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Fermi linearization scheme for itinerant electrons with Clifford variables

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Abstract. We propose an alternative interpretation of the fermi linarization approach to interacting electron systems, based on the requirement that the coefficients of the linearized operators are Clifford-like variables, whose anticommutator equals an unknown constant c. We apply the approximation to the Falicov–Kimball model, explicitly solving the self-consistency equation for the unknown, which turns out to behave as an order parameter. We discuss its relation with a metal–insulator transition and some thermodynamical quantities. In particular we show that our approximation in the $T = 0$ limit reproduces exactly the Gutzwiller results for the Hubbard model.

1. Introduction

Both systems of itinerant interacting electrons on an infinite lattice, and simple systems of a few electrons interacting with bosons, are generally described by Hamiltonians whose dynamical algebra is infinite-dimensional. Various approximation techniques have been developed in order to deal with such systems. In particular, in a set of recent papers [1–3] an approximation scheme was proposed, referred to as a fermionic linearization scheme, which can be applied to a generic many-fermion Hamiltonian. It consists of replacing in the Hamiltonian certain bilinear products of (sums of) electron creation or annihilation operators, say a_1 and a_2, by terms linear in some fermion operator f multiplied by appropriate Grassmann-like coefficients θ,

$$a_1 a_2 + a_2^\dagger a_1^\dagger \sim \theta f + f^\dagger \bar{\theta} \tag{1}$$

where $\{\theta, \bar{\theta}\} = 0$, and $\{\theta, f\} = \{\bar{\theta}, f\} = 0 = \{\theta, a_i\} = \{\bar{\theta}, a_i^\dagger\}$ $(i = 1, 2)$. The anticommutation relations of f and $f^\dagger$ are uniquely determined by a_1 and a_2, and depend on the problem studied. The fact that both the operators f, $f^\dagger$ and the Grassmann coefficients θ, $\bar{\theta}$ satisfy anticommutation relations guarantees that the bilinear products on the right-hand side of (1) have the same 'statistics' of the bilinear operators on the left-hand side.

Once substitution (1) is performed, the scheme allows one to obtain the spectrum of the linearized Hamiltonian—after recognizing that the 'effective' model has a dynamical algebra which is a $\mathbb{Z}_2$-graded algebra—via an inner automorphism of the algebra itself (which generalizes the customary Bogolubov rotation).

In the present note, we propose a new view of the fermionic linearization scheme, which consists of requiring that the variables $\theta, \bar{\theta}$ satisfy a Clifford-like instead of the Grassman-like algebra. More precisely, we set

$$\{\theta, \bar{\theta}\} = c^2 \qquad c \in \mathbb{R} \tag{2}$$

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with c an indeterminate, to be defined for each specific problem. Notice that the requirement (2) on the θs implies that the dynamical algebra of the linearized model is no longer graded, but simply a Lie algebra. In other words, we require that the θs behave as operators rather than anticommuting numbers. Indeed, by inspection of (1) one can easily verify that, in the simple case in which a_1 and a_2 are single-electron operators, and $\{f, f^\dagger\} = 1$, equation (1), with $c = 1$, maps a two-electron operator into another two-electron operator, hence the approximation of the right-hand term of (1) becomes exact. In general, this is not true, and a value of c has to be determined self-consistently according to (1). So the self-consistency equations reconduct the exact results for the linearized model to approximate (mean-field-like) results for the original Hamiltonian.

In the following, we will use this approximation to the solution of the Falicov–Kimball model. The latter gives a very simplified description of a system of itinerant fermions interacting only locally. In this case, prescription (1) is applied to the itinerant part of the Hamiltonian, reducing it to an effective single-site operator, while it leaves unchanged the interaction term. Thus the resulting approximation in principle goes well beyond the standard weak-coupling mean-field theory, and indeed it turns out to be capable of describing a metal–insulator transition.

Let us observe that the approximation (2) was already used in a different context [4] with a fixed value for c, i.e. $c = 1$.

2. The Falicov–Kimball model

The Falicov–Kimball model [5] provides a very simple description of large systems of itinerant interacting fermions, by considering two different species of electrons (say with up and down spin) on a lattice Λ, one of each itinerates on Λ, the electrons with opposite spins being fixed at their sites, and assuming that the electrons interact only via an on-site Coulomb repulsion term. The grand-canonical Hamiltonian reads

$$H_{\mathrm{FK}} = -\mu_n \sum_{\mathbf{i}} N_{\mathbf{i}} - \mu_d \sum_{\mathbf{i}} D_{\mathbf{i}} - 2t \sum_{\langle \mathbf{i},\mathbf{j}\rangle} A_{\mathbf{i}}^\dagger A_{\mathbf{j}} + U \sum_{\mathbf{i}} N_{\mathbf{i}} D_{\mathbf{i}} \qquad (3)$$

where $t > 0$ is the hopping amplitude, and $U > 0$ is the local electron–electron repulsion. $A_{\mathbf{i}}^\dagger, A_{\mathbf{i}}$ are operators which create and annihilate the itinerant electrons ($\{A_{\mathbf{i}}, A_{\mathbf{j}}\} = 0$, $\{A_{\mathbf{i}}^\dagger, A_{\mathbf{j}}\} = \delta_{\mathbf{i},\mathbf{j}}\mathbb{I}$, $N_{\mathbf{i}} \doteq A_{\mathbf{i}}^\dagger A_{\mathbf{i}}$, $\mathbf{i}, \mathbf{j} \in \Lambda$), and $\langle \mathbf{i}, \mathbf{j}\rangle$ stands for non-oriented nearest neighbours (NN) in Λ. Moreover $D_{\mathbf{i}}$ is the number operator of the non-itinerant electrons. As the operators $\sum_{\mathbf{i}} N_{\mathbf{i}}$ and $\sum_{\mathbf{i}} D_{\mathbf{i}}$ both commute with the Hamiltonian, the chemical potentials μ_n and μ_d allow one to fix the average number of electrons of the two species.

The Falicov–Kimball model was introduced for studying the metal–insulator transition in transition metal oxides, and can be considered as a simplified version of the Hubbard model [6]. The exact statistical mechanical solution for the model described by H_{FK} is known only for large dimensions [7]. However, a few general theorems are known [8] for the symmetric (or neutral) case $\mu_n = \mu_d = U/2$, and in particular an Ising-like phase transition is expected for dimension $D \geqslant 2$ at some critical temperature, whose value should vanish both for small and large U. Moreover, there are a number of investigations of the ground-state phase diagram depending on the configuration of fixed spins [9]. Also, a strong-coupling ($U \gg t$) thermodynamic mean-field theory—based on the $D = \infty$ exact solution—was proposed [10].

The fermionic linearization approach [1–3], mentioned in the introduction, also provides a powerful approximation scheme for Hubbard-like models in the strong-coupling limit. In fact it treats in an exact way the Coulomb interaction term, whereas it acts only on the hopping term. Let us write the latter as

$$\sum_{(\mathbf{i},\mathbf{j})} A_{\mathbf{i}}^{\dagger} A_{\mathbf{j}} = \frac{q}{2} \sum_{\mathbf{i}} \left(\Theta_{\mathbf{i}}^{\dagger} A_{\mathbf{i}} + A_{\mathbf{i}}^{\dagger} \Theta_{\mathbf{i}} \right) \tag{4}$$

with $\Theta_{\mathbf{i}} \doteq (1/q) \sum_{\mathbf{j}\mathrm{NN}\mathbf{i}} A_{\mathbf{j}}$, q denoting the number of nearest neighbours of a site in Λ. Of course, the operators $\Theta_{\mathbf{i}}$ have non-trivial anticommutation relations among themselves as well as with the $A_{\mathbf{i}}$s. On the other hand, in [1–3] the $\Theta_{\mathbf{i}}$s were approximated by variables $\theta_{\mathbf{i}}$s anticommuting among themselves as well as with the fermion operators, i.e. $\{\theta_{\mathbf{i}}, \theta_{\mathbf{j}}\} = 0 = \{\bar{\theta}_{\mathbf{i}}, \bar{\theta}_{\mathbf{j}}\}$, $\{\bar{\theta}_{\mathbf{i}}, A_{\mathbf{j}}\} = 0 = \{\theta_{\mathbf{i}}, A_{\mathbf{j}}\}$, $\forall \mathbf{i},\mathbf{j} \in \Lambda$. The former prescription is exact only for $\mathbf{i}$ and $\mathbf{j}$ far enough, depending on the lattice Λ, whereas it is definitely too simple for $\mathbf{i}$ and $\mathbf{j}$ coinciding or having nearest neighbours in common.

Here we propose to improve the fermionic approximation scheme by replacing the operators $\Theta_{\mathbf{i}}$ by variables $\theta_{\mathbf{i}}$ still anticommuting with the fermion operators, and satisfying the following algebra (which is a straightforward generalization of (2))

$$\{\theta_{\mathbf{i}}, \bar{\theta}_{\mathbf{j}}\} = c^2 \delta_{\mathbf{i},\mathbf{j}} \qquad \{\theta_{\mathbf{i}}, \theta_{\mathbf{j}}\} = 0 . \tag{5}$$

Once the above approximation is inserted into (3), one obtains a reduced Hamiltonian $\mathcal{H}_{\mathrm{FK}}$ which is a sum over lattice sites of single-particle Hamiltonians, $\mathcal{H}_{\mathbf{i}}$, commuting with each other:

$$\mathcal{H}_{\mathbf{i}} = -\mu_n N_{\mathbf{i}} - \mu_d D_{\mathbf{i}} - tqc(\bar{\eta}_{\mathbf{i}} A_{\mathbf{i}} + A_{\mathbf{i}}^{\dagger} \eta_{\mathbf{i}}) + U N_{\mathbf{i}} D_{\mathbf{i}} \tag{6}$$

with $\eta_{\mathbf{i}} \doteq \theta_{\mathbf{i}}/c$, so that $\{\bar{\eta}_{\mathbf{i}}, \eta_{\mathbf{j}}\} = \delta_{\mathbf{i},\mathbf{j}}$.

The $D_{\mathbf{i}}$s are to be considered as classical, Ising-like, variables, whose two possible eigenvalues 0 and 1 label two orthogonal projections of $\mathcal{H}_{\mathbf{i}} \doteq \mathcal{H}_{\mathbf{i}}^{(0)} \oplus \mathcal{H}_{\mathbf{i}}^{(1)}$. The problem of finding the spectrum of Hamiltonian (3) is thus reduced, after linearization, to that of diagonalizing the local effective Hamiltonian $\mathcal{H}_{\mathbf{i}}^{(D_{\mathbf{i}})}$. In order to do it, one should first identify the dynamical algebra, $\mathcal{A}$, of (6); it is easily verified that the latter coincides with $u(2)$, generated by

$$\mathcal{A} \equiv u(2) = \left\{ N_{\mathbf{i}} \pm \bar{\eta}_{\mathbf{i}} \eta_{\mathbf{i}} ;\ \bar{\eta}_{\mathbf{i}} A_{\mathbf{i}} \pm A_{\mathbf{i}}^{\dagger} \eta_{\mathbf{i}} \right\} . \tag{7}$$

The transformation which rotates the Hamiltonian into its diagonal form $\tilde{\mathcal{H}}_{\mathrm{FK}}$ is then obtained by acting on $\mathcal{H}_{\mathbf{i}}^{(D_{\mathbf{i}})}$ with

$$\exp(\mathrm{ad}\, Z) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} [Z, [Z, \ldots, [Z, \bullet] \ldots]]$$

where Z is an appropriate skew-Hermitian non-Cartan element of $\mathcal{A}$, $Z = p(\bar{\eta}_{\mathbf{i}} A_{\mathbf{i}} - A_{\mathbf{i}}^{\dagger} \eta_{\mathbf{i}})$. It is easily verified that the choice $p = \tanh^{-1}(2\tau/U D_{\mathbf{i}} - \mu_n)$, with $\tau = cqt$, implies

$$\tilde{\mathcal{H}}_{\mathrm{FK}} = \tfrac{1}{2} [\epsilon_{\mathbf{i}} (\bar{\eta}_{\mathbf{i}} \eta_{\mathbf{i}} + N_{\mathbf{i}}) \pm \sqrt{\epsilon_{\mathbf{i}}^2 + 4\tau^2} (\bar{\eta}_{\mathbf{i}} \eta_{\mathbf{i}} - N_{\mathbf{i}})] - \mu_d D_{\mathbf{i}} \tag{8}$$

with $\epsilon_i \doteq U D_i - \mu_n$; $\tilde{\mathcal{H}}_{FK}$ is manifestly diagonal.

The result (8) is also interesting from the point of view of statistical mechanics, in that the partition function $\mathcal{Z}$ is immediately obtained from (8) as

$$\mathcal{Z} = \sum_{N_i, D_i, \eta_i \eta_i = 0,1} \exp\left(-\beta \tilde{\mathcal{H}}_{FK}\right). \tag{9}$$

Predictions for physical quantities can then be obtained from $\mathcal{Z}$ once the average numbers of electrons of the two species are fixed through the chemical potentials, according to

$$n \doteq \langle N_i \rangle = \frac{1}{\beta \mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \mu_n} \tag{10a}$$

$$d \doteq \langle D_i \rangle = \frac{1}{\beta \mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \mu_d} \tag{10b}$$

where $\langle \bullet \rangle$ denotes the thermodynamical average in the Gibbs ensemble of operator $\bullet$, i.e.

$$\langle \bullet \rangle = \mathcal{Z}^{-1} \sum_{N_i, D_i, \eta\eta = 0,1} \bullet \exp\left(-\beta \mathcal{H}_i^{(D_i)}\right)$$

$$\equiv \mathcal{Z}^{-1} \sum_{N_i, D_i, \eta\eta = 0,1} \exp(\mathrm{ad}Z)(\bullet) \exp\left(-\beta \tilde{\mathcal{H}}_{FK}\right).$$

Moreover, in order to have quantitative predictions, a numerical value for c still has to be self-consistently determined. Indeed, the prescription of substituting in the hopping term the Θ_i operators with the θ_is can be implemented once more in (4), giving rise to the self-consistency equation

$$\langle \bar{\eta} A_i + A_i^{\dagger} \eta \rangle = 2c \langle \bar{\eta} \eta \rangle \tag{11}$$

in which we have assumed translational invariance of the lattice, implying $\eta_i \equiv \eta, \forall i \in \Lambda$.

The three equations (10*a*), (10*b*), and (11) have interesting features. First of all, we notice that (10*b*) can be solved explicitly for μ_d, and gives the result

$$\exp \beta \mu_d = \frac{d}{1-d} \frac{1 + e^{\beta \mu_n} + 2e^{\beta \mu_n / 2} \cosh \frac{1}{2} \beta \sqrt{\mu_n^2 + 4\tau^2}}{1 + e^{\beta(\mu_n - U)} + 2e^{\beta(\mu_n - U)/2} \cosh \frac{1}{2} \beta \sqrt{(\mu_n - U)^2 + 4\tau^2}}. \tag{12}$$

Moreover, it is easy to check that (11) always factorizes a solution $c = 0$, which correspond to the insulating behaviour. Besides this solution, in general the system formed by (10*a*)–(11), with μ_d given by (12), is highly nonlinear, and must be dealt with numerically. It turns out that it has different non-zero solutions. The physical one is to be chosen as that which minimizes the Gibbs free energy f, $f = -(1/\beta) \ln Z$. In the next section we shall discuss the results of the numerical analysis, as well as the analytical results which can be obtained in some limiting cases.

3. Results and discussion

In figure 1 we report the mean-field parameter c versus temperature kT/qt, at half-filling and for the symmetric case $n = d = \frac{1}{2}$. In this case it is easy to check that the solution to (10.1)–(10.2) is $\mu_n = \mu_d = U/2$. c is plotted for different U values, and exhibits a typical order-parameter-like behaviour. For $U = 0$ (non-interacting case) it rises from zero, in the high-temperature regime, to 1, at $T = 0$. For generic $U \leqslant 4qt$, it is possible to show rigorously that, in the limit $T \to 0$, c reaches a value c_0 given by

$$c_0^2 = 1 - \tfrac{1}{16}\tilde{U}^2 \tag{13}$$

where $\tilde{U} \doteq U/qt$. This suggests that the value $c = 1$ used in [4] is correct at half-filling, only in a low-temperature non-interacting regime or for $D = \infty$. On the contrary, for $U > 4qt$, the only solution to (11) is $c = 0$.

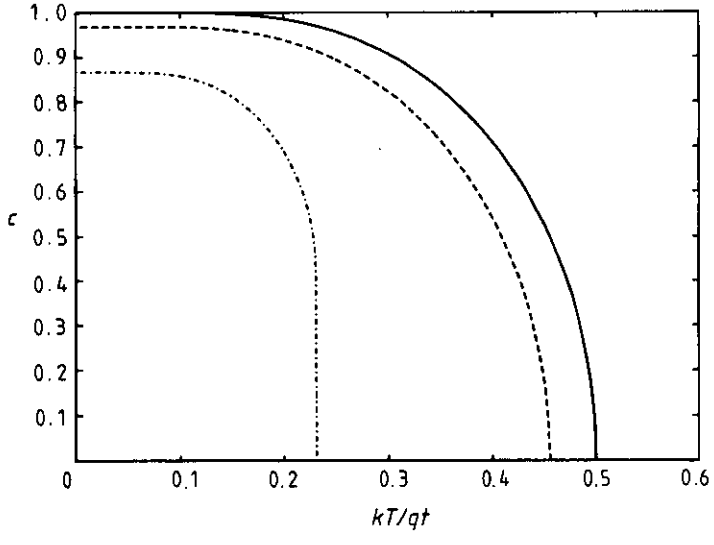

Figure 1. c versus kT/qt at different $\tilde{U}$ values: $\tilde{U} = 0$ (full curve), $\tilde{U} = 1$ (broken curve), $\tilde{U} = 2$ (chain curve).

The expression (13) for c_0 clarifies the physical meaning of the parameter c. Indeed, recalling that on a hypercubic lattice q is twice the dimension of the lattice, (13) reproduces exactly the Gutzwiller result [11] for the discontinuity in the single-particle occupation number at the Fermi surface, obtained for the conventional Hubbard model when $T = 0$. This is not surprising as, on the one hand, the Gutzwiller result for the Hubbard model was in fact obtained by neglecting the kinetic energy of one species of electron, thus in an approximation very similar to that at the basis of the Falicov–Kimball model. On the other hand, according to (4), (5), and (11), at half-filling c coincides with the expectation value of the hopping term, and hence is related to the discontinuity in its Fourier transform.

Notice that when $U = 0$, $c_0 = 1$, and the ground state has all the electrons below the Fermi level. For any $c \neq 0$, the ground state has some electrons above the Fermi

level, but the gap is still there, and, according to (5), the generic lattice site on which one has confined the linearized Hamiltonian is still interchanging fermions with the rest of the lattice. When $c_0 = 0$, on the other hand, the gap in the density of states disappears, and at half-filling we have exactly one electron per site. In this case, the remaining part of the lattice behaves as a system of correlated 'average' fermions (i.e. as if they were frozen at their own sites) and we are in presence of an insulating phase.

The above analysis suggests that c may be able to describe the transition from a conducting to an insulating state. Indeed, again in agreement with the Gutzwiller result, at $T = 0$ we find that the double occupancy expectation value, $\mathcal{P} \doteq \langle N_\uparrow D_\downarrow \rangle$, vanishes precisely at $\tilde{U} = 4$. Explicitly, analytic calculation shows that

$$\mathcal{P} = \begin{cases} \frac{1}{4}\left(1 - \frac{\tilde{U}}{4}\right) & \text{for } \tilde{U} \leqslant 4 \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

It is worth noticing that the result (14) coincides with the exact result both in the limit $\tilde{U} = 0$ and in the limit $\tilde{U} \gg 1$.

A deeper analysis of figure 1 shows that the transition from non-zero to vanishing c is of different order depending on the value of $\tilde{U}$. Indeed, by requiring that (11) also vanishes around $|c| = 0$, one can verify that there exists a tri-critical point at $\tilde{U} = U_t$, where U_t is solution of

$$\tanh \frac{U_t}{2(1 - U_t^2/8)} = \frac{U_t}{2}. \tag{15}$$

One finds a numerical value $U_t \simeq 1.845$. For $\tilde{U}$ smaller than U_t the transition is second order, and the critical temperature is found analytically as the solution T_c of the following equation (obtained by requiring that (11), upon factorizing the $c = 0$ solution, still vanishes for $c = 0$):

$$\tanh \frac{\tilde{U}}{4\Theta_c} = \frac{\tilde{U}}{2} \tag{16}$$

with $\Theta_c \doteq kT_c/qt$, and k the Boltzmann constant. On the other hand, when $\tilde{U}$ is larger than U_t, the transition is first order, and the critical temperature can be evaluated numerically. Figure 2 shows the behaviour of T_c versus $\tilde{U}$ in the two regions. The value $\tilde{U} = 4$ correspond to the vanishing of both the critical temperature and c_0.

Figure 2 can be compared with the rough estimate of the critical temperature of the long-range order phase whose existence is proved for the Falicov–Kimball model in [8]. If one assumes that the phase with $c \neq 0$ could possibly be the long-range ordered phase, the qualitative behaviour of T_c is in agreement with that given by Kennedy and Lieb for large U, whereas it is in contrast with the latter for vanishing U. One should notice however that our approximation is expected to be more realistic for finite U.

Finally, in figure 3 we give the behaviour of c versus T for various fillings, still for a symmetric state ($n = d$). The figure shows that the transition is present at different fillings, again in agreement with the features of the long-range ordered phase described in [8].

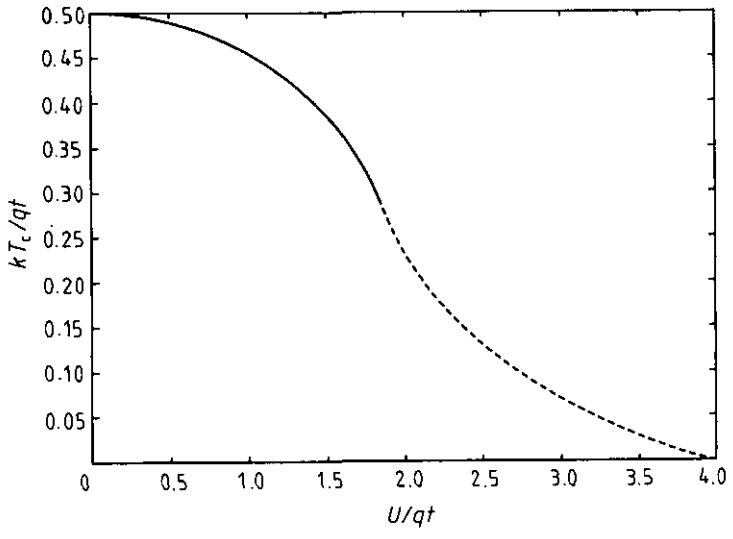

Figure 2. kT_c/qt versus $\tilde{U}$: full curve represents second order transition; broken curve, first order transition.

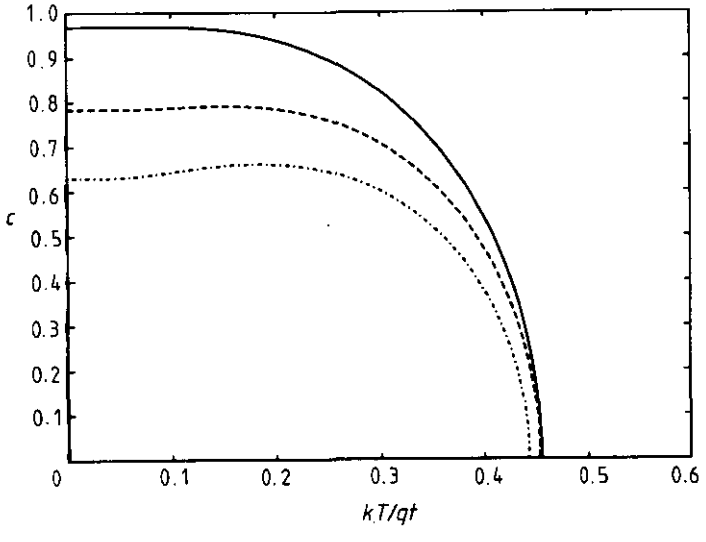

Figure 3. c versus kT/qt at $\tilde{U} = 1$ and different fillings, in the neutral case ($n = d$): $n + d = 1$ (full curve), $n + d = 0.8$ (broken curve), $n + d = 0.6$ (chain curve).

4. Conclusions

In this paper we have proposed an improvement of the Fermi linearization technique for electron systems, based on the requirement that the coefficients of the linearized operators are Clifford-like variables, with their anticommutator equal to an unknown constant c. As an example, we applied such a method to the Falicov–Kimball model, also giving the self-consistency equation which determines the unknown. The latter

turned out to behave as a true order parameter, which at $T = 0$ and at half-filling was shown to coincide with the discontinuity in the single-particle occupation number at the Fermi level in the Gutzwiller approximation to the Hubbard model. The behaviour of c was thus related to the existence of a metal–insulator transition, which again was shown to coincide at $T = 0$ with that hypothesized by Brinkman and Rice [12].

The above results suggest that our approximation could be a natural extension of the Gutzwiller approach to the case $T \neq 0$. They also provide a physical interpretation to the method, which consists of replacing the hopping term by a term which locally still allows the creation and annihilation of electrons, but with an amplitude proportional to the discontinuity in the single-particle average number at the Fermi surface.

Moreover, contrary to the case in which the coefficients of the linearized operators were Grassmann variables, the present approximation produces non-trivial results even in the case $U = 0$.

This paper was intended as a presentation of the method, and little effort was devoted to the numerical results in the various cases. Nevertheless, in view of the promising results obtained, work is in progress in order both to provide a complete phase space at $T = 0$ and to discuss the $T \neq 0$ behaviour of the physical quantities. We also expect that in this case the use of a cluster Bethe version of our approximation [3] should give more accurate quantitative results.

Finally, let us stress that the method is of further generality. In particular, we expect that it can be straightforwardly applied to the conventional Hubbard model, as well as to generalized Hubbard models which have been proposed for the study of high-T_c superconductivity.

Acknowledgments

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