{ij}. In recent years one has referred to the Hamiltonian (1) as the Kondo-lattice model, nevertheless sf, sd, or (for very large J) double-exchange model are probably more suitable descriptions.

Despite the large variety of systems to which the s-f model can be applied,[5] a convincing approximation scheme is still missing. Previous attempts developed along two principal directions. On the one hand the Green's function hierarchy of equations of motions has been restricted by some decoupling schemes.[6] Even though these efforts allowed a fair description of magnetic semiconductors such as europium chalcogenides,[7] this kind of approximation always suffers from a lack of controllability. On the other hand, a classical treatment of the localized spins lead to some substantial results obtained using dynamical mean-field theory[8] or Monte Carlo techniques.[9] However, it has been shown that the quantum-mechanical character of the spins has indeed a substantial impact on the electronic properties of the concerned materials.[10,11]

Therefore, an analytical and numerical treatment of the s-f model should be aspired to, which retains the quantum nature of the spins and ensures the controllability. A perturbational approach would be a good candidate for the latter. However, the incorporation of quantum-spin operators causes difficulties since Wick's theorem, which is generally used to evaluate Feynman diagrams, is not applicable to this class of operators. This is probably the reason why up to now only few attempts exist in this direction. These are mostly limited to special situations such as one-dimensional systems or half-filling.[12,13]

We suggest to circumvent these difficulties by using the projection-operator method (POM) as introduced by Mori.[14,15] Its goal is the expansion of resolvents such as the one-particle Green's functions in a continued fraction. The further one goes in the expansion of the continued fraction, the higher is the accuracy of the results obtained. It has already been applied successfully for a weak-coupling approach to the Hubbard model where it leads to convincing results.[16,17] Its application to the s-f model would be an obvious development, even though straightforward test calculations were not very successful.[11]

A weak-coupling approach to the s-f model is undoubtedly very interesting, both from an experimental and a theoretical point of view. First of all, the parameter regime is probably important for diluted magnetic semiconductors. Second, the well-known Rudderman-Kittel-Kasuya-Yosida exchange mechanism,[18–20] usually used for a qualitative description of magnetism in these materials, is also nothing else but the application of second-order perturbation theory to Hamiltonian (1). However, the goal of this approach is the determination of the ground-state energy, leading to an effective Heisenberg interaction. In contrast to that, here we will show that we are able to analyze the much richer spectrum of dynamical properties of the s-f model to the same order of the coupling constant and beyond it.

Whenever a second-order perturbation theory (SOPT) description is performed in many-body theory there are principally three different ways of treating emerging propagators: a *conventional* SOPT uses only free propagators, a SOPT *relative to Hartree-Fock* (HF) replaces these propagators by the corresponding mean-field expressions, and a *self-consistent treatment* of the SOPT replaces all propagators by (functionals of) the full propagators as obtained in the previous step of iteration. *A priori* it is usually not known which version yields the most reliable results. Of course, the *self-consistent* version includes a summation of more diagrams than the other methods. However, since only a partial class of diagrams is summed, it is unclear which important diagrams are

being missed out or canceled, double counted, or even taken wrongly. There are more profound considerations as put forward by Baym and Kadanoff[21] arguing that the self-consistent approach is a conserving approximation which automatically satisfies the Luttinger theorem[22] and Fermi-liquid properties. However, it is uncertain to which degree this applies to a model which is not exclusively composed of fermions.

Even for more established models such as the periodic Anderson model (PAM), the Falicov-Kimball model (FKM), or the Hubbard model (HM) the question of the most appropriate version has been discussed intensively. For the PAM Yamada and Yosida[23–25] started the perturbational investigations directly by considering deviations from the nonmagnetic HF solution. Later Schweitzer and Czycholl[26] were able to numerically compare this approach with a self-consistent SOPT. Even though this version obeys more of the Luttinger sum rules,[22] the self-consistent version (in contrast to the version relative to HF) failed to show the one-particle peaks near E_f and $E_f + U$ in the f-electron spectral function. The FKM is another example of a model where a not fully self-consistent SOPT treatment qualitatively reproduces exact results, whereas the self-consistent SOPT does not.[26] For the HM the situation is slightly more complicated. One can show that SOPT relative to HF does not yield a metal-insulator transition and does not show a breakdown of the Fermi-liquid behavior.[27] On the other hand, a straightforward application of a self-consistent SOPT does not reproduce the Hubbard bands in the atomic limit.[28] More sophisticated methods such as the interpolation scheme of Edwards and Hertz[29,27] (a version relative to HF) or the iterative perturbation theory of Georges and Kotliar[30] (a self-consistent version) are required. For the latter approach the restriction to half filling has been removed by the modified perturbation theory (MPT) of Kajueter and Kotliar,[31] and Potthoff, Wegner, and Nolting.[32] The MPT is probably the most convincing analytical approach to the HM.[33]

With the present paper we extend this kind of discussion to the electronic part of the periodic s-$d(f)$ exchange model. We will argue that it is indeed a self-consistent ansatz for the electronic self-energy which is the most promising for this model. Other possible weak-coupling approaches are ruled out after a direct comparison with the results of our method of choice. It can be shown that minor changes in the analytical method have drastic effects on one-particle properties, such as the density of states. We believe that a more profound analysis of the s-f model (e.g., by a combination with band-structure calculations) can be based on these considerations.

The paper is organized as follows: As a starting point we derive in Sec. II a SOPT for the s-f model which makes use of the POM. In Sec. III we will study in some detail the exactly soluble limit of a single conduction electron in a ferromagnetically saturated semiconductor. This limit is an excellent testing ground for the implementation of the POM. Even more important, the experience with other models shows that it is indispensable to have nonperturbative, exact statements which can be used to judge the quality of the results obtained. In the next step (Sec. IV) the experiences

for an improvement of this limit are generalized to arbitrary parameter configurations. With all these preparations we are able to present the results of the self-consistent calculation and a comparison with other methods in Secs. V and VI. The findings are summarized in Sec. VII.

It is worth mentioning that our approach seems to be related to a moment-conserving interpolation scheme of the self-energy as published by Nolting et al.[5,34] There, a general structure of the electronic self-energy, which looks similar to the one presented here, has been found by systematically studying all known exact statements on the s-f model. However, their analysis is focused on the low-density limit and ensures the correctness of these statements for $n \rightarrow 0$ (or $n \rightarrow 2$) only. In contrast to that the approach given in this paper concentrates on the weak-coupling behavior. Indeed, independent of the occupation number the correctness of the self-energy up to order $\tilde{J}^2$ in the coupling parameter and up to order E^{-2} in the high-energy expansion is guaranteed. Additionally, we can fulfill the same criteria for $n \rightarrow 0$ as given in the above-mentioned publication. Nevertheless, the two approaches are not identical even for $n = 0$, but otherwise arbitrary parameters.

II. SECOND-ORDER PERTURBATION THEORY

As mentioned above, we use the POM (Refs. 14 and 15) since it allows an expansion of resolvents without the use of Wick's theorem. The approximation consists in considering only a physically relevant subspace of the Liouville space. With the simplest choice the Liouville space is spanned by single-particle states $|c_{\mathbf{k}\sigma}^\dagger)$. Accordingly the projection operator and its orthogonal complement are defined as

$$P = |c_{\mathbf{k}\sigma}^\dagger)(c_{\mathbf{k}\sigma}^\dagger| \quad \text{and} \quad Q = 1 - |c_{\mathbf{k}\sigma}^\dagger)(c_{\mathbf{k}\sigma}^\dagger|. \tag{2}$$

These definitions require the existence of a scalar product, which in our calculations is conveniently chosen to be the thermodynamic average

$$(A|B) \equiv \langle [A^+; B]_+ \rangle. \tag{3}$$

Within the POM the one-particle Green's function is given by the following dynamical equation:

$$G_{\mathbf{k}\sigma} = \left(c_{\mathbf{k}\sigma}^\dagger \left| \frac{1}{\omega - \mathcal{L}} \right| c_{\mathbf{k}\sigma}^\dagger \right) = \frac{\chi_{\mathbf{k}\sigma}}{\omega - [\Omega_{\mathbf{k}\sigma} + M_{\mathbf{k}\sigma}(\omega)]\chi_{\mathbf{k}\sigma}^{-1}}, \tag{4}$$

where $\omega = E + i0^+$ and the Liouville operator $\mathcal{L}$ with its property $\mathcal{L}|A) \equiv |[\mathcal{H}, A]_-)$ has been incorporated. For the choice (2) the susceptibility matrix $\chi_{\mathbf{k}\sigma} = (c_{\mathbf{k}\sigma}^\dagger | c_{\mathbf{k}\sigma}^\dagger)$ is particularly simple: $\chi_{\mathbf{k}\sigma} \equiv 1$. The frequency matrix

$$\Omega_{\mathbf{k}\sigma} = (c_{\mathbf{k}\sigma}^\dagger | \mathcal{L} | c_{\mathbf{k}\sigma}^\dagger) = \varepsilon_{\mathbf{k}} - \tilde{J} z_\sigma \langle S^z \rangle, \tag{5}$$

on the other hand, corresponds to the mean-field result

$$G_{\mathbf{k}\sigma}^{(\mathrm{MF})}(\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + \tilde{J} z_\sigma \langle S^z \rangle} \tag{6}$$

for the Green's function. Here, we have used the abbreviations $\tilde{J} = \frac{1}{2}J$ and $z_{\uparrow,\downarrow} = \pm 1$. All the interesting physics is included in the memory matrix

$$M_{\mathbf{k}\sigma}(\omega) = \left(Q \mathcal{L} c_{\mathbf{k}\sigma}^\dagger \left| \frac{1}{\omega - Q\mathcal{L}Q} \right| Q \mathcal{L} c_{\mathbf{k}\sigma}^\dagger \right), \quad (7)$$

which again has the structure of a resolvent, resulting in a form of $G_{\mathbf{k}\sigma}$ in Eq. (4) involving continued fractions.

The expression for the memory matrix cannot be treated exactly. However, at this stage we are only aiming at a perturbational expansion of the self-energy $\Sigma_{\mathbf{k}\sigma}$ in the form

$$\Sigma_{\mathbf{k}\sigma} = -\tilde{J} z_\sigma \langle S^z \rangle + \tilde{J}^2 \gamma_{\mathbf{k}\sigma} + \cdots. \quad (8)$$

This allows some simplifications. In Eq. (7) already the $\mathcal{H}_{sf}$ contribution in $|Q\mathcal{L} c_{\mathbf{k}\sigma}^\dagger)$ gives rise to a factor $\tilde{J}^2$. Hence, any approximation of the Liouville operator in the denominator is still correct in this order and is thus consistent with Eq. (8). A conventional SOPT implies a replacement of $\mathcal{L}$ by its free part $\mathcal{L}_0$. A SOPT relative to HF is given by a Liouville operator that corresponds to the Hamiltonian

$$\mathcal{H}_0^{(MF)} = \mathcal{H}_0 - \sum_{\mathbf{k},\sigma} \tilde{J} z_\sigma \langle S^z \rangle \hat{n}_{\mathbf{k}\sigma}. \quad (9)$$

In both cases we obtain a similar result

$$\gamma_{\mathbf{k}\sigma} = -\langle S^z \rangle^2 G_{\mathbf{k}\sigma}^{(0/MF)} + \frac{1}{N^2} \sum_{\mathbf{q}} \langle S_{-\mathbf{q}}^z S_{\mathbf{q}}^z \rangle G_{\mathbf{k}+\mathbf{q},\sigma}^{(0/MF)}$$

$$+ \frac{1}{N^2} \sum_{\mathbf{q}} \{ \langle S_{-\mathbf{q}}^{-\sigma} S_{\mathbf{q}}^\sigma \rangle + 2 z_\sigma \langle S_0^z \hat{n}_{\mathbf{q}+\mathbf{k},-\sigma} \rangle \} G_{\mathbf{k}+\mathbf{q},-\sigma}^{(0/MF)}, \quad (10)$$

where $S_{\mathbf{q}}^\sigma = S_{\mathbf{q}}^x + i z_\sigma S_{\mathbf{q}}^y$. For the expectation values contained in Eq. (10) we make use of the fact that we aim for a result correct to second order in $\tilde{J}$ and evaluate them using the eigenstates of the free/mean-field system.

A self-consistent SOPT on the other hand can be obtained in the same manner as suggested by Bulk and Jelitto[17] for the Hubbard model. Within this procedure the unperturbed part is altered in each iteration cycle by the memory matrix of the previous cycle:

$$\mathcal{H}_0^{(N+1)} = \mathcal{H}_0^{(N)} + \sum_{\mathbf{k}\sigma} M_\sigma^{(N)} \hat{n}_{\mathbf{k}\sigma}. \quad (11)$$

It turns out that this procedure is equivalent to a replacement of the Green's functions at the right-hand side of Eq. (10) by the full propagators as obtained in the previous iteration cycle. In Eq. (11) we use the additional approximation that the memory matrix is summed over $\mathbf{k}$ and hence only a local self-energy is considered.

III. AN EXACT SOLUTION

The model can be restricted to the limit of a ferromagnetically saturated semiconductor. This limit is characterized by

two mathematical consequences: First, a semiconductor is defined by an empty conduction band at zero temperature, hence $\langle \cdots c_{\mathbf{k}\sigma} \rangle = 0$. Second, ferromagnetic saturation leads to trivial spin expectation values: $\langle \cdots S_{\mathbf{q}}^z \rangle = NS \langle \cdots \rangle$, $\langle \cdots S_{\mathbf{p}}^+ \rangle = 0$. An application of these simplifications to the result (10) yields the self-energy

$$\Sigma_{\mathbf{k}\sigma} = \Sigma_\sigma = -\tilde{J} z_\sigma S + \tilde{J}^2 2S \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}-\sigma}^{(0/MF)} \delta_{\sigma\downarrow}. \quad (12)$$

One can see directly that in this limit a *self-consistency* iteration does not yield any further results. This is because the $\sigma = \downarrow$ Green's function is uniquely determined by $\sigma = \uparrow$ propagators, which have the iteration-independent self-energy $\Sigma_\uparrow \equiv -\tilde{J}S$.

Due to the restrictions of this limit the memory matrix can in fact be treated more accurately. Following the intention of continued-fraction expansion the memory matrix (7) can itself be considered as a resolvent, to which the concept of the POM is applied:

$$M(\omega) = \frac{1}{\omega - [\hat{\Omega} + \hat{M}(\omega)]\hat{\chi}^{-1}} \hat{\chi}. \quad (13)$$

The higher-order memory matrix $\hat{M}$ will have a form similar to that given in Eq. (7). Again the Liouville operator $\mathcal{L}$ in the denominator should be approximated to allow for an analytical solution of the associated geometric series. According to conventional perturbation theory it is replaced by $\mathcal{L}_0$, the action of a free, undisturbed system of electrons. After sophisticated calculations, which will be published elsewhere, the self-energy is obtained as

$$\Sigma_\sigma = -\tilde{J} z_\sigma S + \delta_{\sigma\downarrow} \tilde{J}^2 \frac{2S \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}}^{(0)}(\omega)}{1 - \tilde{J}(1-S) \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}}^{(0)}(\omega)}. \quad (14)$$

This is certainly an improvement of Eq. (12) and contains the previous result if expanded up to order $\tilde{J}^2$.

Even though we called it perturbation theory, it is however not correct for the next order in $\tilde{J}$. The exact $\tilde{J}^3$ contribution to the self-energy can actually be shown to be

$$\Sigma_\downarrow^{(3)} = \tilde{J}^3 2S \left\{ \left[\frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}}^{(0)}(\omega) \right]^2 - \frac{S}{N} \sum_{\mathbf{q}} [G_{\mathbf{q}}^{(0)}(\omega)]^2 \right\}. \quad (15)$$

As a matter of fact, the second sum in Eq. (15) is a diverging contribution. This already becomes apparent if one looks at its imaginary part, rewrites the $\mathbf{k}$ sum as an integral over the free DOS, separates a Lorentzian, and considers the fact that 0^+ is infinitesimally small. We were able to show that after a summation over all orders in J the diverging terms cancel. Nevertheless, Eq. (15) demonstrates that for the s-f model a strict perturbation theory is only possible up to second order

in J. The different orders of an expansion of the continued fraction within the POM apparently do not have this limitation.

The result (14) can be further improved, if a perturbation theory relative to HF is chosen. Without going into the details we just provide the result as

$$\Sigma_\sigma = -\tilde{J} z_\sigma S + \delta_{\sigma\downarrow} \tilde{J}^2 \frac{2S \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}-\sigma}^{(\mathrm{MF})}(\omega)}{1 - \tilde{J} \frac{1}{N} \sum_{\mathbf{q}} G_{\mathbf{q}-\sigma}^{(\mathrm{MF})}(\omega)}. \quad (16)$$

This expression is actually identical to the result of an exact calculation, where the Liouville operator has not been reduced or altered. Within the POM we were able to perform the derivation of the memory matrix (7) using the complete operator $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\mathrm{sf}}$. However, it is not necessary to give the lengthy calculations here since its result (16) has already been verified by other methods.[35–39]

The self-energy (16) corresponds to an exact eigenstate of the Hamiltonian (1). For the spin-down electrons this eigenstate, which is the ground state[36] for antiferromagnetic coupling ($J<0$), is called magnetic polaron.[37] Its interesting and nontrivial dynamical features, which give rise to a scattering part and a quasiparticle peak in the density of states have been discussed in detail by Nolting *et al.*[39] Apparently, it is possible to retrieve these features within the projection-operator formalism. The reason why already an approximation yields the correct result is the fact that the resulting two-dimensional Liouville subspace is sufficient to completely describe the physics of a ferromagnetically saturated semiconductor.

Now we have obtained several approximate forms of the electronic self-energy. Formula (12) provides an expression for the first and second order in the coupling constant $\tilde{J}$. The (diverging) third order is given in Eq. (15). An improvement of the SOPT is given in Eq. (14) in a conventional way and in Eq. (16) relative to HF. One can compare these self-energies by looking at their quasiparticle densities of states (QDOSs). Obviously, the spin-↑ spectrum is always a mean-field-shifted free DOS. Hence, we can limit ourselves to the spin-↓ spectrum, which is shown in Fig. 1.

In this figure a relatively large $J = 2\tilde{J}$ has been chosen to reveal the differences more clearly. If one compares the DOS of the conventional SOPT and the SOPT relative to HF with that of the exact solution, one gets the impression that the first one is the better approximation. However, if one compares these two approaches for the second step of the POM (equivalent to a larger relevant Liouville subspace) it is clear that the version relative to HF has to be preferred, since only this one gives the exact result. Nevertheless, result (14) is already a satisfactory approximation. As mentioned above a self-consistent calculation is redundant for the discussed limit.
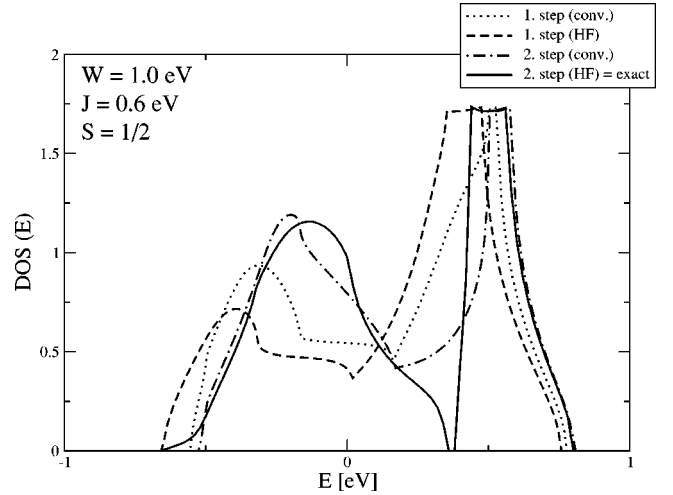

FIG. 1. Comparison of the ↓-QDOS for different self-energies in the limit $n=0$ and $\langle S^z \rangle = S$. The dotted and dashed lines are the results of SOPT (12), conventional and relative to HF, respectively. The dashed-dotted and the solid lines give the corresponding results (14) and (16) for the next step of the POM.

IV. GENERALIZATION TO ARBITRARY CONFIGURATIONS

After these considerations on the magnetic polaron we return to the discussion of the SOPT given in formula (10). As argued before, the limit of a ferromagnetically saturated semiconductor can be used to check the quality of this result. In this limit the SOPT result (12) turns out to be only a poor approximation of the exact solution as demonstrated in Fig. 1. Since the magnetic polaron is indeed an important feature of the s-f model, ways of improving Eqs. (8) and (10) should be considered.

In the preceding section we explained how an improvement can be achieved within this particular limit. A proper application of an additional step within the projection operator method finally leads to the expressions (14) and (16). We generalize the analytical structure of these results to the following *ansatz* for arbitrary band occupations:

$$\Sigma_{\mathbf{k}\sigma}(E) = -\tilde{J} z_\sigma \langle S^z \rangle + \tilde{J}^2 \frac{a_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}(E)}{1 - b_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}(E)}. \quad (17)$$

Although obtained in a completely different manner, this is exactly the kind of a MPT (Ref. 31) which has turned out to be the most promising analytical approach to the Hubbard model.[33]

For the s-f model it has two advantages: First, it does not destroy the correctness of the second-order term proportional to $\tilde{J}^2$, but gives the freedom to fit the parameters $a_{\mathbf{k}\sigma}$ and $b_{\mathbf{k}\sigma}$ such that further criteria are fulfilled. Second, since the SOPT result for the self-energy (8) automatically reproduces the first three moments of the corresponding Green's function correctly, the choice $a_{\mathbf{k}\sigma} = 1$ will ensure the same for the ansatz (17).

It remains to determine the parameter $b_{\mathbf{k}\sigma}$. The most straightforward choice merely ensures the correctness of the ferromagnetically saturated semiconductor ($b_{\mathbf{k}\sigma} = \tilde{J}/2S$).

However, the resulting densities of states have unphysical features. Furthermore, we have learned from the Hubbard model[33] that a fit to the spectral moments of the Green's function yields more promising results. $b_{\mathbf{k}\sigma}$ which is determined by

$$b_{\mathbf{k}\sigma} = \tilde{J}^2 \frac{(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger | \mathcal{L} | Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger) - (Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger | \mathcal{L}_0 | Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)}{(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger | Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)^2}$$

(18)

ensures that the third coefficient of the high-energy expansion of Eq. (18) is identical to the one of the exact self-energy. As explained in more detail in Appendix A this fit is correct for the first four moments of the Green's function.

In a MPT which is based on a conventional SOPT the Liouville operator $\mathcal{L}_0$ in Eq. (18) is understood to correspond to the free part of the Hamiltonian $\mathcal{H}_0$. Then only the $\tilde{J}^3$ contribution in the numerator of $b_{\mathbf{k}\sigma}$ remains to be evaluated and one obtains

$$b_\sigma = \tilde{J} \frac{[S(S+1) - z_\sigma\langle S^z\rangle - \langle S^z\rangle^2](z_\sigma\langle S^z\rangle + 1) + q_\sigma}{[S(S+1) - z_\sigma\langle S^z\rangle - \langle S^z\rangle^2 + 2p_\sigma]^2},$$

(19)

where p_σ and q_σ are sets of further correlation functions, which are given in Appendix B, but have the property to vanish in the limit $n \to 0$. It is instructive to study this limit in more detail. On the one hand it can be combined with the additional constraint of ferromagnetic saturation $\langle S^z\rangle = S$. If the obtained $b_\downarrow$ is placed into the MPT ansatz (17), then the self-energy becomes identical to the one given in Eq. (14). On the other hand, one can consider the zero-bandwidth situation $\varepsilon_{\mathbf{k}} \equiv T_0$ within the limit $n \to 0$. For a dispersionless Green's function all summations in expression (10) for $\gamma_{\mathbf{k}\sigma}$ can readily be performed, and in this limit the self-energy becomes

$$\Sigma_\sigma = -\tilde{J}z_\sigma\langle S^z\rangle + \tilde{J}^2 \frac{[S(S+1) - z_\sigma\langle S^z\rangle - \langle S^z\rangle^2]\dfrac{1}{E - T_0}}{1 - \tilde{J}(z_\sigma\langle S^z\rangle + 1)\dfrac{1}{E - T_0}}.$$

(20)

Comparing this form of Σ_σ to the result of an exact calculation available for the zero-bandwidth limit[5,40] reveals that the expression is correct.

For a SOPT relative to HF the expression for $\mathcal{L}_0$ in Eq. (18) contains an additional term according to the mean-field contribution $\Sigma_\sigma = -\tilde{J}z_\sigma\langle S^z\rangle$ in Eq. (9). This yields a correction

$$\delta b_\sigma = \frac{\Sigma_\sigma[\langle(S^z)^2\rangle - \langle S^z\rangle^2] + \Sigma_{-\sigma}[\langle S^{-\sigma}S^\sigma\rangle + 2z_\sigma\langle S^z\rangle n_{-\sigma}]}{[S(S+1) - z_\sigma\langle S^z\rangle - \langle S^z\rangle^2 + 2p_\sigma]^2}$$

(21)

to the former result (19). We will focus again on the limit $n \to 0$. If combined with the additional constraint of ferromagnetic saturation, the exact result (16) is obtained. A con-

sideration of the zero-bandwidth limit yields the following expression for the self-energy:

$$\Sigma_\sigma = -\tilde{J}z_\sigma\langle S^z\rangle + \tilde{J}^2 Y$$

$$+ \tilde{J}^2 \frac{[S(S+1) - z_\sigma\langle S^z\rangle - \langle S^z\rangle^2]\dfrac{1}{E - T_0 + \tilde{J}z_{-\sigma}\langle S^z\rangle}}{1 - \tilde{J}\left(\dfrac{1}{E - T_0 + \tilde{J}z_{-\sigma}\langle S^z\rangle} + X\right)}.$$

(22)

Apart from the correction terms X and Y this is again the exact result (20). However, both terms are proportional to expressions, which vanish in the paramagnetic regime. Therefore, they also vanish for the zero-bandwidth limit for which the assumption of any finite magnetization does not lead to consistent results.[41]

In the discussion so far we have tested our MPT ansatz (17) in the limit $n \to 0$. One can repeat the same transformations for the opposite case $n \to 2$. By doing this one will notice that the same formulas are obtained. The only difference is the change of the sign of σ and of $b_{\mathbf{k}\sigma}$. This is due to particle-hole symmetry in the system. Therefore, in the same sense as for $n = 0$, our MPT ansatz (17) fulfills the limit of the magnetic polaron and the zero-bandwidth limit for $n = 2$.

V. SELF-CONSISTENT RESULTS

Using the MPT approach of the preceding section we have the possibility to generalize the improvement to the POM for the limit of a ferromagnetically saturated semiconductor to arbitrary parameter regimes. In Sec. III we argued that a self-consistent calculation is redundant in this limit. This does not hold for the generalized version. Here $\gamma_{\mathbf{k}\sigma}$, as given in Eq. (10), does not vanish for spin-$\uparrow$ electrons and consists of propagators for both kinds of spin directions. Consequently, we have performed a self-consistent numerical iteration of the self-energy. This was carried out along the lines sketched at the end of Sec. II. Additionally, the MPT parameter b_σ has to be adjusted such that Σ_σ in Eq. (21) describes the full self-energy and not only its mean-field part.

The details of this procedure are discussed in Sec. VI. If properly performed it is an "upgrading" of the perturbation theory relative to HF in the sense that its properties are maintained. In particular, the evaluation for the ferromagnetically saturated semiconductor yields the previous and exact results of the magnetic polaron. Additionally, the atomic limit is fulfilled for the empty and completely filled conduction band, and the particle-hole symmetry of the system is conserved by the ansatz. In other regimes it is ensured that all results are correct at least to order $\tilde{J}^2$. However, because of the self-consistency the method incorporates more correlations and scattering effects than a straightforward second-order perturbation theory description does. For all these reasons we believe that the self-consistent MPT is not only
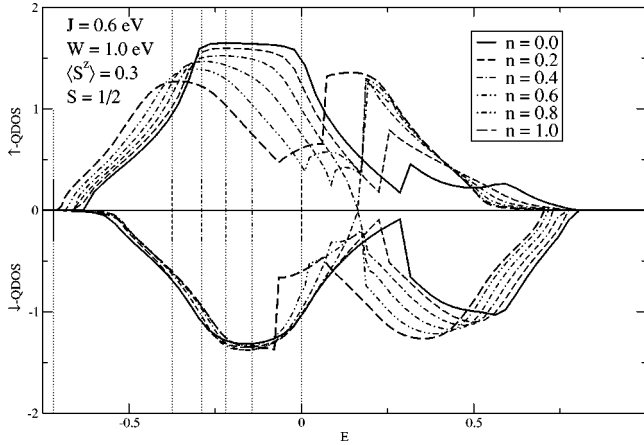
FIG. 2. Dependence on band occupation n for a self-consistent MPT. For free electrons a simple-cubic DOS with bandwidth W is chosen. The parameters are as given. The vertical lines indicate the positions of the Fermi energy to allow for the different values of the band occupation.

correct in the weak-coupling regime, but also for moderate values of $\tilde{J}$.

We discuss the results in terms of the QDOSs. According to our ansatz the QDOS is correct for $n=0, \langle S^z \rangle = S$, however its variation with a change of these parameters is of particular interest. Figure 2 shows the dependence on the first parameter. The dependence on the magnetization (connected to temperature via a Brillouin function) is given in Fig. 3. In both cases a medium value has been chosen for the fixed parameter. It goes without saying that our calculations are also thermodynamically self-consistent. The iteration ensures that the values of the correlation functions are consistent with the obtained one-particle Green's function. Additionally, the chemical potential is adjusted to the desired particle number. Its position is indicated by vertical lines in the figures.

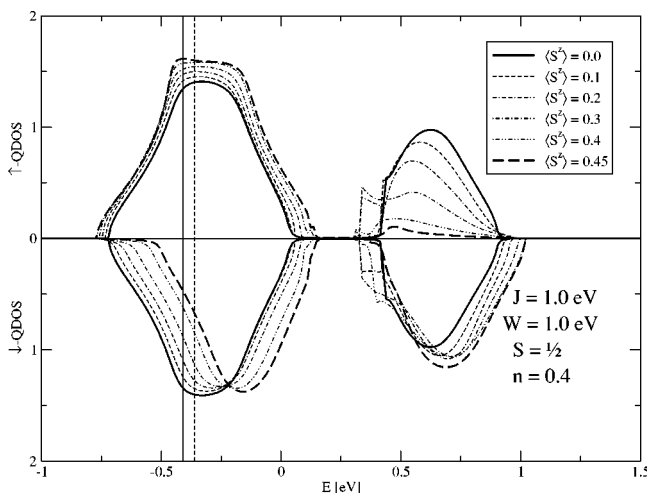In particular, the change of n in Fig. 2 has remarkable

FIG. 3. Change of the QDOS with the magnetization $\langle S^z \rangle$ for a self-consistent MPT. The position of the Fermi energy for the highest and lowest $\langle S^z \rangle$ is marked by vertical lines.

consequences for the QDOS. The clear dependence on the filling of the conduction band points out strong correlation effects, induced by the coupling $\tilde{J}$. For $n=0$ the structure of the QDOS is closely related to the ferromagnetically saturated semiconductor. In particular, the spin-↑ spectrum has the shape of the free (simple cubic) DOS and the scattering part of the spin-↓ spectrum can clearly be seen. Only the polaron subband shows a deformation, due to finite-lifetime effects. Excited spin-↑ electrons can enter the energy region of the polaron, flip their spin, and absorb a magnon since we are not close to saturation.

If the chemical potential (and accordingly the band occupation) is increased, the spectral weight is redistributed between both subbands. For the chosen set of parameters the changes with n are most noticeable in the spin-↑ QDOS, where the upper subband steadily increases in importance at the expense of the lower subband. A sharp jump in the QDOS close to the pseudogap remains a striking feature for all values of n. It is also interesting to note that the lower band edge is shifted by some 0.1 eV in the spin-↑ QDOS, whereas it remains at almost the same position for the spin-↓ QDOS. This behavior is very much different in a MPT relative to HF (Ref. 42), and is a hint that in the self-consistent MPT mainly the majority-spin electrons experience strong correlations.

As the band occupation approaches half filling ($n=1$), the point-symmetric form of the QDOS nicely represents the particle-hole symmetry of the system. The character of the upper spin-↓ subband becomes identical to the lower spin-↑ subband, since the latter is the polaron band for $n=2$. For the same reason we skip the plots for $n>1$, they can be obtained from the band occupations $2-n$.

A higher value for the coupling strength $\tilde{J}$ is chosen in Fig. 3. Therefore, the scattering and the polaron subband are well separated already for a nearly saturated system. The gap remains present for all temperature employed in the calculations. There are only small changes of the position of the bands as a function of the magnetization. Nevertheless, the edge of the lower spin-↑ subband shifts to lower energies if the temperature is lowered from $T=T_C$ ($\langle S^z \rangle = 0$) to smaller values $T \to 0$ (maximum $\langle S^z \rangle$). For semiconductors such an effect is known as the redshift of the optical absorption edge. In metals, since the lower spin-↓ subband is shifted in the opposite direction, it leads to a polarization of the conduction electrons of over 60%. The existence of energy regions well below the Fermi edge occupied entirely by majority-spin electrons is a remarkable result. Similar effects have also been reported in other approximations[43] when studying half-metallic ferromagnets. However, the continuous shift of the chemical potential with magnetization prevents 100% polarization of the conduction electrons in our calculations. The dependence on the chemical potential is such that the effect disappears completely for smaller values ($n \to 0$), where the ↑-QDOS and the ↓-QDOS occupy the same energy region (see Fig. 2).

The situation at the lower edge of the upper subband in Fig. 3 is less systematic. An extra peak in the spin-↑ QDOS obtains its maximum for $\langle S^z \rangle \approx 0.3$ and then vanishes again.

The physical interpretation of this feature is not yet clear. In this context we also have to mention that the choice of the parameter b_σ with its explicit dependence on the self-energy in Eq. (21) substantially increases the numerical effort. In the energy region just mentioned it is particularly difficult to obtain convergence.

The distribution of the spectral weight, on the other hand, is indisputable. It shows the transition from the ferromagnetically saturated configuration (dashed lines), which even for $n = 0.4$ clearly displays the features of the exact solution in Sect. III, to the paramagnetic regime (solid lines), which has to be symmetric with respect to the x axis. Again the more profound changes are observed for the majority-spin electrons. The increasing spectral weight of the upper spin-↑ subband can be explained with higher magnon numbers in this regime.

An artifact of our method is the fact that for both spin directions two subbands are always obtained. With other approaches,[34] one sometimes observes a third band. This is explained by atomic-limit calculations, where for finite band occupations always three out of four subbands have nonvanishing spectral weight. It needs further modifications of our method to retain these features. At the present stage the atomic limit is only correct for $n = 0$ and $n = 2$.

VI. THE PROPER METHOD

The last point brings us to an assessment of our self-consistent approach. Apart from the above-mentioned catalog of analytical properties, a comparison with other conceivable weak-coupling approaches is desirable.

A comparison with a MPT which uses $\gamma_{\mathbf{k}\sigma}$ obtained by conventional SOPT is straightforward. From the analytical considerations in Sec. IV we can conclude that even a MPT based on a SOPT relative to HF should be preferred as compared to one based on a conventional SOPT. This is because the former correctly incorporates the important limiting case of the ferromagnetically saturated semiconductor, whereas the latter does only reproduce, in this limit, the less accurate expression (14). The discussion of the atomic limit does not provide an argument in favor of one of the approaches, since at the end both yield physical expressions of the same quality. In these limits our self-consistent approach has the same properties as the MPT relative to HF.

Our comparison with a MPT relative to HF is based on numerical results with this method. For the same parameters as in Fig. 3 we obtain the set of QDOS given in Fig. 4. Even though its main features look sound again, there are a set of minor aspects which make this approach questionable. The most obvious drawback is prominent and unexplainable peaks close to the Fermi energy. The functional dependence is not smooth and dominated by the free DOS. Also for magnetizations below saturation a gap in the spin-down QDOS is expected from other theories,[5,11] but this does not exist in this approach. Additionally it is noteworthy that the onset of the spin-up QDOS starts for smaller energies as compared to that for the spin-down QDOS.

In the self-consistent MPT of the preceding section most of these peculiarities are not present. A comparison with Fig.
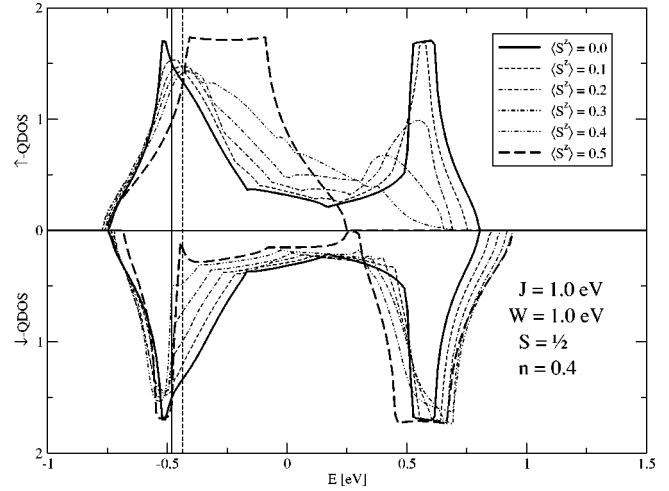

FIG. 4. Change of the QDOS with the magnetization $\langle S^z \rangle$. The MPT calculations are based on a SOPT relative to HF. The parameters are chosen as in Fig. 3.

3 permits the conclusion that the iteration of the self-energy yields shapes of the QDOS which are broader and smoother. This can be understood analytically and is closely related to the fact that the self-energy becomes complex by iteration. These findings make the self-consistent version more reliable.

However, there are several possibilities to incorporate self-consistency into the MPT. An ambiguous point is the order of the applied steps. In contrast to the calculations of the preceding section one could start with the expression of the MPT as obtained in an approach relative to HF and continue by dressing all included propagators as full Green's functions. Hence, the parameters $b_{\mathbf{k}\sigma}$ are fixed, which is still correct for a fit to the high-energy expansion up to order E^{-2}. The consequences for the densities of states are shown in Fig. 5. They look reasonable for values of $\langle S^z \rangle$ close to saturation. However, the single, broad, elliptic band which emerges close the paramagnetic regime is a surprising feature. Not only is this result inconsistent with other approxi-
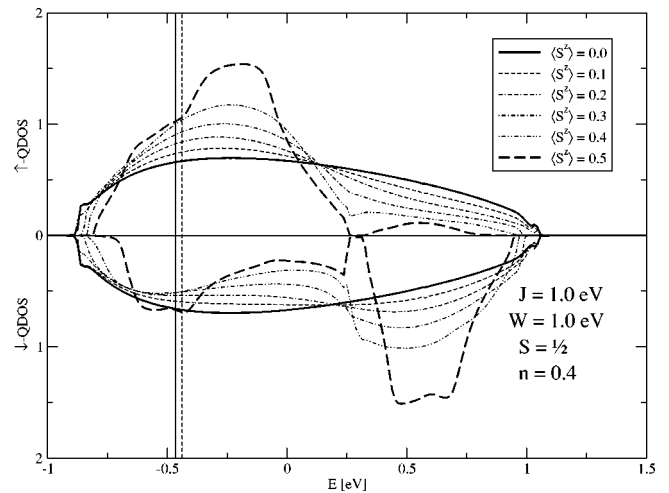

FIG. 5. Dependence on magnetization $\langle S^z \rangle$ for a MPT based on a *self-consistent* SOPT. The parameters are as in Fig. 3.

mations of the s-f model,[5,6,8,34] moreover it is incorrect in the zero-bandwidth limit. This is because the same structure remains in the limit $W \to 0/n \to 0$, where two narrow bands around $-\tilde{J}S$ and $\tilde{J}(S+1)$ are expected as indicated by exact calculations.[40] The shortcoming can already be seen analytically when looking at Eqs. (20) or (22). If the propagators are dressed without a change of b_σ, then an equality is not possible with the exact solution:

$$\tilde{J}^2 \frac{S(S+1)\dfrac{1}{E-T_0-\Sigma}}{1-\tilde{J}\dfrac{1}{E-T_0-\Sigma}} \neq \tilde{J}^2 \frac{S(S+1)\dfrac{1}{E-T_0}}{1-\tilde{J}\dfrac{1}{E-T_0}} = \Sigma. \quad (23)$$

This conflict can be resolved if the order of arguments is changed. Now the starting point is a self-consistent SOPT and only afterwards the result is fitted to the high-energy expansion. The consequence is not a higher accuracy in powers of E^{-1} but an additionally dressed fitting parameter b_σ. According to the correction given in Eq. (21) it now contains the full self-energy and not only its mean-field contribution. This leads to the correct result for the zero-bandwidth limit at $n=0$:

$$\tilde{J}^2 \frac{S(S+1)\dfrac{1}{E-T_0-\Sigma}}{1-(\tilde{J}-\Sigma)\dfrac{1}{E-T_0-\Sigma}} = \tilde{J}^2 \frac{S(S+1)\dfrac{1}{E-T_0}}{1-\tilde{J}\dfrac{1}{E-T_0}}. \quad (24)$$

Additionally, it has serious consequences for all other parameter regions. We compare numerical results for the three different approaches mentioned above in Fig. 6(a). The set of parameters $W, \tilde{J}, S$ is chosen to be close to the atomic limit. The choice $n=0, \langle S^z \rangle = 0$ ensures exactness in this limit. If the input $\gamma_{\mathbf{k}\sigma}$ to the MPT (17) is the result of the SOPT relative to HF (dashed line), then two nearly free subbands at the correct positions are obtained. There seems to be a third flat band between them. To dress only the propagators and not the fitting parameter b_σ (dotted line) is definitely wrong. However, one can convince oneself that an inclusion of the full self-energy in the calculation of b_σ (solid line) really yields a considerable improvement for $n=0$. Here one again observes the two narrow subbands, the excitation energies for an electron that aligns its spin parallel $(-\tilde{J}S)$ or antiparallel $[\tilde{J}(S+1)]$ to the localized spin.

Nevertheless, there remains an uncertainty in the determination of b_σ as far as the correlation function p_σ in Eqs. (19) and (21) is concerned. Its definition is chosen such that it can be calculated with the help of the one-particle Green's function $G_{\mathbf{k}\sigma}$:

$$p_{-\sigma} = -\frac{1}{\pi \hbar \tilde{J} N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} (E-\varepsilon_{\mathbf{k}}) \cdot \frac{\mathrm{Im}G_{\mathbf{k}\sigma}}{e^{\beta E}+1} dE. \quad (25)$$

This form of the spectral theorem has the handicap to be only applicable for determining a sum of correlation functions (B1). Whenever being confronted with a single correlation
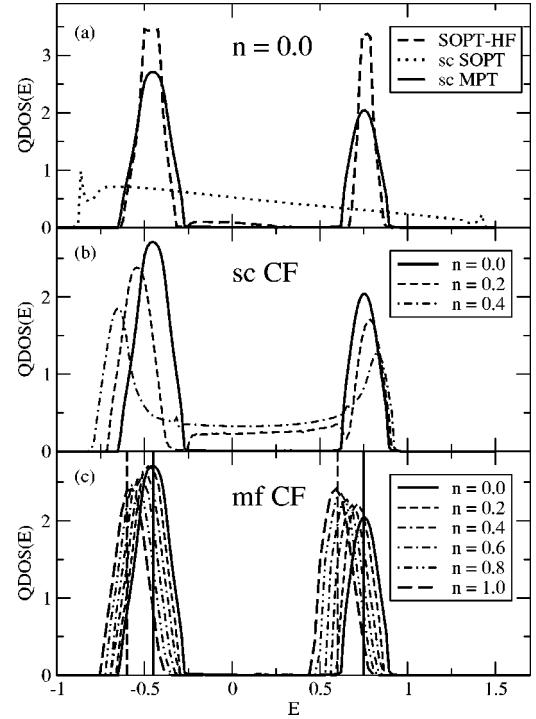

FIG. 6. Comparison of different MPT approaches for parameters close to the atomic limit (bandwidth $W=0.5$ eV, $J=0.6$ eV, $S=3/2$, $\langle S^z \rangle = 0.0$). (a) Dashed line, the MPT is based on a SOPT relative to HF; dotted line, only the SOPT input is treated self-consistently and the parameter b_σ is not altered; and solid line, the self-consistency has also consequences for b_σ. For the latter there are two versions to treat the correlation functions (CF) in b_σ: either self-consistent (b) or mean-field-like (c). The vertical lines indicate the energy positions of the maxima of the subbands.

function contribution to Eq. (25), we are forced to perform a mean-field decoupling: $\langle S^z n_{-\sigma} \rangle = \langle S^z \rangle \langle \hat{n}_{-\sigma} \rangle$. This is still compatible with the expansion in $\tilde{J}$ and E^{-1}. It is therefore straightforward to treat those correlation functions for which relations such as Eq. (25) exist as accurate as possible, and perform approximations for the remaining correlation functions.

The consequences of this methodology for the atomic limit are shown in Fig. 6(b). The QDOS looks sound for $n=0.0$, but shows a broad nonquasiparticle structure between the subbands for $n>0$. Its spectral weight increases with band occupation at the latter's expense. This dependence is qualitatively different compared to that of a third, intermediate band in the QDOS for the SOPT relative to HF, which remains small for all values of n. Here, already for a band occupation of $n=0.4$ the gap is completely filled. It is difficult to find a physical explanation for such a behavior. Small satellite peaks between the subbands were also reported for other approximation methods[5] and were attributed to untrapped electrons which experience the global magnetization $\langle S^z \rangle$ as an effective quantization axis. A shift of the spectral weight within the intermediate structure as a function of the net magnetization has also been observed in our calculations. However, the missing symmetry in the paramagnetic regime and the strong dependence on the band occupation does not

fit into this picture. The accompanying shift of the two sub-bands is also surprising. For these reasons we believe that these features are an artifact of the approximations used as we know that the atomic limit is only correctly included for $n = 0$.

In contrast to the methodology to determine b_σ as accurately as possible, it has apparently a much higher priority to treat all included correlation functions on an equal footing. Figure 6(c) shows results for the QDOS with the same set of parameters as in Fig. 6(b). The only modification in the theory is a mean-field decoupling of all correlation functions in b_σ. The effects on the QDOS is dramatic, as the intermediate structure completely vanishes now. Additionally, the shift of the two subbands happens in a comprehensible way. Due to the particle-hole symmetry we expect for $n = 2$ two subbands at positions $-\tilde{J}(S+1)$ and $+\tilde{J}S$. Since our approach apparently only allows for a single band gap, the change from an $n = 0$ to an $n = 2$ configuration can only be implemented by the system if the two peaks move continuously to their new positions. Accordingly their positions at half filling ($n = 1$) have to be $E_\pm = \pm \tilde{J}(2S+1)/2$, as seen in the figure. Also the redistribution of the spectral weight takes place along these lines.

Based on our experience with the MPT we draw the following conclusion. The most promising weak-coupling approach to the periodic s-$d(f)$ exchange model is the self-consistent MPT. Expression (10) dressed with full propagators $G_{\mathbf{k}\sigma}$ should be used as the input from second-order perturbation theory. Only afterwards the parameters $a_{\mathbf{k}\sigma}$ and $b_{\mathbf{k}\sigma}$ in the MPT ansatz (17) should be determined such that the high-energy expansion is fulfilled to power E^{-2}, which implies that b_σ carries a dependence on the full self-energy. For the correlation functions entering b_σ it is important that they are all treated on the same footing. This is, at this stage, only possible by using a mean-field decoupling.

VII. SUMMARY AND OUTLOOK

Within the presented work we have demonstrated how the projection-operator method can be exploited to find an analytical approach to the periodic s-$d(f)$ exchange model and that it is indeed a valuable tool in this context. Nevertheless, we argued that the second-order perturbation is insufficient and suggested an improvement in the form of a MPT. The principal structure of this ansatz results from a study of the limit of the ferromagnetically saturated semiconductor. We showed that the calculations have to be performed self-consistently. In a further step a clarification of the proper treatment of the fitting parameter b_σ was necessary. At the end we were able to make an informed statement, which of all possible approaches is the most reliable one. On the one hand it is satisfactory that a certain approach was able to produce considerably better results than other attempts. On the other hand, the high sensitivity of the QDOS to the methodology used to treat the correlation functions includes the danger of arbitrariness.

All of the suggested approaches have in common that they are correct up to second order in the coupling parameter J. Nevertheless, our improvements are nonperturbative in the sense that no Taylor expansion is provided. On the one hand this is for technical reasons, since the absence of a Wick's theorem for spin operators significantly complicates the calculation of Feynman diagrams. On the other hand already Shastry and Mattis[37] argued that a perturbation theory in J would fail because of the discontinuities in the physical properties of the model as J changes sign. Additionally, we have pointed out that the J^3 contribution to the exact self-energy in the limit of a ferromagnetically saturated semiconductor diverges although the sum over all orders yields a finite result.

The qualitative properties of the densities of states presented here are very similar to the findings of other approaches.[6] Since the former results were based on decoupling schemes for Green's functions the approximations incorporated into these calculations are difficult to control in their quality. With our results we can confirm *a posteriori* and justify these findings. This includes a complete set of strong correlation effects discussed there.

However, in its present state the documented method is only an approach to the electronic part of the s-f model. Whenever correlation functions that carry a dependence on the properties of localized magnetic moments emerged we had to perform some crude approximations. It is connected to this fact that we only considered a $\mathbf{k}$-independent self-energy by taking the average over the whole Brillouin zone. In this direction there is certainly room for further improvements.

APPENDIX A: HIGH-ENERGY EXPANSION

The high-energy expansion of the Green's function can be obtained from its representation as a resolvent (4):

$$G_{\mathbf{k}\sigma} = \sum_{l=0}^{\infty} \frac{m_{\mathbf{k}\sigma}^{(l)}}{\omega^{l+1}} = \sum_{l=0}^{\infty} \frac{(c_{\mathbf{k}\sigma}^\dagger | \mathcal{L}^l | c_{\mathbf{k}\sigma}^\dagger)}{\omega^{l+1}}. \quad \text{(A1)}$$

The coefficients $m_{\mathbf{k}\sigma}^{(l)}$ are called spectral moments and are determined by an l-fold commutator with the Hamiltonian $\mathcal{H}$. Apart from the mean-field contribution to the frequency matrix (5), the self-energy is identical to the memory matrix (7). Hence, its high-energy expansion $\Sigma_{\mathbf{k}\sigma} = \sum_{m=0}^{\infty} C_{\mathbf{k}\sigma}^{(m)}/\omega^m$ is given by

$$\Sigma_{\mathbf{k}\sigma} = -\tilde{J}z_\sigma \langle S^z \rangle + \sum_{m=0}^{\infty} \frac{(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger | (Q\mathcal{L}Q)^m | Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)}{\omega^{m+1}}. \quad \text{(A2)}$$

Due to the properties of Q, the coefficients $C_{\mathbf{k}\sigma}^{(m)}$ can be expressed in terms of spectral moments:

$$C_{\mathbf{k}\sigma}^{(1)}=m_{\mathbf{k}\sigma}^{(2)}-[m_{\mathbf{k}\sigma}^{(1)}]^2, \tag{A3}$$

$$C_{\mathbf{k}\sigma}^{(2)}=m_{\mathbf{k}\sigma}^{(3)}-2m_{\mathbf{k}\sigma}^{(2)}m_{\mathbf{k}\sigma}^{(1)}+[m_{\mathbf{k}\sigma}^{(1)}]^3. \tag{A4}$$

However, in our second-order perturbation theory the Liouville operator $\mathcal{L}$ is replaced by a part $\mathcal{L}_0$:

$$\begin{aligned}
\Sigma_{\mathbf{k}\sigma}^{(\text{SOPT})}&=-\tilde{J}z_\sigma\langle S^z\rangle+\tilde{J}^2\gamma_{\mathbf{k}\sigma}\\
&=-\tilde{J}z_\sigma\langle S^z\rangle+\sum_{m=0}^{\infty}\frac{(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger|(Q\mathcal{L}_0Q)^m|Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)}{\omega^{m+1}}.
\end{aligned} \tag{A5}$$

If this result is used for the MPT (17), the high-energy expansion of the self-energy is given by

$$\Sigma_{\mathbf{k}\sigma}^{(\text{MPT})}=-\tilde{J}z_\sigma\langle S^z\rangle+\tilde{J}^2a_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}+\tilde{J}^2a_{\mathbf{k}\sigma}b_{\mathbf{k}\sigma}[\gamma_{\mathbf{k}\sigma}]^2+\cdots. \tag{A6}$$

A comparison with the exact expression (A2) shows that $\gamma_{\mathbf{k}\sigma}$ is correct to order ω^{-1}. To ensure correctness to the same order for $\Sigma_{\mathbf{k}\sigma}^{(\text{MPT})}$ the parameter $a_{\mathbf{k}\sigma}$ has to be chosen as 1. To order ω^{-2} the self-energy $\Sigma_{\mathbf{k}\sigma}^{(\text{MPT})}$ has the coefficient

$$(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger|\mathcal{L}_0|Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)+\frac{1}{\tilde{J}^2}b_{\mathbf{k}\sigma}(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger|Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger)^2. \tag{A7}$$

In order to ensure that also this coefficient is exact, it has to be equal to

$$C_{\mathbf{k}\sigma}^{(2)}=(Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger|\mathcal{L}|Q\mathcal{L}c_{\mathbf{k}\sigma}^\dagger). \tag{A8}$$

Equality can be obtained if $b_{\mathbf{k}\sigma}$ is chosen as suggested in Eq. (18) above. As can be seen from Eq. (A4) in the high energy this order expansion implies the correctness of the four moments $m_{\mathbf{k}\sigma}^{(0)},\ldots,m_{\mathbf{k}\sigma}^{(3)}$ of the Green's function.

APPENDIX B: ABBREVIATIONS

For the sake of brevity we have introduced some shorthand notations in this papers. The full expressions are given here.

Equation (19):

$$p_\sigma=z_\sigma\langle S^zn_{-\sigma}\rangle-\langle S^{-\sigma}c_\sigma^\dagger c_{-\sigma}\rangle, \tag{B1}$$

$$q_\sigma=4z_\sigma\langle S^z\rangle p_\sigma-2(x_\sigma-p_\sigma), \tag{B2}$$

$$\begin{aligned}
x_\sigma&=S(S+1)\langle\hat{n}_\sigma\rangle-z_\sigma\langle S^z\hat{n}_\sigma\rangle+2z_\sigma\langle S^z\hat{n}_\sigma\hat{n}_{-\sigma}\rangle\\
&\quad+\langle(S^z)^2(\hat{n}_{-\sigma}-\hat{n}_\sigma)\rangle-z_\sigma\langle S^\sigma S^z c_{-\sigma}^\dagger c_\sigma+\text{H.c.}\rangle\\
&\quad-\langle S^\sigma c_{-\sigma}^\dagger c_\sigma+\text{H.c.}\rangle.
\end{aligned} \tag{B3}$$

We have evaluated x_σ by making use of the equivalence

$$\begin{aligned}
\sum_j T_{lj}(\langle S_l^\sigma c_{-\sigma}^\dagger c_{j\sigma}\rangle&-\langle S_l^\sigma c_{j-\sigma}^\dagger c_{l\sigma}\rangle)\\
&=-\tilde{J}(x_\sigma-S(S+1)\langle n_{-\sigma}\rangle-p_\sigma).
\end{aligned} \tag{B4}$$

and arguing that the left-hand side vanishes for almost all parameter configurations and, in particular, if mean-field decoupling is applied.

Equation (14):

$$\begin{aligned}
X=&\tilde{J}Z\frac{\langle(S^z)^2\rangle-\langle S^z\rangle^2}{S(S+1)-z_\sigma\langle S^z\rangle-\langle S^z\rangle^2}\\
&-2\tilde{J}\frac{z_\sigma\langle S^z\rangle\langle(S^z)^2\rangle-z_\sigma\langle S^z\rangle^3}{S(S+1)-z_\sigma\langle S^z\rangle-\langle S^z\rangle^2}\frac{1}{E-T_0-\tilde{J}z_\sigma\langle S^z\rangle}\\
&+2\tilde{J}Zz_\sigma\langle S^z\rangle\left[\frac{\langle(S^z)^2\rangle-\langle S^z\rangle^2}{S(S+1)-z_\sigma\langle S^z\rangle-\langle S^z\rangle^2}\right]^2,
\end{aligned} \tag{B5}$$

$$Y=Z\frac{\langle(S^z)^2\rangle-\langle S^z\rangle^2}{1-\tilde{J}\left[\dfrac{1}{E-T_0-\tilde{J}z_\sigma\langle S^z\rangle}+X\right]}, \tag{B6}$$

$$Z=\frac{1}{E-T_0+\tilde{J}z_\sigma\langle S^z\rangle}-\frac{1}{E-T_0+\tilde{J}z_{-\sigma}\langle S^z\rangle}. \tag{B7}$$

$\langle S^z\rangle$ vanishes in the paramagnetic regime. Hence, Z becomes zero, which implies the same for $X=Y=0$.

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