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High dimensions – a new approach to fermionic lattice models

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The limit of high spatial dimensions d, which is well-established in the theory of classical and localized spin models, is shown to be a fruitful approach also to itinerant fermion systems, such as the Hubbard model and the periodic Anderson model. Many investigations which are prohibitively difficult in finite dimensions, become tractable in $d = \infty$. At the same time essential features of systems in $d = 3$ and even lower dimensions are very well described by the results obtained in $d = \infty$. A wide range of applications of this new concept (e.g., in perturbation theory, Fermi liquid theory, variational approaches, exact results, etc.) is discussed and the state-of-the-art is reviewed.

1. Introduction

Theoretical investigations of correlated fermion systems are generally exceedingly difficult owing to quantum statistics and the many-body nature of the problem. Even standard methods like perturbation theory and variational approaches meet with severe technical problems when it comes to explicit evaluations. It is therefore of essential importance to find non-trivial limits where such treatments are manageable at all. In this respect the lowest spatial dimension, $d = 1$, is a standard dimension for quantum-theorists, since in $d = 1$ there exist powerful techniques (Bethe-Ansatz, bosonization, etc.) which in many cases allow one to derive exact results. By contrast, in classical statistical physics the limit of large spatial dimensions is well-established, since exact solutions for *spin lattice models* in $d = \infty$ are intimately connected with the respective mean field theories (MFT) [1].

It is therefore natural to ask whether the limit of $d = \infty$ also helps to gain insight into systems with itinerant quantum mechanical degrees of freedom, e.g. *fermionic lattice models*. In fact, Metzner and Vollhardt [2] recently showed that in the limit $d \to \infty$ Hubbard-type models (if properly scaled) and their correlations remain non-trivial, while investigations become substantially simpler.

2. Fermionic lattice models in d = ∞

The Hubbard model is used in various areas of condensed matter theory (e.g., itinerant magnetism, metal–insulator transition, high-T_c superconductivity) because of its relative simplicity and generic nature. It describes electrons with spin $\sigma = \uparrow, \downarrow$ on a lattice with a short-range (effectively zero-range, i.e., on-site) interaction

$$\hat{H}_U = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = U\hat{D} \,, \tag{1a}$$

where $\hat{n}_{i\sigma} = \hat{c}^+_{i\sigma}\hat{c}_{i\sigma}$, such that $\hat{D}$ is the number operator for doubly occupied sites in the system. The electrons can have a general kinetic energy

$$\hat{H}_t = \sum_{\langle ij\rangle,\sigma} t_\sigma \hat{c}^+_{i\sigma}\hat{c}_{j\sigma} \,, \tag{1b}$$

with hopping matrix element t_σ. If nearest-neighbor interactions are included, e.g. by $\hat{H}_V = \Sigma_{\langle ij\rangle}\Sigma_{\sigma\sigma'} V_{\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'}$, a generalized, one-band Hubbard model may be written as

$$\hat{H}_{\mathrm{Hub}} = \hat{H}_t + \hat{H}_U + \hat{H}_V \,. \tag{1c}$$

In the original Hubbard model $V_{\sigma\sigma'} \equiv 0$ and $t_\sigma \equiv -t$. Another important, somewhat related *two-band* model is the periodic Anderson model (PAM) involving c- and f-electrons

$$\hat{H}_{\mathrm{PAM}} = \hat{H}_t^c + \hat{H}_t^f + \hat{H}_U^f + \sum_{k,\sigma} (V_k \hat{f}_{k\sigma}^{+} \hat{c}_{k\sigma} + \mathrm{h.c.}) , \tag{2}$$

which are hybridized via the last term (here V_k is the hybridization matrix element and $\hat{f}_{k\sigma}^{+}$, $\hat{c}_{k\sigma}$, etc. are expressed in momentum representation). The hopping corresponds to an energy dispersion $\varepsilon(\boldsymbol{k})$, which on a hypercubic lattice has the form ($t_\uparrow = t_\downarrow \equiv -t$)

$$\varepsilon(\boldsymbol{k}) = -\frac{t}{L} \sum_{\langle ij \rangle} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{i}-\boldsymbol{j})} = -2t \sum_{i=1}^{d} \cos k_i . \tag{3}$$

Here L is the number of lattice sites and the lattice constant is taken as unity. In the limit of large dimensions, $d \to \infty$, $\varepsilon(\boldsymbol{k})$ is *not* of the order of td, as might be naively expected from eq. (3). In fact, for a randomly chosen momentum eq. (2) yields $\varepsilon(\boldsymbol{k}) \propto -td^{1/2}$ for large d [2] (exceptions are $\boldsymbol{k} = 0$ and $\boldsymbol{k} = \boldsymbol{Q}$ (half a reciprocal lattice vector), but these momenta have zero measure), and the central limit theorem determines the density of states (DOS) as

$$N(E) \overset{d\to\infty}{=} \frac{1}{2t\sqrt{\pi d}} \mathrm{e}^{-[E/(2t\sqrt{d})]^2} \tag{4}$$

This is a Gaussian DOS, free of van Hove singularities, which is finite only if t is rescaled as $t \to \bar{t}/\sqrt{2d}$, whereby $N(E) \to (2\pi\bar{t}^2)^{-1/2} \exp(-E^2/2\bar{t}^2)$ (henceforth $\bar{t} \equiv 1$). Only this scaling with $1/\sqrt{d}$ leads to a finite kinetic energy in the limit $d \to \infty$ and hence to a non-trivial limit for the Hubbard model, in which kinetic energy $\hat{H}_t$ and interaction $\hat{H}_U$ (which needs no rescaling because of its local nature) truely compete. If, in addition, $V_{\sigma\sigma'} \neq 0$ in eq. (1c), it has to be scaled according to $V \to V/2d$, because the interaction involves the *densities* of nearest neighbors, their number being of order $2d$. For other types of lattices and/or range of hopping the scaling of the kinetic energy still has to be performed as discussed above, but the DOS is then in general no longer Gaussian [3]. From the above discussion it is clear that the limit of high dimensions only applies to *lattice* models.

3. Variational wave functions

In view of the substantial difficulties involved in any exact treatment of fermionic many-body systems, variational wave functions (VWFs) have always played an important role in the investigation of such systems. VWFs provide an approximate, but explicit and intuitive approach to the understanding of correlations and, in particular, go beyond standard perturbation theory [4]. In the case of fermionic lattice models with on-site interaction as in eqs. (1a) and (2), the reduction of doubly occupied sites is of particular importance. This is achieved by a Gutzwiller-type wave function [5]

$$|\psi\rangle = g^{\hat{D}} |\psi_0\rangle = \prod_i [1 - (1-g)\hat{D}_i] |\psi_0\rangle , \tag{5}$$

where $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, $g \in [0, 1]$ is a variational parameter and $|\psi_0\rangle$ is an arbitrary one-particle wave function. The projector $g^{\hat{D}}$ reduces the amplitude of those spin configurations with too many doubly occupied sites. When $|\psi_0\rangle$ is taken as the (paramagnetic) Fermi sea, eq. (5) reduces to the well-known Gutzwiller wave function [6]. More generally, $|\psi_0\rangle$ can, e.g., be chosen as a spin density wave with antiferromagnetic long-range order, a BCS-wave function or – in the case of eq. (2) – the wave function for the hybridized ground state of c- and f-electrons at $U = 0$ [5]. In spite of the apparent simplicity of eq. (5), the analytic evaluation of the expectation value $\langle \hat{O} \rangle$ of an operator $\hat{O}$ in terms of eq. (5) is in general not tractable in finite dimensions. However, using a perturbational diagrammatic approach similar to that used in a ϕ^4-theory an exact evaluation of $\langle \hat{O} \rangle$ is possible in the limit $d \to \infty$ [2, 7]. In this approach diagrams are conveniently expressed by the self-energy $S_{\sigma ij}$ in position space, with lines corresponding to $P^0_{\sigma ij} = \langle \psi_0 | \hat{c}^{+}_{i\sigma} \hat{c}_{j\sigma} | \psi_0 \rangle$ and vertices corresponding

to a factor $(g^2 - 1)$. Both, the one-particle density matrix $P_{\sigma ij} \equiv \langle c^+_{i\sigma} c_{j\sigma} \rangle$ (which yields the kinetic energy $\langle \hat{H}_t \rangle$, eq. (1b)) and the on-site interaction $\langle \hat{H}_U \rangle$, eq. (1a), are completely determined by $S_{\sigma ij}$. In the limit $d \to \infty$ the evaluation of the diagrams for $S_{\sigma ij}$ is tremendously simplified due to the fact that $P^0_{\sigma_{ij}}$ vanishes as

$$P^0_{\sigma ij} \propto \mathcal{O}\left[\left(\frac{1}{\sqrt{d}}\right)^{|i-j|}\right], \tag{6}$$

where $|\boldsymbol{i} - \boldsymbol{j}| = \Sigma_{l=1}^{d} |i_l - j_l|$. This implies a drastic collapse of those diagrams in which two vertices are joined by more than two different paths (see fig. 1). This is the case, in particular, for the *proper* self-energy $S^*_{\sigma ij}$, which is the sum over all one-particle irreducible self-energy diagrams. Consequently, $S^*_{\sigma ij}$ is *site-diagonal* in $d = \infty$,

$$S^*_{\sigma ij} = S^*_{\sigma ii} \delta_{ij} \,. \tag{7}$$

Given a starting wave function $|\psi_0\rangle$ in eq. (5) the evaluation of, say, the ground state energy $\langle \hat{H}_{\mathrm{Hub}} \rangle$ can be performed explicitly in $d = \infty$ [8]. In this case only diagrams with bubble structure remain, i.e., correlation functions acquire an overall RPA structure.

As shown by Gebhard [9] the above formalism can be further simplified by a slight redefinition of the wave function $|\psi_0\rangle$ in eq. (5). Thereby results in $d = \infty$ can be obtained without having to calculate a single graph. In particular, the ground-state energy for eq. (1c) or eq. (2) can now be obtained in *closed form* for arbitrary $|\psi_0\rangle$. The result is found to be identical to an earlier one obtained by Kotliar and Ruckenstein [10], who used a saddle point approximation within a slave boson approach. Thus the $d = \infty$ limit reveals an intimate connection between two seemingly different approaches. – Contact with finite dimensions can be made by explicit $1/d$ expansions [7, 9]. In many cases already the $1/d$ correction, together with the appropriate DOS in d dimensions, yields excellent agreement with known results in dimensions as low as $d = 1$. In general, results in $d = 3$ are already found to be very well approximated by those for $d = \infty$.

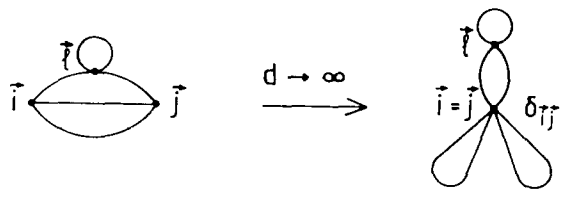

Fig. 1. Collapse of a typical irreducible self-energy diagram in $d = \infty$.

It is interesting to observe that in the case of the Gutzwiller wave function [6] the results of the exact evaluation of the ground state energy of the Hubbard model in $d = \infty$ [2] are identical to those obtained within the so-called Gutzwiller approximation [11]. The latter corresponds to a semi-classical approximation, which evaluates matrix elements by calculating the *classical* statistical weights of spin configurations, thereby neglecting spatial correlations [12]. At half-filling $(n = 1)$ the Gutzwiller approximation leads to a localization transition at finite U (Brinkman–Rice transition [13]). It yields simple, physically sensible results in a number of problems (e.g., metal–insulator transitions [13], normal-liquid ^{3}He [12, 14]) and allows contact to be made with Fermi-liquid theory. The transition itself is an artefact of $d = \infty$, which is not removed by finite orders of $1/d$ corrections [8, 9]. However, in $d = 3$ the approximation is indeed excellent if one is not too close to this transition, and is even better for $n < 1$.

For the investigation of the periodic Anderson model a VWF has been proposed [15] where $|\psi_0\rangle$ in eq. (5) is given by the exact ground state wave function for $U = 0$, with the hybridization amplitude between the c- and f-electrons taken as a variational function. The correlator $g^{\hat{D}}$ in eq. (5) then only acts on the f-electrons. Such an Ansatz is motivated by VWFs used in the single-impurity problem. An exact evaluation of the ground-state energy E [16], correlation functions [17], etc. is again possible in $d = \infty$, the result for E being identical to that obtained by a Gutzwiller-type approximation. In fig. 2 we show the spin–spin and density–density correlation function for the f-electrons as calculated analytically in $d = \infty$ and evaluated with the DOS in $d = 1$ [17], and compare with the results in $d = 1$ ob-

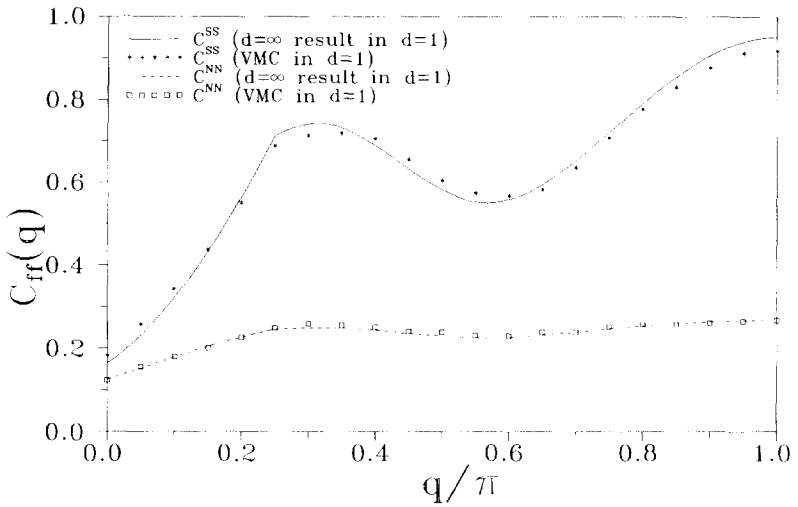

Fig. 2. Variational evaluation of the spin–spin ($C^{SS}(q)$) and density–density ($C^{DD}(q)$) correlation function for f-electrons in the periodic Anderson model. Analytic results for $d = \infty$ (evaluated with the one-dimensional DOS [17]) are compared with variational Monte Carlo (VMC) results in $d = 1$ [18]. Parameters: $n = 1.75$, $U = \infty$, $E_f = 0$, $t = 1$, $V = 0.5$.

tained by variational Monte Carlo [18]. Obviously the two agree extremely well. This shows that the $d = \infty$ limit can even give valuable insight into dimensions as low as $d = 1$.

4. Weak coupling perturbation theory

The diagrammatic collapse discussed above, and the substantial simplifications deriving from it [2], actually occur in any standard perturbational treatment of fermionic lattice models in $d = \infty$. The propagator (Green function) of the noninteracting system always obeys eq. (6), which is a consequence of the scaling $t \to t/\sqrt{2d}$ [19]. Therefore, within a site representation, two vertices in a diagram collapse, if they are connected by more than two lines: for nearest neighbor sites a propagator is of order $d^{-1/2}$, and there are of order d sites which are to be summed; hence the contribution to a diagram, in which two vertices are on different sites and are joined by three and more lines, vanishes unless the two sites coincide. In particular, e.g. for skeleton diagrams, the irreducible self-energy $\Sigma^*_{\sigma ij}$, this collapse involves *all* vertices, i.e., the contribution is purely site-diagonal ('local') as given by eq. (7) [3, 19].

A simple illustration of these simplifications is provided by weak coupling expansions, e.g. for the correlation energy $E_c \equiv E_{exact} - E_{HF}$ for the Hubbard model [2], which is the difference between the exact ground-state energy and the Hartree–Fock energy. Within Goldstone perturbation theory the second-order contribution to E_c is given by $E_c^{(2)} \propto U^2$, which is an integral over four momenta $\boldsymbol{k}_i$, $i = 1, \ldots, 4$, which are constrained by momentum conservation (thus yielding a $3d$-fold integration). This constraint (a δ-function) can be expressed as a lattice sum (effectively the sum over the relative position $\boldsymbol{f} = \boldsymbol{i} - \boldsymbol{j}$ of the two vertices $\boldsymbol{i}$ and $\boldsymbol{j}$ of the diagrams on the lattice). In $d = \infty$ the collapse implies $\boldsymbol{i} = \boldsymbol{j}$ and hence only the term $\boldsymbol{f} = 0$ contributes. This may be interpreted as an irrelevance of momentum conservation at vertices, because the δ-function is replaced by a constant [3]. Thus the evaluation of $E_c^{(2)}$ in $d = \infty$ reduces to a *one-dimensional* integral over probability functions and is therefore the simplest of all dimensions. The density dependence of $E_c^{(2)}$ is shown in fig. 3 and is compared with the respective numerical results for $d = 1$ and 3. Clearly the result for

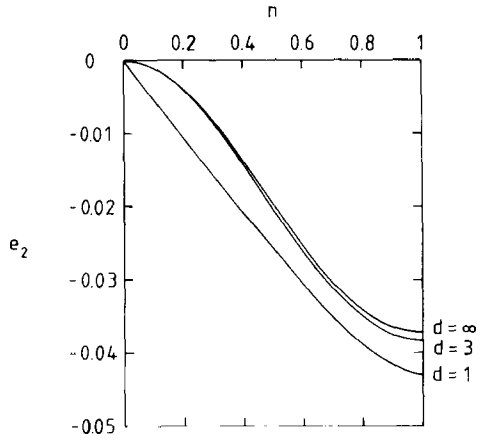

Fig. 3. Second-order correlation energy for the Hubbard model, $e_2 = 2(E_c^{(2)}/|\bar{\varepsilon}_0|)/(U/|\bar{\varepsilon}_0|)^2$, as a function of the density n for several dimensions d; $|\bar{\varepsilon}_0|$ is the kinetic energy for $U = 0$ [2].

$d = \infty$, which is easily obtained, is seen to provide a very good approximation for the case in $d = 3$, whose evaluation involves considerable numerical efforts. It should be noted that the neglect of the terms $f \neq 0$ in the above lattice sum ('local approximation') has already been used earlier [20] as a pragmatic approximation within a perturbational treatment of transition metals in $d = 3$. This approximation is now understood to be exact in the limit $d \to \infty$.

It should be noted that the collapse not only occurs in one-particle quantities; the totally irreducible part of the *two*-particle vertex function also collapses completely, i.e., becomes independent of momenta (but care has to be taken at relative momenta $\boldsymbol{q} = 0$ and $\boldsymbol{Q}$). Hence the momentum dependence of the two-particle propagator is given by the parquet equations [21]. There is, however, no collapse concerning the time variable, i.e., energy, such that the unsueing problem, e.g. the calculation of response and correlation functions, is still complicated. It should also be mentioned that, provided perturbation theory is valid at all, the contribution to the electrical conductivity due to vertex corrections vanishes for $d = \infty$, so that the conductivity is given by the 'zeroth-order bubble', owing to the odd parity of the current vertex [22].

An immediate consequence of the proper self-energy being site-diagonal is that its Fourier transform is *momentum independent*, i.e., only depends on frequency ω [3]

$$\Sigma(\boldsymbol{k}, \omega) \overset{d=\infty}{\to} \Sigma(\omega) . \tag{8}$$

The one-particle propagator thus has the form

$$G(\boldsymbol{k}, \omega) = [\omega - \varepsilon(\boldsymbol{k}) + E_F - \Sigma(\omega)]^{-1} , \tag{9}$$

and depends on $\boldsymbol{k}$ only via the $\varepsilon(\boldsymbol{k})$. As pointed out by Müller–Hartmann [19] this has several very interesting implications concerning a Fermi-liquid description of the lattice models under consideration, some of which we list below. (Note, that for an A–B lattice and nearest neighbor hopping the Hubbard model has a 'perfect-nesting' instability at half-filling, leading to an insulating state with antiferromagntic correlations independent of d; in this case the system is of course not a Fermi liquid. However, by including hopping to next-nearest neighbors one may open a 'Fermi liquid window' at small U, such that the above considerations apply; here we assume that the symmetry also remains unbroken otherwise):

(i) For $\omega \to 0$ the system has quasiparticle properties, owing to

$$\mathrm{Im}\, \Sigma(\omega) \propto \omega^2 . \tag{10}$$

(ii) Since $\varepsilon(\boldsymbol{k}) - E_F + \Sigma(0) = 0$ determines the Fermi surface (reducing to $\varepsilon(\boldsymbol{k}) = E_F^0$ in the non-interacting case) the $\boldsymbol{k}$-independence of $\Sigma(0)$ implies that its shape is *not* changed by the interaction. (This shape may be quite complicated due to the lattice structure.) The Fermi surface volume hence does not change (Luttinger theorem).

(iii) The DOS at the Fermi surface is not renormalized.

(iv) The mass renormalization is simply given by

$$\frac{m^*}{m} = 1 - \left.\frac{\mathrm{d}\Sigma}{\mathrm{d}\omega}\right|_{\omega=0} \geqslant 1 . \tag{11}$$

We note, that in microscopic calculations the $\boldsymbol{k}$-dependence of Σ is frequently neglected for simplicity. For lattice models this *approximation* is seen to be *exact* in $d = \infty$.

(v) The momentum distribution $n_k \equiv n(\varepsilon_k)$ has a discontinuity at E_F given by

$$n(E_F - 0) - n(E_F + 0) = \left(\frac{m^*}{m}\right)^{-1}. \qquad (12)$$

In $d = 2$, 3 weak coupling expansions of the self-energy etc., are very complicated to compute explicitly, owing to the large number of momentum integrations. In particular, self-consistent, numerical calculations turn out to be prohibitively difficult for this reason, even using the largest computers. Here the limit of large dimensions opens a new avenue. Indeed, the simplifications arising from the collapse of diagrams and the ensueing momentum independence of the proper self-energy allows one to perform self-consistent calculations for the first time. In the case of the Hubbard model Müller–Hartmann [21] performed conserving approximations within second-order perturbation theory and thereby extracted the Fermi-liquid parameters F_0^s and F_0^a from the respective charge- and spin-susceptibilities $\chi_c/\chi_{co} = (m^*/m)/(1 + F_0^s)$ and $\chi_s/\chi_{so} = (m^*/m)/(1 + F_0^a)$. One finds that, compared with Hartree–Fock, m^*/m and F_0^s are strongly enhanced, while $|F_0^a|$ becomes smaller. In fact, F_0^a levels off at ~ -0.4, rather than approaching -1, and thus stabilizes the paramagnetic phase. By the same method partial summations, e.g. of bubble and ladder diagrams to the self-energy, can also be calculated explicitly [23].

The periodic Anderson model was studied by Schweitzer and Czycholl [24], who performed the first fully selfconsistent calculation of the f-electron self-energy and spectral function to second order in U, including their temperature and density dependence. The self-consistency guarantees that all Luttinger sum rules are fulfilled. In this model, which is used to describe heavy fermion systems, perturbation theory should be particularly valuable since in the Kondo limit the effective mass can become arbitrarily large even for *small* repulsion [25]. These authors also showed how the $d = \infty$ limit can be employed to determine the full $\boldsymbol{k}$-dependent self-energy in low dimensions ($d = 1, 2, 3$) [26]. For a given dimension d they started from the 'local approximation' (see the beginning of this section) and then included the contribution from nearest, next-nearest neighbors, etc., until convergences was reached. This corresponds to an effective $1/d$-expansion and converges even in $d = 1$. In fig. 4 we show their results for the f-electron spectral function in $d = 3$, where the result for $d = \infty$ is compared with that for the $\boldsymbol{k}$-dependent self-energy obtained by summation up to the third neighbor shell. Clearly, the $d = \infty$ result already provides a very good approximation.

5. Exact solutions

In spite of the diagrammatic simplifications occurring in $d = \infty$, fermionic lattice models such as eqs. (1c) and (2), remain non-trivial and so far an exact solution for the Hubbard model in $d = \infty$ has not been possible. However, a simplified Hubbard model, where only one of the two spin species can hop (i.e., $t_\uparrow = 0$ and $t_\downarrow \equiv -t$ in eq. (1b)) and which serves as a model for semiconductor–metal transition or, alternatively, for crystallization, has been solved by Brandt

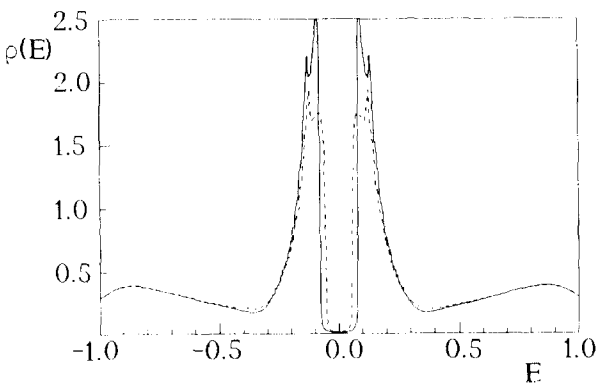

Fig. 4. f-electron spectral function of the periodic Anderson model in $d = 3$. Parameters: $n = 2$, $U = 1$, $E_f = -0.5$, $t = 1/6$, $V = 0.3$. Dashed line: result with full $\boldsymbol{k}$-dependent self-energy; full line: result for $d = \infty$ [26].

and Mielsch [27]. They made explicit use of the fact that in $d = \infty$ the proper self-energy is site-diagonal and can itself be expressed by the site-diagonal propagator. Hence they showed that it is sufficient to solve an *atomic* problem in a generalized time-dependent external field.

There arises a fundamental question here: in what sense has the exact solution in $d = \infty$ of a fermionic lattice model with on-site interaction a 'mean field' character, and how does this mean field theory look like? (Note that the on-site interaction is the only dynamical interaction in $d = \infty$ [3] and that Hartree–Fock cannot become exact in $d = \infty$ because it decouples this interaction [28].) An answer was recently provided by van Dongen and Vollhardt [28] who showed that even for models with an on-site interaction a mean field Hamiltonian can be constructed, which – in analogy with spin lattice models – becomes exact in $d \rightarrow \infty$. Here, 'mean fields' are collective fermion operators, rather than numbers. The solution shows that the issue of mean field theories is much more subtle in this class of problems than in the case of classical and localized models.

6. Discussion

Within a short time investigations of lattice fermion systems in the limit of high spatial dimensions have yielded new insight into the properties and the behavior of Hubbard-type models. Provided that the kinetic energy is scaled properly, these models and the correlations described by them remain non-trivial even in $d = \infty$. At the same time perturbational calculations become much simpler than in finite dimensions. This property makes variational calculations, microscopic many-body methods, etc. tractable in $d = \infty$ which are prohibitively difficult in lower dimensions. Most importantly, many essential features of systems in $d = 3$, and even lower dimensions, are very well described by the results in $d = \infty$ or expansions around this limit. In this sense $d = 3$ may already by considered a 'high dimension'. Indeed, on a lattice the important quantity is not so much d itself, but the number of nearest neighbors ($Z = 2d$ on a hypercubic lattice). The limit of large d also allows one to understand the nature of mean field theories for fermionic lattice models, which is much more subtle than in classical systems. The investigation of Hubbard-type models in high dimensions has only begun. There are still many open questions, whose answer will help to provide a better understanding of these important models.

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