# Gapless metallic charge-density-wave phase driven by strong electron correlations

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We analyze the transformation from insulator to metal induced by thermal fluctuations within the Falicov-Kimball model. Using the dynamic mean field theory (DMFT) formalism on the Bethe lattice we find rigorously the temperature dependent density of states (DOS) at half filling in the limit of high dimensions. At zero temperature ($T = 0$) the system is ordered to form the checkerboard pattern and the DOS has the gap $\Delta$ at the Fermi level $\varepsilon_F = 0$, which is proportional to the interaction constant $U$. With an increase of $T$ the DOS evolves in various ways that depend on $U$. For $U > U_{cr}$ the gap persists for any $T$ (then $\Delta > 0$), so the system is always an insulator. However, if $U < U_{cr}$, two additional subbands develop inside the gap. They become wider with increasing $T$ and at a certain $U$-dependent temperature $T_{MI}$ they join with each other at $\varepsilon_F$. Since above $T_{MI}$ the DOS is positive at $\varepsilon_F$, we interpret $T_{MI}$ as the transformation temperature from insulator to metal. It appears that $T_{MI}$ approaches the order-disorder phase transition temperature $T_{\text{O-DO}}$ when $U$ is close to 0 or $U_{cr}$, but $T_{MI}$ is substantially lower than $T_{\text{O-DO}}$ for intermediate values of $U$. Moreover, using an analytical formula we show that $T_{MI} = 0$ at $U = \sqrt{2} < U_{cr}$, so we prove that the quantum critical point exists for the ordered metal at ($T = 0$, $U = \sqrt{2}$). Having calculated the temperature dependent DOS we study thermodynamic properties of the system starting from its free energy $F$. Then we find how the order parameter $d$ and the gap $\Delta$ change with $T$ and we construct the phase diagram in the variables $T$ and $U$, where we display regions of stability of four different phases: ordered insulator, ordered metal, disordered insulator, and disordered metal. Finally, we use a low temperature expansion to demonstrate the existence of a nonzero DOS at a characteristic value of $U$ on a general bipartite lattice.

## I. INTRODUCTION

One of the most successful methods for describing strongly correlated electron systems is the dynamical mean-field theory (DMFT) [1,2]. This formalism appears to be particularly useful in studying the Falicov-Kimball model (FKM) [3], as it enables us to get analytical, or high precision numerical results, which become exact in the limit of large dimensions. Most of the findings have been obtained in the high-temperature homogeneous phase [1], but the ordered phase was also considered in a few papers [2,4–11]. The results presented in these papers are remarkable, as they give a clear evidence that the static mean field theory is not an adequate tool for describing correlated electron systems. Indeed, physical quantities obtained using the static and dynamic mean field approach are substantially different one from another. This discrepancy is particularly clearly demonstrated by Hassan and Krishnamurthy [10], and by Matveev, Shvaika, and Freericks [11]. Both teams analyzed the spinless FKM at half filling in the ordered charge-density-wave (CDW) phase having the form of the checkerboard phase. Hassan and Krisnamurthy [10] considered the square lattice and the Bethe lattice in the limit of infinite dimension and focused mostly on spectral properties, whereas Matveev, Shvaika, and Freericks [11] examined the hypercubic lattice in the limit of high dimensions and focused mainly on transport properties. It is quite interesting that even though these studies were performed on different lattices, they lead to similar spectral properties of the model. Namely, in all the cases the energy spectrum has a gap at the Fermi level at $T = 0$ and with an increase of $T$ two

additional subbands develop inside the gap in such a way, that the density of states (DOS) at the Fermi level becomes positive still in the ordered phase (above a certain temperature $T_{MI}$), i.e. below the order-disorder transition temperature $T_{\text{O-DO}}$. In fact, the energy subbands developing inside the gap in the ordered checkerboard phase were already noticed by Freericks and Zlatić [2]. Here it is noteworthy that the Monte Carlo calculations performed on the 2D systems also give results similar to those obtained within DMFT [12,13].

On the other hand, the data based on the static mean field theory calculations show that the gap disappears only at $T_{\text{O-DO}}$ [14]. Indeed, according to a conventional mean field theory this gap gradually diminishes with an increase of temperature, but still persists until the CDW phase exists, i.e., until the order-disorder (O-DO) phase transition temperature $T_{\text{O-DO}}$ is reached [14]. Surprisingly, the same conclusion was also formulated by van Dongen, who studied the FKM on the Bethe lattice using a different variant of DMFT [5,6]. In fact, van Dongen derived analytical formulas on the temperature Green functions in the ordered phase, but he analyzed them only in the limiting cases of small and large coupling parameter $U$. Since in these two limits the gap is always present in the ordered phase, he concluded that it exists for any $U$. However this is in contradiction to the results reported in Refs. [10,11].

Since the demonstration of the existence of the gapless ordered phase in Refs. [10,11] is quite surprising, in this contribution we develop studies of the subject. Our purpose is to perform a more detailed analysis of spectral properties of the system, focusing mainly on intermediate values of the

parameter $U$. Following the approach derived by van Dongen [5] we perform nonperturbative calculations that allow us to reconstruct in a simple way the data obtained by Hassan and Krisnamurthy [10] and to get analytical expressions for some different characteristics of the spectrum. Our analytical calculations, which expand the results obtained by Hassan and Krisnamurthy [10], give proof of the existence of the quantum critical point at $U = \sqrt{2}$. In addition, we calculate the internal energy as a function of $T$ and show that it behaves smoothly without any noticeable kink around the temperature $T_{MI}$ of metal-insulator (MI) transformation. Hence, we conclude that the transformation is not a phase transition in the usual sense.

Our analysis of the single electron energy spectrum of the spinless FKM is based on exact formulas for the temperature-dependent DOS $\rho(\varepsilon)$ derived for the Bethe lattice within a version of the DMFT formalism derived by van Dongen [5,6]. There are two types of localized particles $A$ and $B$ in the system, whose densities $\rho_A$ and $\rho_B$, respectively, are equal to each other and equal to 1/2, ($\rho_A = \rho_B = 1/2$) and spinless electrons. The localized particles may correspond, for example, to two different components of an alloy. We focus on the half-filling case, when the density of electrons $\rho_d = 1/2$. Then the ground state has the checkerboard-type structure composed of two interpenetrating sublattices $+$ and $-$, each of which is occupied only by one type of particle: the sublattice $+$ by $A$ particles and the sublattice $-$ by $B$ particles, respectively. Consequently, the density $\rho_A^+(\rho_B^-)$ of particles $A(B)$ on the sublattice $+(-)$ is equal to 1 ($\rho_A^+ = \rho_B^- = 1$), whereas the density $\rho_B^+(\rho_A^-)$ of particles $B(A)$ on the sublattice $+(-)$ is equal to 0 ($\rho_B^+ = \rho_A^- = 0$).

With an increase of temperature the densities $\rho_A^+$, $\rho_B^-$ ($\rho_A^+ = \rho_B^-$) diminish below 1, while $\rho_B^+$, $\rho_A^-$ ($\rho_B^+ = \rho_A^-$) increase above 0, and in the disordered phase all these densities are equal to 1/2. Then the quantity $d = \rho_A^+ - \rho_B^+ = \rho_B^- - \rho_A^-$ is equal to 1 at $T = 0$ and equal to 0 in the high-temperature disordered phase, thus it is chosen to be the order parameter. It turns out that changes of $d$ cause significant changes in the DOS. In particular, some energy states appear within the energy gap if $0 < d < 1$. If it happens around the Fermi level, it corresponds to the MI transformation.

In fact, the DOS depends explicitly on the order parameter $d$ and its temperature dependence comes out entirely from the temperature dependence of $d$. Consequently, the order parameter $d(U;T)$ and the DOS $\rho(U,T;\varepsilon)$ are determined self consistently from the following procedure. First we determine the $d$-dependent DOS $\rho(U,d;\varepsilon)$ and from that the free energy $F(U,d;T)$. Next we find the temperature dependence of the order parameter $d(U;T)$ from minimization of $F(U,d;T)$ over $d$. Then, we find the temperature dependent DOS $\rho(U,T;\varepsilon)$ by inserting $d(U;T)$ into $\rho(U,d;\varepsilon)$. Finally we calculate the internal energy $E(U,T)$, the energy gap $\Delta(U;T)$, and the value of DOS at the Fermi level $\rho(U,T;\varepsilon_F = 0)$.

The Hamiltonian we use is (see Ref. [7])

$$H = t \sum_{\langle m,n \rangle} d_m^+ d_n + U \sum_m w_m n_m^d \qquad (1)$$

where $\langle m,n \rangle$ means the nearest neighbor lattice sites $m$ and $n$, $d_m(d_m^+)$ is an annihilation(creation) operator of itinerant electrons, whereas $n_m^d$ is their particle number operator. The

quantity $w_m$ is equal to $1/2(-1/2)$ for the lattice site occupied by the particle A(B), so the Coulomb-type on-site interaction between itinerant electrons and the localized particles amounts to $U/2(-U/2)$. The hopping electron amplitude $t$ we henceforth set equal to one for our energy scale. We suppose that our results should be relevant to various experimental systems that display charge density or magnetic order such as for example $BaBiO_3$, $Ba_{1-x}K_xBiO_3$ (see Ref. [11] and the citations given therein), or perovskite compounds $Ca(Mn_{3-x}Cu_x)Mn_4O_{12}$ and $TbBaCo_{2-x}Fe_xO_{5+\delta}$ [15,16].

In the next section we provide a detailed analysis of the DOS as a function of $d$ and $U$ and in Sec. III we show the temperature dependence of the DOS. In Sec. III we also discuss the relationship between the O-DO and MI transformations and present the phase diagram of the system. Then the existence of a nonzero DOS at a characteristic value of $U$ is derived within a low temperature expansion on a general bipartite lattice (Sec. IV). Finally, the last section contains some concluding remarks on our findings and a summary.

## II. DENSITY OF STATES (DOS)

All physical properties analyzed in this paper are derived from $\rho(U,d;\varepsilon)$ calculated from the Laplace transformation of the retarded Green function $G(U,d;\varepsilon)$ defined for complex $z$ with $\text{Im}(z) > 0$ using the standard formula

$$\rho(U,d;\varepsilon) = -\frac{1}{\pi}\text{Im}G(U,d;\varepsilon + i0). \qquad (2)$$

In the remainder of this paper we will sometimes use simplified notations $G$ or $G(\epsilon)$ instead of $G(U,d;\epsilon)$ and $\rho(\epsilon)$ instead of $\rho(U,d;\epsilon)$, respectively.

For the two sublattice system one has

$$G(\varepsilon) = G^+(\varepsilon) + G^-(\varepsilon), \qquad (3)$$

where the corresponding system of two equations for Green functions $G^+(z)$ and $G^-(z)$ on the Bethe lattice reported by van Dongen [5] is as follows:

$$G^+(z) = \frac{z + \frac{1}{2}Ud - G^-(z)}{[z + \frac{1}{2}U - G^-(z)][z - \frac{1}{2}U - G^-(z)]}$$

$$G^-(z) = \frac{z - \frac{1}{2}Ud - G^+(z)}{[z + \frac{1}{2}U - G^+(z)][z - \frac{1}{2}U - G^+(z)]}. \qquad (4)$$

At zero temperature $d = 1$, so the system of equations (4) reduces to the following simple form:

$$G^+(z) = \frac{1}{z - \frac{1}{2}U - G^-(z)}$$

$$G^-(z) = \frac{1}{z + \frac{1}{2}U - G^+(z)}, \qquad (5)$$

and the Green functions are expressed by the analytical formulas

$$G^+(z) = \frac{4z^2 - U^2 - \sqrt{(4z^2 - U^2)(4z^2 - U^2 - 16)}}{4(2z - U)}$$

$$G^-(z) = \frac{4z^2 - U^2 - \sqrt{(4z^2 - U^2)(4z^2 - U^2 - 16)}}{4(2z + U)}. \qquad (6)$$

It comes out from Eq. (6) that the imaginary parts of $G^+(z)$ and $G^-(z)$, so the DOS, have nonzero values within the intervals $-(\sqrt{U^2 + 16})/2 < \varepsilon < -U/2$ and $U/2 < \varepsilon < (\sqrt{U^2 + 16})/2$. Then the energy gap at the Fermi level is equal to $U$. Consequently, for any nonzero $U$ the system is an insulator at zero temperature.

The situation is quite different at high temperatures, when the system is in a disordered, homogeneous state. In this case $d = 0$, so $G^+(z) = G^-(z) = G(z)$ and the system of equations (4) reduces to one polynomial equation of third rank [Eq. (7)] on $G(z)$. In fact, Eq. (7) was first derived and analyzed already by Hubbard in his alloy analogy paper [17] (within the Hubbard-III-approximation of the Hubbard model). Then it was re-derived by Velicky *et al.* [18] and later on by van Dongen and Leinung [6]. Here we rewrite it in the following form:

$$G^3 - 2zG^2 + (1 + z^2 - U^2/4)G - z = 0. \qquad (7)$$

The Eq. (7) has nontrivial analytic solutions that are significantly different for small and large $U$. Consequently, for $U < U_{cr} = 2$ there is no gap in the electronic energy spectrum, whereas for $U > U_{cr} = 2$ there is the finite gap at the Fermi level that increases with $U$. So the system is a conductor when $U$ is smaller than the critical value $U_{cr} = 2$, otherwise it is an insulator.

In Fig. 1 we display the DOS in the ordered phase at $T = 0$ (left column) and in the disordered phase (right column) for a few representative values of $U$. It comes out that for $U > U_{cr} = 2$ the energy gap at the Fermi level persists in the disordered phase, then the system is an insulator. On the other hand, for $U < U_{cr}$ the gap disappears in the high-temperature phase, so the order-disorder phase transition is accompanied by the insulator-metal transformation. However, it turns out that temperatures where these two transformations occur are usually different.

The natural question that now arises is how the DOS evolves with temperatures starting from $T = 0$ and ending at high temperature, where the system is in the disordered phase. As we mentioned in the Introduction, preliminary studies of the DOS for the ordered phase at finite temperatures were already reported in the review paper by Freericks and Zlatic [2]. Then this problem was examined by Hassan and Krishnamurthy [10] and independently by Matveew, Shvaika, and Freericks [11]. In all these papers the authors calculated $\rho(\varepsilon)$ numerically by finding a self-consistent solution of a set of few nonlinear equations [2]. Here we get similar results using a simpler method that also allows us to get analytical expressions on some physically relevant quantities, as it is shown further in this paper. Namely, we solve the system of equations (4) for arbitrary $d$ and then we calculate $\rho(\varepsilon)$ from equations (2) and (3). In fact, the system of equations (4) reduces to the polynomial equation of fifth rank on $G^+(z)$ [see Eq. (8)] or $G^-(z)$ [not displayed, but knowing $G^+(z)$ one can find $G^-(z)$ from (4)]:

$$a_0 + a_1 G^+ + a_2 (G^+)^2 + a_3 (G^+)^3 + a_4 (G^+)^4 + a_5 (G^+)^5 = 0. \qquad (8)$$

The coefficients $a_0$, $a_1$, $a_2$, $a_3$, $a_4$, $a_5$ are functions of $z$, $U$, and $d$. Since the expressions on these coefficients are rather lengthy, we put them into Appendix A. One can easily check that for $d = 1$ Eq. (8) factorizes to the following form:

$$(U - 2z + 2G^+)^2 [4 - (2z + U)^2 + 2(2z + U)G^+]$$
$$\times [2(2z + U) + (U^2 - 4z^2)G^+ + 2(2z - U)(G^+)^2] = 0, \qquad (9)$$

from which the upper part of Eq. (6) can be derived. On the other hand, if $d = 0$ then Eq. (8) factorizes to the form

$$16[-z + (1 + z^2 - U^2/4)G^+ - 2z(G^+)^2 + (G^+)^3]$$
$$\times (-4z^2 + 4z^4 + U^2 - 2z^2 U^2 + U^4/4$$
$$+ (4z - 8z^3 + 2zU^2)G^+ + (4z^2 - U^2)(G^+)^2), \qquad (10)$$

from which Eq. (7) can be obtained.

In a general case of arbitrary $d$ Eq. (8) does not factorize, so one needs to solve it numerically, but with a very high precision. The resulting DOS is displayed in Fig. 2 for $U = 0.8$ and a set of $d$ values, and in Fig. 3 for $d = 0.95$ and a set of $U$ values. By viewing Fig. 2 one can see how $\rho(\varepsilon)$ evolves when the system undergoes the MI transformation, and by viewing
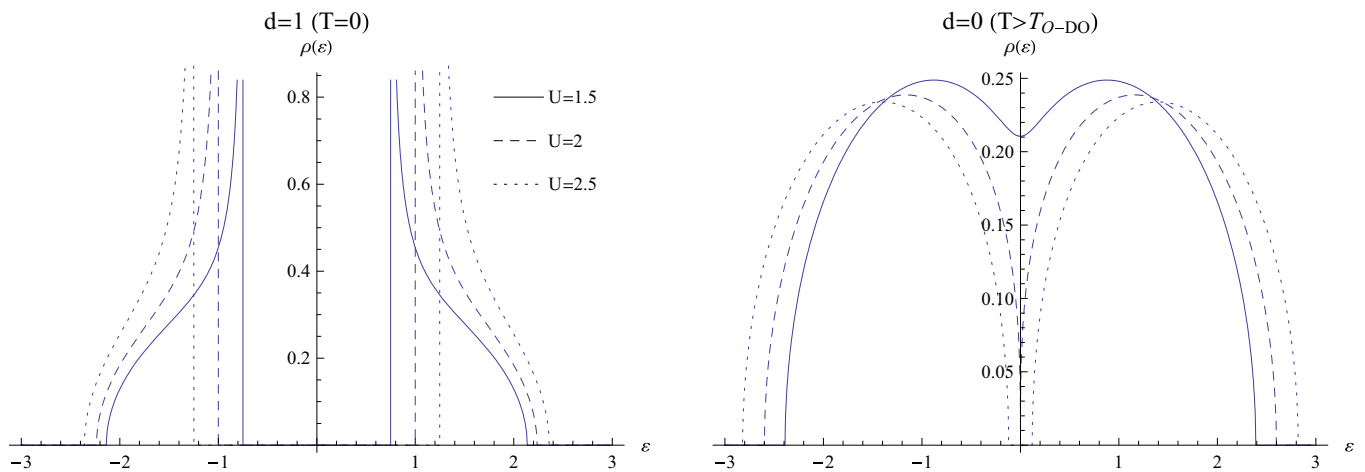


d=1 (T=0)

$\rho(\varepsilon)$

d=0 (T>$T_{O-DO}$)

$\rho(\varepsilon)$

FIG. 1. (Color online) DOS in the fully ordered phase ($d = 1$) at $T = 0$ (left panel) and in the disordered phase ($d = 0$) at $T > T_{\text{O-DO}}$ (right panel) for $U = 1.5$ (the solid lines), $U = 2$ (the dashed lines) and $U = 2.5$ (the dotted lines), respectively.
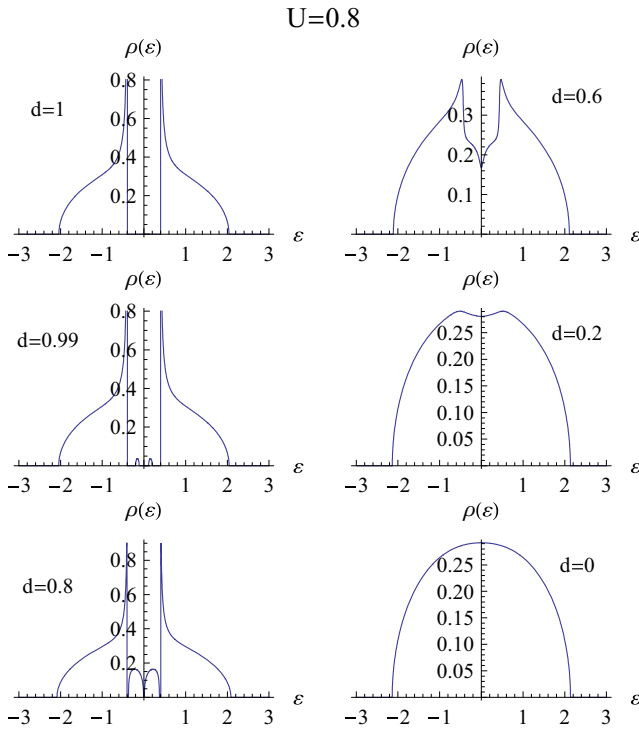
FIG. 2. (Color online) Evolution of the DOS with a change of the order parameter $d$ from the fully ordered phase at $T = 0$ ($d = 1$) to the high-temperature disordered phase ($d = 0$) for $U = 0.8$. In this case the insulator-metal transformation occurs in the system (at $d = 4\sqrt{21}/25 \approx 0.733$).
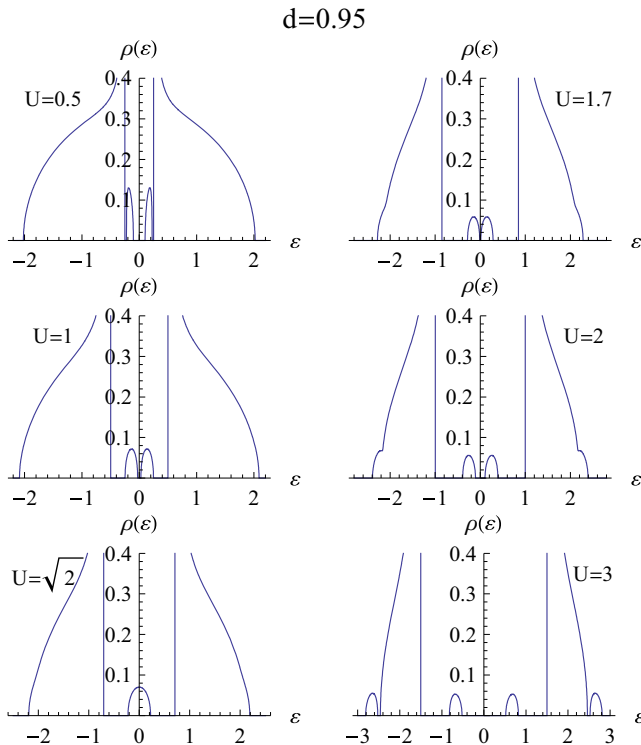


FIG. 3. (Color online)  Evolution of the DOS with $U$ for the fixed value of the order parameter $d = 0.95$.

Fig. 3 one can notice how the process of filling in the gap starts up when the order parameter $d$ begins to be less than one. It appears that our results, part of which are analytical, confirm numerical findings reported in Refs. [10,11]. In particular, there is a filling of the gap that occurs due to two additional subbands developing inside the gap. These additional subbands are located symmetrically with respect to the Fermi level and their initial positions depend on $U$ (for $d$ just below 1). With a decrease of $d$ the width of the subbands increases, and they merge together to form one band at a certain value $d_{\text{crit}}(U)$, if $0 \leqslant U < U_{cr} = 2$.

As we already mentioned before, this filling is quite surprising, since it is completely different from the expectations based on the conventional mean field theory [14]. Indeed, according to this theory the process of closing the gap is due to gradual increase in the width of two DOS subbands: one lying just below and the other just above the Fermi level. As a result, the upper edge of the valency band and the lower edge of the conduction band converge to each other if, and only if, $d = 0$.

From our calculations it was easy to obtain a simple analytical formula for DOS at the Fermi level $\rho(\varepsilon = \varepsilon_F)$ as a function of $U$ and $d$. Indeed, it appears that at this special point the polynomial in Eq. (8) factorizes, so that Eq. (8) has the following simple form:

$$U(4G^+ - 4(G^+)^3 + 2dU + G^+U^2)$$
$$\times (8dG^+ + 4U + 4(G^+)^2U - U^3) = 0. \quad (11)$$

Then Eq. (11) can be solved analytically and the resulting DOS is as follows:

$$\rho(\varepsilon_F) \equiv \rho(U,T; \varepsilon = \varepsilon_F) = \frac{1}{\pi} \text{Im} \left( \frac{\sqrt{4d^2 - 4U^2 + U^4}}{2U} \right). \quad (12)$$

Hence it follows that inside the whole interval $0 < U < 2$ the system is metallic (i.e., $\rho(\varepsilon_F) > 0$) not only in the disordered phase where $d = 0$ [then $\rho(\varepsilon_F) = \frac{\sqrt{4-U^2}}{2\pi}$], but also in the ordered phase, if only $d < d_{\text{crit}}(U) = \frac{U}{2}\sqrt{4 - U^2}$. Moreover, at $U = \sqrt{2}$ the maximum value $d_{\text{crit}}(U) = 1$ is attained, so the system is then metallic even for $d$ infinitesimally close to the limit $d = 1$, that corresponds to the fully ordered phase at $T = 0$.

Having the formula for DOS derived from the system of equations (4) we are also able to analyze the insulating phase characterized by its energy gap at the Fermi level $\Delta(\varepsilon_F)$ [then obviously $\rho(\varepsilon_F) = 0$]. If $U \geqslant 2$ the system is an insulator both in the disordered and ordered phase for any $d$. On the other hand, if $0 < U < 2$, then it is an insulator only for $d_{\text{crit}}(U) \leqslant d \leqslant 1$. As we already mentioned before, at $T = 0$, i.e., in the fully ordered phase ($d = 1$) one has $\Delta(\varepsilon_F)(U) = U$. However, $\Delta(\varepsilon_F)$ is not a continuous function of $d$ at $d = 1$ due to the appearance of the subgap bands for $d = 1 - 0^+$. Indeed, when $d < 1$ and $d \to 1$ (i.e., $T = 0^+$) we got the following analytical formula

$$\Delta(\varepsilon_F) = \left| \frac{\sqrt{1 + 4U^2} - U^2 - 1}{U} \right|, \quad d \to 1 \ (d < 1) \quad (13)$$
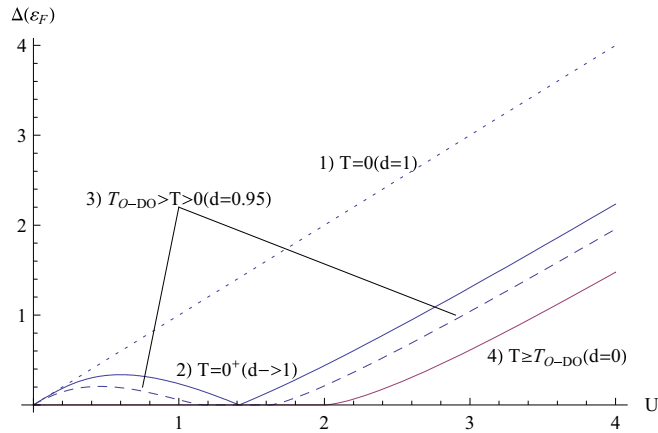
FIG. 4. (Color online) Energy gap $\Delta(\varepsilon_F)$ at the Fermi level as a function of U for a few fixed values of the order parameter $d$.
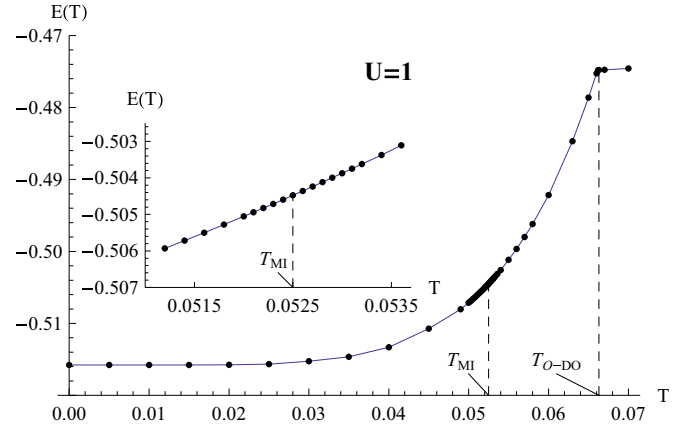


FIG. 5. (Color online) Internal energy $E(U,T)$ as a function of $T$ for $U = 1$. The temperature interval close to $T_{MI}$ is displayed in the inset. Drawn lines are guides to the eye.

and also the analytical expression for $d = 0$ ($T > T_{\text{O-DO}}$) [see Eq. (14)]:

$$\Delta(\varepsilon_F) = \begin{cases} 0 & \text{for } d = 0, U < 2 \\ \sqrt{10 + U^2 - 2\frac{1+\sqrt{(1+2U^2)^3}}{U^2}} & \text{for } d = 0, U > 2 \end{cases}.$$

(14)

In Fig. 4 we display how the energy gaps $\Delta(\varepsilon_F)$ change with $U$ for a set of a few fixed values of $d$. At $T = 0$ ($d = 1$) $\Delta(\varepsilon_F)(U)$ is represented by the straight dotted line $\Delta(\varepsilon_F)(U) = U$. However, for $d < 1$, but $d$ being infinitesimally close to 1 the function $\Delta(\varepsilon_F)(U)$ behaves nonmonotonically. Starting from zero at $U = 0$ it first increases, attains its local maximum equal to $\frac{4\sqrt{18-2\sqrt{17}}+\sqrt{17}-15}{2\sqrt{14-2\sqrt{17}}} \approx 0.33675$ at $U = \frac{\sqrt{\frac{7-\sqrt{17}}{2}}}{2} \approx 0.6$, and then goes down to 0 at $U = \sqrt{2}$. In the opposite limit of the homogeneous phase ($d = 0$) one has $\Delta(\varepsilon_F)(U) = 0$ for $U \leqslant 2$ and the curve $\Delta(\varepsilon_F)(U)$ starts to rise up for $U \geqslant 2$ according to the formula (14). The behavior of $\Delta(\varepsilon_F)(U)$ between these two limits is represented in Fig. 4 for $d = 0.95$ by the dashed line.

Note also that when $U \to 0$, from the formula (13) one has $\Delta(\varepsilon_F) \to |U|$, and when $U \to \infty$, from (14) one gets $\Delta(\varepsilon_F) \to |U| - 2$. This is why the exact analytical calculations performed in the limiting cases of small and large $U$ by van Dongen [5] could not detect the gapless checkerboard phase.

## III. ORDER-DISORDER VERSUS INSULATOR-METAL TRANSITION

Having calculated $\rho(U,d;\varepsilon)$ we can determine the free energy functional using the formula (see Refs. [19,20])

$$F(U,d,T) = T \int_{-\infty}^{\infty} d\varepsilon \rho(U,d;\varepsilon) \ln \frac{1}{1 + \exp(-\varepsilon/k_B T)}$$
$$+ T \left( \frac{1+d}{2} \ln \frac{1+d}{2} + \frac{1-d}{2} \ln \frac{1-d}{2} \right)$$

(15)

and by minimizing $F(U,d,T)$ over $d$ we can find the order parameter $d(U;T)$. Then, by inserting $d(U;T)$ into $\rho(U,d;\varepsilon)$ we get $\rho(U,T;\varepsilon)$. Next, from $\rho(U,T;\varepsilon)$ we determine the internal energy $E(U,T)$ using the standard formula (16)

$$E(U,T) = \int_{-\infty}^{\infty} d\varepsilon \rho(U,T;\varepsilon) \frac{\varepsilon}{1 + \exp(\varepsilon/k_B T)}$$

(16)

and the temperature dependence of two quantities characterizing the MI transformation: the energy gap $\Delta(U;T)$ and the DOS at the Fermi level $\rho(\varepsilon_F = 0;T)$. We display $E(U = 1,T)$ as a function of $T$ in Fig. 5, where it can be seen that this function has a kink at $T_{\text{O-DO}}$, but no kink or any noticeable anomaly at $T_{MI}$. This is why we conclude that the metal-insulator transformation at $T_{MI}$ is not a phase transition in the usual sense. On the other hand, at $T_{\text{O-DO}}$ the system undergoes a typical order-disorder phase transition.

The temperature dependencies of $d$, $\rho(\varepsilon_F)$ and $\delta$ for $U = 1$ are displayed in Fig. 6, where $\delta = \Delta(T)/\Delta(T = 0)$ is the relative value of the gap. Note that $\delta$ has a jump at $T = 0$ because $\Delta(T = 0) = U$ but, as it comes from Eq. (10), $\Delta(T = 0^+) < U$. Then, for $U = 1$ one has $\delta(T = 0) = 1$ and
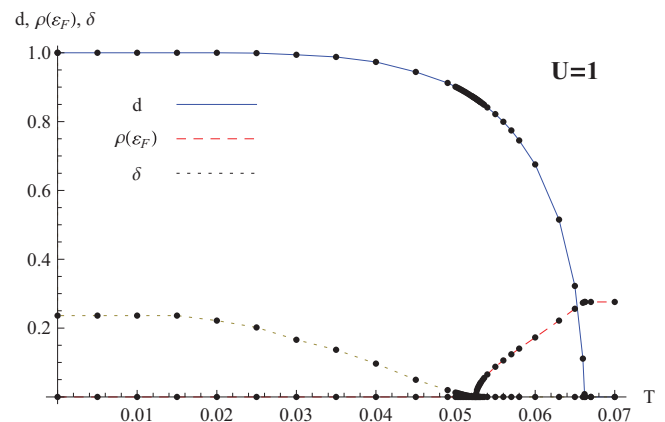


FIG. 6. (Color online) Temperature dependence of the order parameter $d$, DOS $\rho(\varepsilon_F)$ at the Fermi level and the relative value of energy gap $\delta$ for $U = 1$. Drawn lines are guides to the eye.
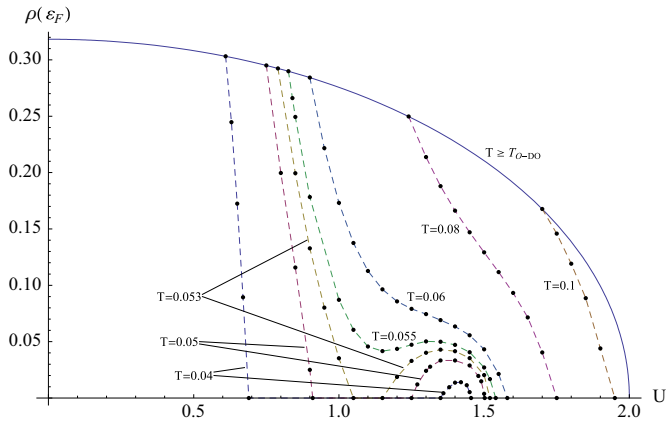
FIG. 7. (Color online) DOS $\rho(\varepsilon_F)$ as a function of $U$ for a representative set of temperatures. Drawn lines are guides to the eye.

$\delta(T = 0^+) = \sqrt{5} - 2 \approx 0.236$. Obviously, the energy gap $\Delta$, and so $\delta$, is positive in the insulating phase, i.e., for $T < T_{\mathrm{MI}}$ and is equal to zero in the metallic phase. On the other hand, $\rho(\varepsilon_F)$ is equal to zero in the insulating phase, but is positive in the metallic phase.

By viewing Fig. 6 one can see that $T_{\mathrm{MI}} \approx 0.052$ and $T_{\mathrm{O\text{-}DO}} \approx 0.0662$ for $U = 1$, so $T_{\mathrm{MI}}$ is substantially smaller than $T_{\mathrm{O\text{-}DO}}$. One can also notice that MI transformation occurs when the order parameter $d \approx 0.9$, so $d$ is still close to its maximum value 1. Another interesting observation is that $\rho(\varepsilon_F)$ clearly increases with temperature up to the maximum value $\rho(T = T_{\mathrm{O\text{-}DO}}; \varepsilon_F)$ attained at $T_{\mathrm{O\text{-}DO}}$ and this value is preserved for higher temperatures.

After inserting $d(U; T)$ into (9) we get $\rho(\varepsilon_F)$ as a function of $U$ and $T$. This function is quite nontrivial as can be seen in Figs. 7 and 8. In Fig. 7 we display $\rho(\varepsilon_F)$ as a function of $U$ for a set of fixed temperatures, and in Fig. 7 one can observe $\rho(\varepsilon_F)$ as a function of $T$ for a few $U$ values.

After collecting the data on $T_{\mathrm{O\text{-}DO}}$ and $T_{\mathrm{MI}}$ for a representative set of $U$ values we constructed the phase diagram of the system that is displayed in Fig. 9. This phase diagram is similar to the one presented in Ref. [10]. Nevertheless,
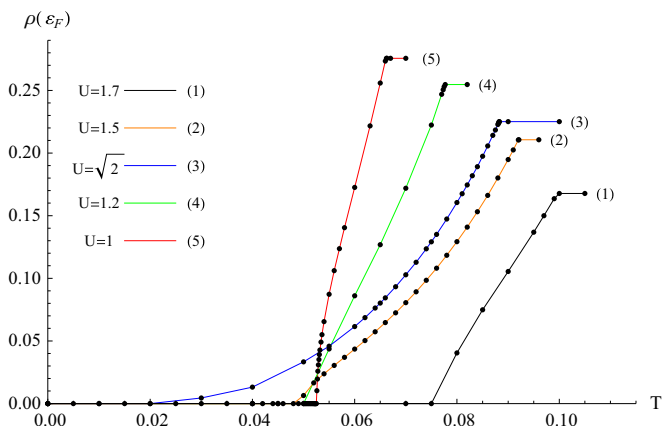


FIG. 8. (Color online) DOS $\rho(\varepsilon_F)$ as a function of $T$ for a few $U$ values. Drawn lines are guides to the eye.
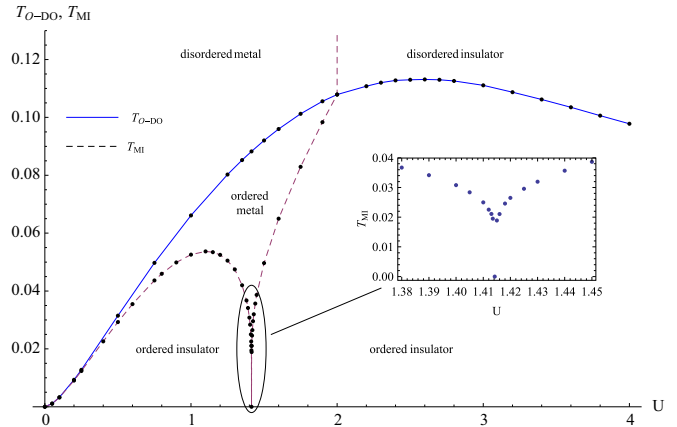


FIG. 9. (Color online) Phase diagram of the system at finite temperatures. $T_{\mathrm{O\text{-}DO}}$ is the order-disorder transition temperature (displayed by points and the solid line, that is a guide to the eye; online in blue) and $T_{\mathrm{MI}}$ is the metal-insulator transformation (displayed by points and the dashed line that is a guide to the eye). The solid line separates the disordered phase (the upper part of the diagram) from the ordered phase (the lower part of the diagram) and the dashed line separates the insulating phase (on the right) from the conducting phase (on the left). In the middle of the diagram there is an area of stability of the ordered metallic phase.

due to difference in calculation techniques used in the two cases, there is a substantial difference between the two diagrams at $U = \sqrt{2}$. Indeed, in Ref. [10] the end point of the homogeneous phase at $U = \sqrt{2}$ lies slightly above $T = 0$, whereas in our case it is located precisely at $T = 0$, which shows the existence of the quantum critical point. We were able to fix this quantum critical point using the analytical formula (12). Then the question arises about quantum effects related to the MI transformation for this particular value of $U$. In order to clarify this point some additional studies need to be done.

Let us note that in the diagram displayed in Fig. 9 the region of ordered insulator phase located below $T_{\mathrm{O\text{-}DO}}$ (continuous) line consists of two parts corresponding to insulating phases separated by an ordered metallic phase. This is quite an unexpected finding obtained neither within the conventional mean field theory [14], nor through the exact procedure of expanding in series for large or small $U$ values [5]. In fact, the finding is not inconsistent with the result obtained by Van Dongen [5], as indeed, for small and large $U$ the gap exists in the ordered phase up to $T_{\mathrm{O\text{-}DO}}$. However, for intermediate $U$ values the metallic ordered phase appears below $T_{\mathrm{O\text{-}DO}}$ down to $T_{\mathrm{MI}}$. What's more, for $U = \sqrt{2}$ the metallic phase can be stable down to $T_{\mathrm{MI}} = 0$.

## IV. LOW-TEMPERATURE EXPANSION ON THE LATTICE

Now we consider a grand-canonical ensemble with the spinless Falicov-Kimball Hamiltonian (1) on a $d$-dimensional bipartite lattice. To distinguish the following calculation from the previous one on the Bethe lattice, we introduce lattice coordinates $r$, $r'$. With $n_r = w_r + 1/2$, where the absence (presence) of a heavy fermion at site $r$ is represented as a classical binary number $n_r = 0$ ($n_r = 1$), we can write for the

Hamiltonian matrix

$$\tilde{H}_{r,r'} = h_{r,r'} - (\mu - U n_r)\delta_{r,r'} \qquad (17)$$

with the chemical potential $\mu$. At half filling we have for the latter $\mu = U/2$.

According to Ref. [21], the heavy particles are distributed by the thermal distribution at the inverse temperature $\beta = 1/k_B T$,

$$P(\{n_{\mathbf{r}}\}) = e^{\beta\mu \sum_r n_r} \det(\mathbf{1} + e^{-\beta\tilde{H}})/Z,$$
$$Z = \sum_{\{n_r=0,1\}} e^{\beta\mu \sum_r n_r} \det(\mathbf{1} + e^{-\beta\tilde{H}}), \qquad (18)$$

which we can approximate by an Ising distribution as

$$e^{\beta\mu \sum_r n_r} \det(\mathbf{1} + e^{-\beta\tilde{H}}) = e^{-2\beta t^2 \sum_{<r,r'>}(n_r-1/2)(n_{r'}-1/2)+o(t^3)}. \qquad (19)$$

Adding or removing a heavy particle from the ground state (staggered configuration) appears then with the weight $w^{-\beta}$, where

$$w \sim e^{-2t^2/U}. \qquad (20)$$

This provides us a low temperature expansion for the density of states (cf. Appendix B) by adding or removing particles from the ground state configuration:

$$\rho = w^{-\beta}(U^3 g^2/4)\delta(1 - gU^2/2) + o(w^{-2\beta}). \qquad (21)$$

Thus, in order $w^{-\beta}$ we have a Dirac delta function for the DOS which is peaked at $U^2 = 2/g$ and has a weight $w^{-\beta}U^3 g^2/4$, where the parameter can be calculated as an integral for a given lattice with known hopping term $h_k$:

$$g = \int_{\mathbf{k}} \frac{1}{U^2/4 + |h_k|^2}. \qquad (22)$$

The contribution to the DOS in Eq. (21) vanishes with decreasing temperature, similar to the DOS in Figs. 7 and 8. With increasing temperature we must include higher order terms in $w^{-\beta}$ which might lead to a broadening of the DOS around $U = \sqrt{2/g}$. These results indicate that the singular DOS around a special value of $U$ in Fig. 7 is not an artifact of the DMFT or the Bethe lattice but a general feature of the FK model on any bipartite lattice.

## V. FINAL REMARKS AND CONCLUSIONS

Here we focus on the quantitative analysis of a relationship between the degree of disorder in a correlated electron system and the transformation from insulator to metal. Using exact formulas for the temperature-dependent DOS for the FK model on the Bethe lattice we demonstrate the effect of closing of the energy gap in the DOS in the insulating phase (for not too large $U$) and then of increasing of the DOS value at the

Fermi level in the metallic phase with an increase of degree of disorder. Our results confirm and extend the findings presented in Refs. [10,11], where the most important extension is to prove the existence of the quantum critical point at $U = \sqrt{2}$.

One of the most surprising conclusions drawn from all these studies is that an increase of disorder may lead to a closure of the energy gap before the system transforms into a completely disordered phase. In view of this result, we suggest a re-examination of those experiments, in which transition temperatures $T_{\text{O-DO}}$ and $T_{\text{MI}}$ are found to be the same [15,16,22]. But one should keep in mind that the distinction between $T_{\text{O-DO}}$ and $T_{\text{MI}}$ can be difficult to detect in some systems, as a clear difference between these temperatures was found only in a relatively narrow range of values of the parameter $U$. An additional difficulty is that just above $T_{\text{MI}}$ the DOS at the Fermi level is still small, as only above $T_{\text{MI}}$ it begins to rise with temperature, starting from zero and reaching a maximum value at $T_{\text{O-DO}}$ (see Fig. 7). Therefore, we expect that one will be able to notice a difference between $T_{\text{MI}}$ and $T_{\text{O-DO}}$ only in precise enough experiments.

As we have demonstrated within a low temperature expansion, the results emerging from the DMFT calculation on the Bethe lattice might be quite general. The reason is that the FK model, called by some authors the simplified Hubbard model [23], contains basic ingredients that are present in many other models of the correlated electron system. On the other hand, properties of the DOS relevant for these studies, such as the existence of the gap in the homogeneous phase for sufficiently large $U$ and closing the gap with decreasing $U$ in the homogeneous phase but not in the ordered phase, are common for all examined lattices (hypercubic 1D, 2D, 3D, and the infinite D, as well as the Bethe lattice in the infinite D limit) [5,6,12,13,23].

Interestingly enough, there are some similarities between our phase diagram displayed in Fig. 6 and the phase diagram found for the Hubbard model with disorder [24]. In fact, we cannot directly compare our results with those reported in Ref. [24], as the latter were obtained not for the FK model but for the Hubbard model, and only at zero temperature. However, in these two cases the same sort of phases appear on the phase diagram; only insulating phases survive for large $U$ and the ordered metallic phase occupies a relatively small region in the phase diagram. Finally, let us hope that the existence of the gapless checkerboard-type charge density wave phase found first for the FK model will be confirmed by studies on the Hubbard model and other models of strongly correlated electrons.

## APPENDIX A: COEFFICIENTS OF THE POLYNOMIAL GIVEN IN EQ. (8)

Here are the coefficients $a_0$, $a_1$, $a_2$, $a_3$, $a_4$, $a_5$ given in Eq. (8) that are obtained from the transformation of the system

of equations (4):

$$a_0 = -2(4z^2 - U^2)(8z^3 + 4dz^2 U$$
$$- dU(-4 + U^2) - 2z(4 + U^2))$$

$$a_1 = 64z^6 + 192dz^3 U - 48dzU^3 - 16z^4(-8 + 3U^2)$$
$$+ U^2(16 + 16d^2 - U^4) + 4z^2(-32 - 8U^2 + 3U^4)$$

$$a_2 = -16(16z^5 + 20dz^2 U - 8z^3 U^2$$
$$- dU(2 + U^2) + z(-4 + U^4))$$

$$a_3 = 8(48z^4 + 24dzU + U^4 - 16z^2(1 + U^2))$$

$$a_4 = -32(8z^3 + dU - 2z(1 + U^2))$$

$$a_5 = 64z^2 - 16U^2.$$

## APPENDIX B: GREEN'S FUNCTION ON THE BIPARTITE LATTICE

Then the Green's function of the light fermions reads as an average with respect to a grand-canonical distribution of the heavy fermions

$$G = \langle (H - i\delta)^{-1} \rangle \equiv \sum_{\{n_{\mathbf{r}}=0,1\}} P(\{n_{\mathbf{r}}\})(H - i\delta)^{-1}. \quad \text{(B1)}$$

At half filling, where $\mu = U/2$, the ground state of the heavy particles on a bipartite lattice is a staggered (or generalized checkerboard) configuration. Using a sublattice representation for the hopping of the light fermions, we obtain

$$\bar{H} = \begin{pmatrix} U/2 & h \\ h^T & -U/2 \end{pmatrix}, \quad \text{(B2)}$$

where the sublattice 1 (2) has the effective potential $U/2$ ($-U/2$). Here we have assumed that the hopping is only between nearest neighbors. Therefore, the hopping terms are $h$, $h^T$ in the off-diagonal elements of our sublattice matrix. Now we apply a Fourier transformation on the translational invariant sublattice to get as Fourier components $2 \times 2$ matrices

$$\bar{H}_k = \begin{pmatrix} U/2 & h_k \\ h_k^* & -U/2 \end{pmatrix} \quad \text{(B3)}$$

with the two-band dispersion $E_k = \pm\sqrt{U^2/4 + |h_k|^2}$. The sum over other configurations in (B1) is now an expansion in powers of a weight $w^{-\beta}$. This implies for the Green's function

$$G = \sum_{\{n_{\mathbf{r}}=0,1\}} P(\{n_{\mathbf{r}}\})(\bar{H} + Un - i\delta)^{-1} \quad \text{(B4)}$$

$$= (\bar{H} - i\delta)^{-1} + w^{-\beta} \sum_r [(\bar{H} + V_r - i\delta)^{-1}$$

$$+ (\bar{H} + W_r - i\delta)^{-1}] + o(w^{-2\beta}) \quad \text{(B5)}$$

with

$$V_r = \begin{pmatrix} -U & 0 \\ 0 & 0 \end{pmatrix}, \quad W_r = \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}. \quad \text{(B6)}$$

The latter expressions mean that $V_r$ ($W_r$) removes (adds) a heavy particle at site $r$ on sublattice 1 (2). The expressions $(\bar{H} + V_r - i\delta)^{-1}$, $(\bar{H} + W_r - i\delta)^{-1}$ can be easily computed

by using the identity

$$(A + \eta)^{-1} = A^{-1} - A^{-1}(\mathbf{1} + \eta A^{-1})_S^{-1} \eta A^{-1}, \quad \text{(B7)}$$

where $S$ refers to the projection of the matrix space with nonzero $\eta$. In our case $S$ is just the single site $r$, such that this identity reads with $\bar{G} = (\bar{H} - i\delta)^{-1}$

$$(\bar{H} + V_r - i\delta)_{r'j,r'j}^{-1} = \bar{G}_{r'j,r'j} - \bar{G}_{r'j,r1}\frac{-U}{1 - U\bar{G}_{r1,r1}}\bar{G}_{r1,r'j}$$

$$\text{(B8)}$$

$$(\bar{H} + W_r - i\delta)_{r'j,r'j}^{-1} = \bar{G}_{r'j,r'j} - \bar{G}_{r'j,r2}\frac{U}{1 + U\bar{G}_{r2,r2}}\bar{G}_{r2,r'j}.$$

$$\text{(B9)}$$

The elements of the Green's function $\bar{G}$ can be evaluated from their Fourier components as

$$\bar{G}_{r1,r1} = (U/2 + i\delta)g, \quad \bar{G}_{r2,r2} = (-U/2 + i\delta)g,$$

$$g = \int_{\mathbf{k}} \frac{1}{U^2/4 + \delta^2 + |h_k|^2} \quad \text{(B10)}$$

such that

$$(\bar{H} + V_r - i\delta)_{r'j,r'j}^{-1}$$

$$= \bar{G}_{r'j,r'j} - \bar{G}_{r'j,r1}\frac{-U}{1 - gU^2/2 - iUg\delta}\bar{G}_{r1,r'j} \quad \text{(B11)}$$

$$= \bar{G}_{r'j,r'j} + \frac{U(1 - gU^2/2 + iUg\delta)}{(1 - gU^2/2)^2 + U^2g^2\delta^2}\bar{G}_{r'j,r1}\bar{G}_{r1,r'j}$$

$$\text{(B12)}$$

$$(\bar{H} + W_r - i\delta)_{r'j,r'j}^{-1}$$

$$= \bar{G}_{r'j,r'j} - \bar{G}_{r'j,r2}\frac{U}{1 - gU^2/2 + iUg\delta}\bar{G}_{r2,r'j} \quad \text{(B13)}$$

$$= \bar{G}_{r'j,r'j} - \frac{U(1 - gU^2/2 - iUg\delta)}{(1 - gU^2/2)^2 + U^2g^2\delta^2}\bar{G}_{r'j,r2}\bar{G}_{r2,r'j}.$$

$$\text{(B14)}$$

Since we have a gap $U$, the Green's function $\bar{G}$ is real in the limit $\delta \to 0$. Therefore, the density of states reduces to

$$\rho = \frac{1}{\pi} \lim_{\delta \to 0} \text{Im} G_{rj,rj}$$

$$= w^{-\beta} \frac{1}{\pi} \lim_{\delta \to 0} \frac{U^2 g\delta}{(1 - gU^2/2)^2 + U^2g^2\delta^2}\bar{G}_{r'j,r'j}^2 + o(w^{-2\beta})$$

$$\text{(B15)}$$

$$= w^{-\beta} U \bar{G}_{r'j,r'j}^2 \delta(1 - gU^2/2) + o(w^{-2\beta}) \quad \text{(B16)}$$

with the Dirac delta function $\delta(x)$.

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