Hubbard model in infinite dimensions

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We present an exact mapping of the Hubbard model in infinite dimensions onto a single-impurity Anderson (or Wolff) model supplemented by a self-consistency condition. This provides a mean-field picture of strongly correlated systems, which becomes exact as $d \to \infty$. We point out a special integrable case of the mean-field equations, and study the general case using a perturbative renormalization group around the atomic limit. Three distinct Fermi-liquid regimes arise, corresponding to the Kondo, mixed-valence, and empty-orbitals regimes of the single-impurity problem. The Kondo resonance and the satellite peaks of the single-impurity model correspond to the quasiparticle and Hubbard-bands features of the Hubbard model, respectively.

Despite intensive theoretical work, the physics of strongly correlated fermions still contains numerous unsolved problems, even in its simplest formulation such as the single-band Hubbard model. In particular, there is no widely accepted mean-field theory which becomes exact in some limit. In a number of statistical-mechanics problems (including spin glasses, fully frustrated models, and lattice gauge theories) the mean-field theory obtained by taking the limit of large space dimensionality provided great insights. In a pioneering paper,[1] Metzner and Vollhardt pointed out that this limit is also of great interest for quantum many-body models, which simplify remarkably while retaining the main features, making their physics nontrivial. In this paper, we construct a mean-field picture of the Hubbard model, which becomes exact as $d \to \infty$ and unravels a connection with the single-impurity Anderson model. This analogy elucidates many features of the Hubbard model in infinite dimensions. A different mean-field approach has been recently proposed[2] by Van Dongen and Vollhardt for the Falicov-Kimball model.

As usual in statistical mechanics, the limit $d \to \infty$ must be taken while scaling the parameters in a definite way, in order to avoid the situation that a single term in the Hamiltonian dominates all others. For the Hubbard model on a d-dimensional hypercubic lattice with nearest-neighbor hopping t_{ij}, the on-site U need not be scaled, while t_{ij} must be scaled[1] as $1/\sqrt{d}$ in order to keep both the kinetic and potential energy per site finite. Specifically, we shall choose

$$H = \frac{-1}{2\sqrt{d}} \sum_{\langle ij \rangle, \sigma} (C_{i\sigma}^{\dagger} C_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{1}$$

With this scaling, the model remains an itinerant system with correlations. The free ($U=0$) density of states (DOS) acquires a Gaussian form[1] in the $d \to \infty$ limit: $D(\varepsilon) = 1/\sqrt{\pi} e^{-\varepsilon^2}$. It displays band tails extending from $-\infty$ to $+\infty$, but in many instances, the effective bandwidth is given by the variance of the density of states.

Metzner and Vollhardt's observation stimulated a number of subsequent works,[3] concentrating mainly on the study of variational wave functions and weak-coupling expansions, which simplify enormously in $d = \infty$. Furthermore, in a remarkable piece of work,[4] Brandt and Mielsch (BM) obtained the exact solution of the infinite-dimensional Falicov-Kimball model, a simplified Hubbard model in which only one of the two spin species is allowed to hop. For reasons which will appear later, the infinite-dimensional Hubbard model cannot be solved exactly, but the BM method does provide a very useful framework for its study. The goal of the method is to find a set of equations allowing the calculation of the self-energy Σ, defined from the interacting single-electron Green's function $G(\mathbf{k}, i\omega_n)$ by

$$G(\mathbf{k}, i\omega_n) = [i\omega_n + \mu - \varepsilon_{\mathbf{k}} - \Sigma]^{-1} . \tag{2}$$

(Unbroken translational and spin symmetries are assumed here, see the discussion below.) In $d = \infty$, the self-energy depends only on frequency[1,5] in Fourier space, $\Sigma = \Sigma(i\omega_n)$.

To compute Σ we consider an auxilliary impurity problem with the single-site action:

$$S = U \int_0^{\beta} d\tau \, n_{\uparrow}(\tau) n_{\downarrow}(\tau) - \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{\sigma} c_{\sigma}^{\dagger}(\tau) G_0^{-1}(\tau - \tau') c_{\sigma}(\tau') . \tag{3}$$

Here, G_0, the "bare" Green's function of this local dynamics, contains the information of all the other sites which have been integrated out. G_0 *does not* coincide with the noninteracting site-diagonal Green's function of the Hubbard model. This impurity problem has a self-energy $\Sigma_{\text{imp}}[G_0, i\omega_n]$ defined from the interacting Green's function $G(i\omega_n)$ of (3) by

$$G(i\omega_n) = \langle c^{\dagger}(i\omega_n) c(i\omega_n) \rangle_S = [G_0^{-1} - \Sigma_{\text{imp}}(G_0, i\omega_n)]^{-1} . \tag{4}$$

The mean-field equations require that the site-diagonal Green's function of the Hubbard model [equal to the sum of (2) over momenta, $\sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n)$] actually coincides

with (4), provided $\Sigma=\Sigma_{\rm imp}(i\omega_n)$. This reads

$$G(i\omega_n)=\int_{-\infty}^{+\infty} d\varepsilon \frac{D(\varepsilon)}{i\omega_n+\mu-\Sigma_{\rm imp}(i\omega_n)-\varepsilon}. \quad (5)$$

Notice that the nature of the lattice enters the mean-field equations via the density of states $D(\varepsilon)$ only.

For a Gaussian $D(\varepsilon)$, the Hilbert transform on the right-hand side of (5) equals $-i\sqrt{\pi}e^{-\zeta^2}\mathrm{erfc}(-i\zeta)$, where erfc denotes the complementary complex error function and $\zeta=i\omega_n+\mu-\Sigma_{\rm imp}(i\omega_n)$. Equations (3)–(5) are the mean-field equations for the Hubbard model which are exact in infinite dimensions, and fully determine G, G_0, and $\Sigma=G_0^{-1}-G^{-1}$, in principle.

Equations (3)–(5) generalize the BM equations[4] to the case of the Hubbard model. They follow from the observation, of Müller-Hartmann,[5] that the skeleton functional expressing the dependence of the Hubbard model self-energy on the *interacting* Green's function actually depends only on the *site-diagonal* Green's function in $d=\infty$. As a result, only frequency conservation has to be insured in the skeleton expansion, and all the action takes place on a single site.

It is instructive to check these equations in the two solvable limits $U=0$ and $t_{ij}=0$. In the former, the solution of (3) and (4) is trivially $G=G_0$, thus $\Sigma=0$ and (5) correctly assigns its free value to G; in the latter, $D(\varepsilon)$ becomes a δ function: Thus, (4) and (5) imply $G_0(i\omega_n)=(i\omega_n+\mu)^{-1}$ and (3) indeed reduces to the (Hamiltonian) atomic limit.

We would like to point out that Eqs. (3)–(5) have a very natural physical interpretation as a *mean-field picture* of a quantum many-body system; they mean that due to the freezing of spatial fluctuations, one-particle properties can be understood by looking at a single fixed site of the lattice. Because the model is itinerant, the occupation of this site undergoes quantum fluctuations (in imaginary time) between empty, occupied by an "up" or a "down" spin, and doubly occupied. The quantum dynamics of these processes is described by (3), where G_0 is an *effective* quantity determined by all the processes happening on the other sites. G_0 should be thought of as the appropriate generalization to itinerant systems of the effective field h_i acting on the sites of a localized spin model. Equation (4) expresses the local Green's function $G(i\omega_n)$ in terms of G_0, in the same way as solving the mean-field Hamiltonian $\sum_i h_i S_i$ yields the magnetization in terms of h_i: $m_i=\tanh(\beta h_i)$ (for Ising spins). In this framework, (5) can be thought of as analogous to the self-consistency requirement $h_i=\sum_{j(i)}J_{ij}m_j$. Of course, it is always possible to think in terms of an effective dynamics for a single site: The simplification in $d=\infty$ is that this dynamics factorizes into products of two-particle processes described solely by G_0.

The rest of this paper is devoted to a discussion of the physics resulting from Eqs. (3)–(5). Let us point out that these describe the paramagnetic solution only, which will not be the *actual* one below the Néel temperature, if U and the density are such that spin and/or translational symmetry is actually broken. At half-filling, for example, antiferromagnetic order is expected. However, the discussion below is relevant even there, not only because following the paramagnetic solution is interesting in itself, but also because the critical U for ordering depends on the lattice, and certain next-nearest-neighbor hoppings can push it to a nonzero value while leaving (for $d=\infty$) the DOS $D(\varepsilon)$ unchanged.[5] As it stands, the local dynamics (3) might *a priori* undergo a *spontaneous* spin-symmetry breaking. Indeed, solving it in the Hartree-Fock approximation $G_{\mathrm{HF},\sigma}^{-1}=G_{0\sigma}^{-1}-Un_{-\sigma}$ and taking (5) into account leads to the usual Stoner criterion $UD(\mu_0)>1$ for the appearance of ferromagnetism in the Hubbard model. However, this instability of the local model will be shown below to be washed away by quantum fluctuations. This *does not mean* that no ferromagnetic transition exists for the infinite-dimensional Hubbard model, but rather that the description of phases *with* broken symmetries require a slightly different impurity model. As in the Falicov Kimball model[4] the local dynamics (3) is unchanged except for explicit spin dependence of G_0, and the self-consistency relation (5) is modified to account for a broken translational symmetry.

It is useful to think of (3) as describing a single fermion c_σ coupled to a bath of "conduction electrons" which generate G_0. This is precisely the Anderson model[6] of a magnetic impurity hybridized with a conduction band:

$$H_{\rm AM}=\sum_{k\sigma}E_k a_{k\sigma}^\dagger a_{k\sigma}+\varepsilon_d\sum_\sigma d_\sigma^\dagger d_\sigma+Un_{d\uparrow}n_{d\downarrow}+\sum_{k\sigma}[V_k a_{k\sigma}^\dagger d_\sigma+\mathrm{H.c.}], \quad (6)$$

where we have kept the standard notation d_σ for the impurity. $H_{\rm AM}$ is quadratic in the $a_{k\sigma}$'s which can thus be integrated out, yielding a dynamics for d_σ identical to (3), with

$$G_0^{\rm AM}(i\omega_n)^{-1}=i\omega_n-\varepsilon_d-\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\pi}\frac{\Delta(\varepsilon)}{i\omega_n-\varepsilon}, \quad (7)$$

where $\Delta(\varepsilon)=\pi\sum_k V_k^2\delta(\varepsilon-E_k)$ is a combined measure of the hybridization and of the DOS of the conduction electrons. Equivalently, it may be more natural in the present context to view (3) as describing a Wolff model (i.e., a free lattice gas with a local Green's function G_0 and U acting only on a single site).

The representation (7) is general enough to reproduce any G_0 with a suitably chosen form of $\Delta(\varepsilon)$; however, the standard form discussed in the context of the Anderson model is a constant $\Delta(\varepsilon)=\Delta$ inside the conduction band $-W_0/2<\varepsilon<W_0/2$, and zero outside. The Bethe ansatz solvable case corresponds furthermore to $W_0\to\infty$, i.e., $G_0^{-1}(\omega+i0^+)=\omega-\varepsilon_d+i\Delta$. Here, $\Delta(\varepsilon)$ is a self-consistently determined quantity which evidently does not have this shape in general. It is remarkable, however, that, if $D(\varepsilon)$ was a Lorentzian $L(\varepsilon)=\Delta/\pi[(\varepsilon-\varepsilon_0)^2+\Delta^2]$ instead of a Gaussian, the self-consistency condition (5) would imply that $G_0^{-1}=\omega+\mu-\varepsilon_0+i\Delta$ precisely has the integrable form. Furthermore, it is easily shown in that case that the free-energy coincides with the free-energy of the impurity model. This means that Eqs. (3)–(5) can be solved, in the case of a Lorentzian density of states to obtain all the thermodynamics of the model in closed form. This allows us to study in detail, in a soluble model, the renormalizations caused by strong correlations. Detailed results will be presented elsewhere; let us simply point out

here that this model has a Mott transition at half filling at $U_c=\infty$. The spin susceptibility diverges $\chi\approx 1/\sqrt{Ut}\times\exp(\pi U/8t)$, the compressibility vanishes $\partial n/\partial\mu\approx 4t/\pi U^2$. The Wilson ratio γ/χ stays finite as predicted by Brinkman and Rice. There is no ferromagnetic phase away from half filling at any finite value of U. We suspect that the Lorentzian density of states corresponds to an infinite-dimensional Hubbard model with a particular form of long-range hopping. The fact that $U_c=\infty$ is particular to this case in which the expectation value of the kinetic energy is infinite.

In this paper we shall use the Lorentzian case mainly as the starting point of a renormalization-group (RG) approach showing that the three known Fermi-liquid regimes of the single-impurity Anderson model correspond to three Fermi-liquid regimes of the paramagnetic solution of the Hubbard model in $d=\infty$ (with Gaussian DOS).[7] The underlying idea is that the low-frequency physics depends only on the low-energy properties of $\Delta(\varepsilon)$, and not on its detailed shape. More precisely, we write $D(\varepsilon)=L(\varepsilon)+\delta D(\varepsilon)$, where the parameters ε_0 and Δ characterizing $L(\varepsilon)$ are to be specified below; then, from (5),

$$G(\omega+i0^+)=[\omega+\mu-\varepsilon_0-\Sigma(\omega+i0^+)+i\Delta]^{-1}+\delta G(\omega)$$

and $G_0=[\omega+\mu-\varepsilon_0+i\Delta]^{-1}+\delta G_0(\omega)$. Let us first assume that $\mathrm{Im}\Sigma(i0^+)=0$ and that $\Sigma(i0^+)$ is finite; then we show that ε_0 and Δ can be chosen in such a way that *both δG and δG_0 vanish at zero frequency*, namely,

$$\Delta=\frac{\sqrt{\pi}\exp(\zeta_0^2)}{\pi+\left[\int_0^{\zeta_0}e^{t^2}dt\right]^2},\quad \varepsilon_0=\zeta_0-2\Delta/\sqrt{\pi}\int_0^{\zeta_0}e^{t^2}dt\,, \tag{8}$$

with $\zeta_0=\mu-\Sigma(i0^+)$. Δ is thus seen to always be nonzero. A perturbative RG *in the hybridization* Δ has been devised by Haldane for the Anderson model[8] for $\Delta\ll U$. The same approach can be followed here, further treating δG_0 in perturbation theory. Because $\delta G_0(\omega+i0^+)$ vanishes as $\omega\to 0$, it only induces *irrelevant terms* in the RG equations. [Equivalently, in an approach like the Anderson-Yuval-Hamman one, $\delta G_0(\tau-\tau')$ is less singular than $1/(\tau-\tau')$, and thus does not contribute to the Coulomb gas charge.] The scaling equations to one-loop order are thus identical to Haldane's, and yield two scaling invariants: Δ and $E_d^*=\varepsilon_d(W)+\Delta/\pi\ln(W/\Delta)$ $[=\varepsilon_0-\mu+\Delta/\pi\ln(U/\Delta)$ at the bare level]. $\varepsilon_d(W)$ increases upon scaling, and thus scaling is effectively towards small U. The low-frequency behavior then obeys all $T=0$ Fermi-liquid requirements, described by Langreth[9] for the Anderson model and recently by Müller-Hartmann[10] in the present context; in particular, $\mathrm{Re}\Sigma(\omega+i0^+)=\Sigma(0)+(1-1/Z)\omega+\cdots$, $\mathrm{Im}\Sigma(\omega+i0^+)=\gamma\omega^2+\cdots$. Luttinger and Ward identities imply that Luttinger theorem is satisfied: $\mu-\Sigma(i0^+)=\mu_0(n)$, where n is the total density of electrons, and $\mu_0(n)=\mathrm{erfc}^{-1}(2-n)$ is the noninteracting chemical potential. Using this in (8) yields the explicit dependence of Δ and ε_0 on density; note furthermore that the low-frequency behavior of the Green's function is unchanged by the interaction. The above proof of the Fermi-liquid nature of the paramagnetic phases of the infinite-dimensional Hubbard model is *not based on perturbation theory in U*, in contrast with previous work;[10] rather, it is based on a perturbation expansion in Δ/U, and therefore can be viewed as an expansion around the atomic limit $U/t\gg 1$ (a RG is needed because this limit is singular). Note that it is based on a single assumption, namely, $\mathrm{Im}\Sigma(i0^+)=0$ and that $\Sigma(i0^+)$ is finite, which is certainly always correct for the paramagnetic solution, except perhaps at half filling, where a nonzero imaginary part might signal a transition to a Mott insulating state for $U>U_c$. Indeed, whether a finite U_c exists should be clarified in future work.

Next, we discuss the various Fermi-liquid regimes resulting from the scaling analysis, together with the finite frequency structure of the $T=0$ one-particle spectral density: $\rho(\omega)=-1/\pi\sum_{\mathbf{k}}\mathrm{Im}G(\mathbf{k},\omega+i0^+)$. Quantitatively, the latter depends on the detailed shape of $\Delta(\varepsilon)$; however, the same qualitative differences between various regimes as for the Anderson model with a structureless $\Delta(\varepsilon)$ are expected here. For very small U (well below the Hartree-Fock instability), $\rho(\omega)$ has a shape close to the noninteracting one $D(\omega+\mu_0)$, with some narrowing of the peak (by the factor $Z<1$), and some of the spectral weight transferred to the tails. [Note that because of (8), $\rho(0)$ remains "pinned" for all U at its noninteracting value,[10] $\rho(0)=D(\mu_0)$]. For larger U, there are three distinct regimes,[8] depending on the ratio of the two scaling invariants.

(i) When $E_d^*/\Delta\ll -1$ (i.e., close to the particle-hole symmetric half-filled case $\mu=-\varepsilon_d=U/2$), $\rho(\omega)$ has a three-peaked structure: a narrow quasiparticle peak (the Abrikosov-Suhl resonance) of width the Kondo temperature T_K, and two "satellite peaks" roughly centered at the position of the two magnetic Hartree-Fock solutions. In the Hubbard model framework, those correspond to the upper Hubbard band for particles and holes, respectively. In this "local moment" regime, the empty state $|0\rangle$ (and, of course, $|\uparrow,\downarrow\rangle$) is almost decoupled, and the single-site dynamics consists of spin fluctuations between $|\uparrow\rangle$ and $|\downarrow\rangle$, with almost frozen charge fluctuations. These spin fluctuations are quenched by the Kondo effect below the Kondo temperature T_K. The quasiparticle residue Z (which is also related here[10] to the effective mass by $m^*/m=1/Z$) is of the order of T_K.

(ii) For $|E_d^*/\Delta|<1$, there is a "mixed-valence" regime with both on-site charge and spin fluctuations (between $|0\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$). $\rho(\omega)$ has two peaks in this regime: a somewhat broadened quasiparticle peak, and the "upper Hubbard band" for $\omega>0$.

(iii) The last regime $E_d^*/\Delta\gg 1$ corresponds to the dilute limit, where a given site is most of the time empty. $\rho(\omega)$ has a broad single peak in this regime, with possibly some shoulder reflecting the transfer of spectral weight to high energy.

We believe (and we have confirmed below by weak-coupling calculations and by the exact solution of the model with a Lorentzian density of states) that for moderate and large U, the paramagnetic solution of the Hubbard model on the square lattice displays all three regimes as the density is varied. μ has a very steep variation with n close to half filling and for U large, and thus the lo-

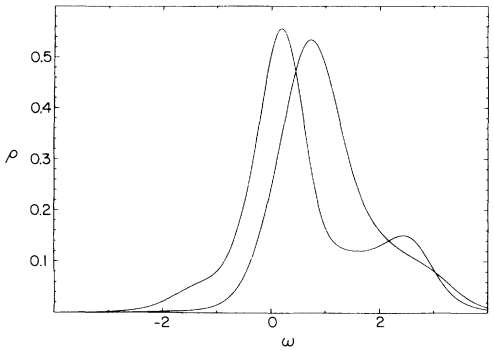

FIG. 1. Local spectral density for $U=2.5$ and densities $n=0.6$, $n=0.2$ (from left to right), obtained by the procedure described in the text.

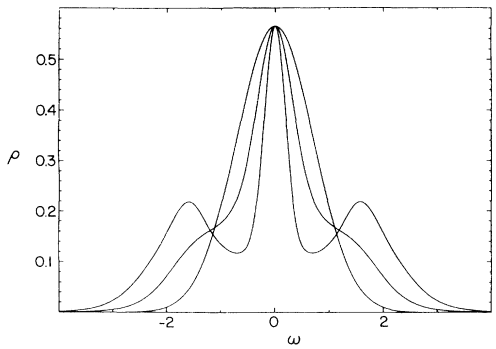

FIG. 2. Local spectral density of the paramagnetic solution at half filling ($n=1$) for $U=0$, $U=1.5$, and $U=2.5$.

cal moment regime for large U is likely to arise only quite close to $n=1$ for large U. Most densities are then in the mixed-valence regime, with the dilute regime setting in roughly near the Hartree-Fock boundary.

Finally, we present results obtained by solving (3)–(5) using second-order perturbation theory for the single-site dynamics (3). A previous weak-coupling study was carried out by Müller-Hartmann,[10] using self-consistent perturbation theory, i.e., inserting the full propagator **G** into the calculation of the second-order proper irreducible self-energy. Our method and results differ significantly from this approach. Indeed, it has been shown by Yosida and Yamada[11] that perturbation theory in U is quite well behaved for the Anderson model, *provided the expansion is made around the nonmagnetic Hartree-Fock solution,* i.e., that $U(n_\uparrow - n/2)(n_\downarrow - n/2)$ is treated as a perturbation. Only this procedure is able to handle correctly the position of the resonance (see Ref. 12 for subsequent work along these lines in the asymmetric case). Thus, given a G_0, we use modified "Hartree-Fock" propagators $G_{\mathrm{HF}}^{-1} = G_0^{-1} - Un/2$ to calculate the second-order correction $\Sigma^{(2)}$ to $\Sigma = Un/2 + \Sigma^{(2)}$. This is then used in (5) to find G, and define an alternate G_0 from $G_0^{-1} = G^{-1} + \Sigma$. The process is iterated numerically until it converges, so that the self-consistency condition (5) is satisfied. The same techniques than in Ref. 10 can be used here to reduce the computation to one-dimensional Fourier transforms, thus making the solution numerically easy. In Figs. 1 and 2, we present some results for the spectral density $\rho(\omega)$: Fig. 1 gives the result for $U=2.5$ and the two densities $n=0.6$ and $n=0.2$, which are clear examples of regimes (ii) and (iii), respectively. For the paramagnetic solution at half filling, the results for $U=0, 1.5, 2.5$ in Fig. 2 clearly show how regime (i) is reached from the weak-coupling side. These results differ considerably from those of Ref. 10, in which a single-peaked structure is always found, together with much larger values of Z close to half filling [the values of Z estimated from the results of Fig. 2 at $n=1$ are $Z(U=1.5)\simeq 0.65$, $Z(U=2.5)\simeq 0.32$]. A very recent work[13] involving bubble and ladder summations gives values much closer to ours for Z, but still fails to reproduce high-energy (Hubbard band) features: We believe that this is a general flaw of fully self-consistent approaches, in contrast to direct perturbation theory. The Hartree shift is responsible for the appearance of the upper-band satellite peaks, as also pointed out recently by Schweitzer and Czycholl at half-filling in a related context [Ref. 14 has results qualitatively close to ours; the effect of satisfying (5) is to push down the upper band to lower energies and to somewhat reduce Z further].

As a conclusion, we believe that the infinite-dimensional Hubbard model provides a very natural mean-field description of strongly correlated Fermi liquids. It captures both the itinerant and atomic aspects and their interplay, which is at the heart of the strong correlation problem. The connection to a single-impurity problem clarifies the analytic structure of the perturbation theory in the weak- and strong-coupling regimes, it explains how the Hubbard bands emerge in the spectral function of the Hubbard model, and suggests useful approximation schemes to extract the essential physics of the Hubbard model in infinite dimensions. The exactly soluble Lorentzian case illustrates in a soluble example how Fermi-liquid theory works in the presence of strong correlations. It also allows us to understand the incoherent regime above the Kondo temperature which is characterized by strong correlations but small mass renormalizations and is dominated by spin fluctuations. The renormalization-group approach to the strong-coupling $d=\infty$ Hubbard model outlined in this paper should allow one to make considerable quantitative progress in the near future: Numerical methods[15] allowing a direct $T=0$ study of impurity models seem very promising in this respect. Magnetic phases should also be a subject of future investigation, as recently done by Brandt and Mielsch for the Falicov-Kimball model. Finally let us emphasize that the above method can also be used to devise *approximations* to finite-dimensional systems [the simplest one being just to replace the Gaussian $D(\varepsilon)$ with the finite-dimensional DOS; see also Ref. 14].

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