Temperature and filling dependence of the superconducting pi-phase in the Penson-Kolb-Hubbard model

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Fabrizio Dolcini and Arianna Montorsi
Dipartimento di Fisica and Unità INFM, Politecnico di Torino, I-10129 Torino, Italy
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We investigate in the Hartree approximation the temperature and filling dependence of the superconducting π phase for the Penson-Kolb-Hubbard model. Due to the presence of the pair-hopping term, the phase survives for repulsive values of the on-site Coulomb interaction, exhibiting an interesting filling and temperature dependence. The structure of the self-consistent equations peculiar to the π phase of the model allows us to explicitly solve them for the chemical potential. The phase diagrams are shown and discussed in dimension 2 and 3. We also show that, when a next-nearest-neighbors hopping term is included, the critical temperature of the superconducting region increases, and the corresponding range of filling values is shifted away from half-filling. Comparisons with known exact results are also discussed.

I. INTRODUCTION

Interest in strongly correlated electron systems and superconductivity has motivated some attention on the wide class of extended Hubbard models:[1] indeed, a number of interesting results[2–15] show that for some of these models a superconducting phase exists. The Hamiltonian of the extended Hubbard models reads

$$H_{\mathrm{EH}}=H_{\mathrm{Hub}}+H_X+H_{\tilde{X}}+H_V+H_W+H_Y, \tag{1}$$

where

$$H_{\mathrm{Hub}}=-t\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+U\sum_{\mathbf{i}} n_{\mathbf{i},\uparrow}n_{\mathbf{i},\downarrow} \quad \text{(Hubbard)},$$

$$H_X=X\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} (n_{\mathbf{i},-\sigma}+n_{\mathbf{j},-\sigma})c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma} \quad \text{(bond charge)},$$

$$H_{\tilde{X}}=\tilde{X}\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} n_{\mathbf{i},-\sigma}n_{\mathbf{j},-\sigma}c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma} \quad \text{(correl. hopping)},$$

$$H_V=\frac{V}{2}\sum_{\langle \mathbf{i},\mathbf{j}\rangle} n_{\mathbf{i}}n_{\mathbf{j}} \quad \text{(neighboring site charge)},$$

$$H_W=\frac{W}{2}\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma,\sigma'} c^{\dagger}_{\mathbf{i},\sigma}c^{\dagger}_{\mathbf{j},\sigma'}c_{\mathbf{i},\sigma'}c_{\mathbf{j},\sigma} \quad \text{(exchange)},$$

$$H_Y=Y\sum_{\langle \mathbf{i},\mathbf{j}\rangle} c^{\dagger}_{\mathbf{i},\uparrow}c^{\dagger}_{\mathbf{i},\downarrow}c_{\mathbf{j},\downarrow}c_{\mathbf{j},\uparrow} \quad \text{(pair hopping)}.$$

Here $c^{\dagger}_{\mathbf{i},\sigma}$ and $c_{\mathbf{i},\sigma}$ are fermionic creation and annihilation operators, where $\mathbf{i}$ runs over the L^d sites of a d-dimensional lattice Λ, and $\sigma\in\{\uparrow,\downarrow\}$ is the spin label; the usual anticommutation rules $\{c_{\mathbf{i},\sigma'},c_{\mathbf{j},\sigma}\}=0$, $\{c_{\mathbf{i},\sigma},c^{\dagger}_{\mathbf{j},\sigma'}\}=\delta_{\mathbf{i},\mathbf{j}}\delta_{\sigma,\sigma'}$ hold. The symbol $\langle \mathbf{i},\mathbf{j}\rangle$ stands for nearest neighbors in Λ. Finally, $n_{\mathbf{i},\sigma}=c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{i},\sigma}$ is the number of electrons with spin σ at site $\mathbf{i}$, and $n_{\mathbf{i}}=n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow}$. For the ordinary Hubbard model H_{Hub} no exact result supports the existence of a superconducting phase at finite values of U, and even within a mean-field scheme this is achieved only for $U<0$. On the contrary, for appropriate nonvanishing values of the other coupling constants, the superconducting phase can be proved to exist by means of exact integrability methods; the latter results involve the states known as η_{ϕ} pairs, namely

$$|\eta\rangle_{\phi}=(K^{\dagger}_{\phi})^{m}|0\rangle; \quad K^{\dagger}_{\phi}=\sum_{\mathbf{j}\in\Lambda} e^{i\boldsymbol{\phi}\cdot\mathbf{j}}c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}=\sum_{\mathbf{k}\in B} c^{\dagger}_{\boldsymbol{\phi}-\mathbf{k}\downarrow}c^{\dagger}_{\mathbf{k}\uparrow}, \tag{2}$$

where $\boldsymbol{\phi}$ is a d-dimensional vector $(\phi,\phi,\ldots)$, B is the first Brillouin zone in the reciprocal lattice, and $m=1,\ldots,L^d$. Noticeably, the states $|\eta\rangle_{\phi}$ enjoy the property of ''off diagonal long range order'' (ODLRO), which implies superconductivity.[10] Therefore much effort has been done through the last years to find which are the relations among the coupling parameters in Eq. (1) guaranteeing that an $|\eta\rangle_{\phi}$ is the ground state.

A first set of remarkable results was obtained in 1D for the subclass of Hamiltonians characterized by the constraint $X=t$. In Refs. 6 and 7 the phase diagram U vs filling for the AAS model $X=t,\tilde{X}=W=V=Y=0$ (reported in Fig. 1) was derived at $T=0$: one can see a superconductive filling-independent region, where the $|\eta\rangle_{\phi}$ are degenerate ground states for any ϕ, and a filling dependent zone (again superconducting because it contains at least $|\eta\rangle_0$ pairs) rising up to positive values of U. Unfortunately, in contrast to the real case of superconducting materials, the superconducting phase turns out to have a maximum at half filling. A similar phase diagram (see Fig. 1) was also obtained in Refs. 4 and 5 for the EKS Hamiltonian, characterized by $X=t,\tilde{X}=0$, $Y=W=V=-1$. There the filling independent phase is made of $|\eta\rangle_{\phi}$ with only $\phi=0$, since $Y\neq 0$: in fact a nonvanishing pair-hopping term removes the degeneracy of $|\eta\rangle_{\phi}$, $|\eta\rangle_0$ being energetically favorite for $Y<0$, while $|\eta\rangle_{\pi}$ is favorite for $Y>0$. Moreover, as Fig. 1 shows, a nonvanishing Y also contributes to rise up the superconducting region towards positive values of U.

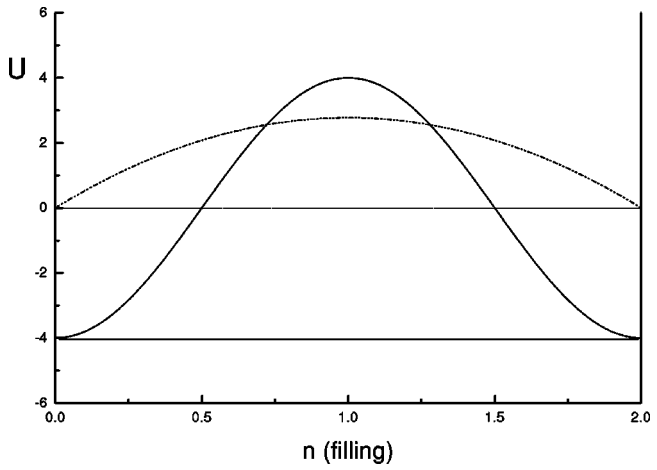

FIG. 1. Phase diagram in $d=1$ at $T=0$ of AAS model (solid curve) and EKS model (dot-dashed curve). In the filling-independent (superconducting) region the η_ϕ pairs are ground state. Above it, a filling-dependent region (still superconducting) exists. In the EKS model the *pair hopping* term contributes to extend the superconducting zone towards positive values of U. In such exactly solved 1D models the phase diagram reaches a maximum around half filling.

More recently, it has also been realized[3] that, at least in order to obtain the filling independent superconducting region, some of the constraints on the parameters (in particular $X=t$, which is not very physical) are not necessary, provided that a pair-hopping term is present. Also, as long as $X\neq t$, only $|\eta\rangle_\pi$ states could become ground states, the other choices of ϕ in Eq. (2) giving states that cannot be eigenstates of Eq. (1).

On the contrary, no exact result is available concerning the existence of the more structured filling dependent superconducting region when the above constraints on the parameters are removed. It is one purpose of the present paper to investigate within the Hartree scheme such possibility, as well as to test how the superconducting region modifies at $T\neq 0$.

Due to the relevance of the pair-hopping term to stabilize the η_π-pairs phase, and in order to make the physical mechanism more clear, we shall focus on a subcase of the extended model in which, apart from the pure Hubbard terms, only the pair hopping amplitude is taken different from zero. This is known in the literature as Penson-Kolb-Hubbard model. We want to emphasize here that the presence of other terms in Eq. (1) is not expected to affect our results in a qualitative way, as other recent numerical studies confirm.[11,12]

In Sec. II we give the Hamiltonian and derive within the Hartree scheme the temperature dependent equations for the filling and the self-consistent superconducting order parameter. In Sec. III we solve the equations in dimension 2 and 3, and show the temperature and filling dependence of the superconducting phase in these cases. In Sec. IV we add to the Hamiltonian a next-nearest-neighbors contribution to the hopping term, and we show how this affects the filling and temperature dependence of the superconducting phase. Finally, in Sec. V we discuss our results and give some conclusions.

II. PENSON-KOLB-HUBBARD MODEL AND HARTREE APPROACH TO THE π PHASE

The Penson-Kolb-Hubbard Hamiltonian reads

$$H_{\mathrm{PKH}}=H_{\mathrm{Hub}}+H_Y+\mu\sum_{\mathbf{i}} n_{\mathbf{i}}, \tag{3}$$

where H_{Hub} and H_Y are given in Eq. (1) and the last term is the chemical potential. The case $U=0$ in 1D was first examined by Penson and Kolb[13] to study a short range interaction between electron pairs of small radius (actually zero), in contrast with the BCS theory, where the size of the Cooper pairs is comparatively large. This led to envisage a *real space* formulation for the electron pairing, which is very interesting in many contexts of condensed matter physics.

Later on, the Coulomb repulsion term U was also taken into account by Ref. 14, where the PKH Hamiltonian was proposed as an effective phenomenological model capturing the main physical features of doped materials, such as high-T_c superconductors. Indeed if we assume that, due to some (yet unknown) microscopic mechanism, localized pairs can be formed, then their displacement in the lattice should be described by a pair hopping term competing with a single carrier hopping amplitude t. The Coulomb repulsion term should account for the insulating phase.

More recently a slave boson wide study of the different possible phases of the model at zero temperature has also been done.[15] In particular, a region characterized by a non-vanishing value of the order parameter $x_\pi=(1/L^d)\langle K_\pi^\dagger\rangle$ was found; here $K_\pi^\dagger$ is given by the $K_\phi^\dagger$ in Eq. (2) with $\phi=\pi$, and $\langle\,\rangle$ stands for the average value on the grand canonical statistical ensemble. In the following we shall denote such a phase as π phase. The latter turns out to be favorite with respect to other ϕ phases with different ϕ values for $Y>0$. At zero temperature, the analysis performed in Ref. 15 by means of different approximation schemes clarifies for which range of parameters the π phase is energetically favorite also with respect to other (nonsuperconducting) ordered phases. Within this range, we expect that for low enough temperatures the thermal energy is not sufficient to let other phases emerge. The Hartree approximation then decomposes the PKH Hamiltonian into the following sum of k-space commuting Hamiltonians:

$$H_{\mathrm{PKH}}\approx\sum_{\mathbf{k}\in B}\,(-(t\epsilon_{\mathbf{k}}+\overline{\mu})n_{\mathbf{k}\uparrow}-(t\epsilon_{\boldsymbol{\pi}-\mathbf{k}}+\overline{\mu})n_{\boldsymbol{\pi}-\mathbf{k}\downarrow} + \tilde{U}[x_\pi c_{\mathbf{k}\uparrow}^\dagger c_{\boldsymbol{\pi}-\mathbf{k}\downarrow}^\dagger + x_\pi^* c_{\boldsymbol{\pi}-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}]-\tilde{U}|x_\pi|^2), \tag{4}$$

where $\tilde{U}=U-qY$ (q being the number of nearest neighbors, equal to 2D for a hypercubic lattice), and $\overline{\mu}=\mu-nU/2$ is the Hartree-renormalized chemical potential. The sum in Eq. (4) runs over the Brillouin zone B and the $\mathbf{k}$ vectors are measured in units of the inverse lattice spacing (i.e., $-\pi\leqslant k_i\leqslant\pi$).

In contrast with Eq. (3), the linearized Hamiltonian (4) does not preserve the number of particles; indeed in a Hartree picture the π phase has to be thought of as a superposition of η_π pairs involving different number of pairs, the *average* number of electrons being fixed through the chemi-

cal potential. A standard calculation allows to derive the Hartree grand potential (per particle) ω in the thermodynamic limit as

$$\omega = -\frac{1}{(2\pi)^d}\int_B d\mathbf{k}\left(A_{\mathbf{k}} + \frac{1}{\beta}\sum_{s=\pm 1}\ln\left[2\cosh\beta\frac{D_{\mathbf{k}}+sR_{\mathbf{k}}}{2}\right]\right),$$

with $D_{\mathbf{k}} = t(\epsilon_{\mathbf{k}} - \epsilon_{\pi-\mathbf{k}})/2$, $A_{\mathbf{k}} = C_{\mathbf{k}}^2 + \tilde{U}|x_\pi|^2$, $R_{\mathbf{k}} = (C_{\mathbf{k}}^2 + \tilde{U}^2|x_\pi|^2)^{1/2}$ and $C_{\mathbf{k}} = \bar{\mu} + t(\epsilon_{\mathbf{k}} + \epsilon_{\pi-\mathbf{k}})/2$. In order to investigate the thermodynamical properties of the system one has to implement the self-consistency equation $\partial\omega/\partial x_\pi = 0$ for the order parameter. Such equation gives, as usual, a solution $x_\pi \equiv 0$ for $T \geqslant T_c$, and a solution $x_\pi \neq 0$ for $T \leqslant T_c$. It can be shown that the π phase (i.e., $x_\pi \neq 0$) exists only when $\tilde{U} = U - qY \leqslant 0$, that is when the pair-hopping $Y > 0$ term renormalizes the interaction $U > 0$ to an effective *attractive* regime. Investigating in particular the $T \leqslant T_c$ regime, the self-consistency relation can be written as

$$\tilde{U}^{-1} = -\frac{1}{(2\pi)^d}\int_B d\mathbf{k}\frac{1}{4R_{\mathbf{k}}}\sum_{s=\pm 1} s\tanh\beta\frac{D_{\mathbf{k}}+sR_{\mathbf{k}}}{2}. \quad (5)$$

Moreover, one must also satisfy the filling equation, $n = \partial\omega/\partial\mu$, which reads

$$n = 1 + \frac{1}{(2\pi)^d}\int_B d\mathbf{k}\frac{C_{\mathbf{k}}}{2R_{\mathbf{k}}}\sum_{s=\pm 1} s\tanh\beta\frac{D_{\mathbf{k}}+sR_{\mathbf{k}}}{2}. \quad (6)$$

Equations (5) and (6) constitute the *parametric* form of the equation of state. In order to get to one *closed* form, one should in principle invert Eq. (6) obtaining $\bar{\mu}$ as a function of n, T and $\tilde{U}$, and then insert it into Eq. (5). The thermodynamics of the model will then be expressed in terms of n, T and $\tilde{U}$. Noticeably, comparing Eqs. (5) and (6) it is easy to show that whenever $\epsilon_{\pi-\mathbf{k}} = -\epsilon_{\mathbf{k}}$ the chemical potential can be *exactly* inverted. In this case we have

$$\bar{\mu} = \frac{1-n}{2}\tilde{U}. \quad (7)$$

We wish to stress that for a given model, even within the Hartree approximation, it is not obvious at all that the chemical potential can be inverted exactly: in the PKH model this is a peculiar feature of the π phase (not shared by 0 phase). Equation (7) holds in any dimension for a hypercubic lattice when dealing with a *nearest-neighbors* hopping term, since the dispersion relation is $\epsilon_{\mathbf{k}} = \sum_{i=1}^{d} 2\cos k_i$. However, when a *next-nearest-neighbors* term is included, the form of $\epsilon_{\mathbf{k}}$ changes so that Eq. (7) does not hold any longer (see Sec. IV).

III. TEMPERATURE AND FILLING DEPENDENCE OF THE PHASE DIAGRAM IN $d=2$ AND $d=3$

In this section we consider the case of a nearest neighbors hopping term. We aim to derive the features of the critical values of $\tilde{U}$ versus n for a given temperature T, in order to compare them with known solution of similar models (see Sec. V). The critical curve $\tilde{U}_c = \tilde{U}_c(n)$ is obtained from Eqs. (5) and (6) by setting $x_\pi = 0$ into $R_{\mathbf{k}}$.

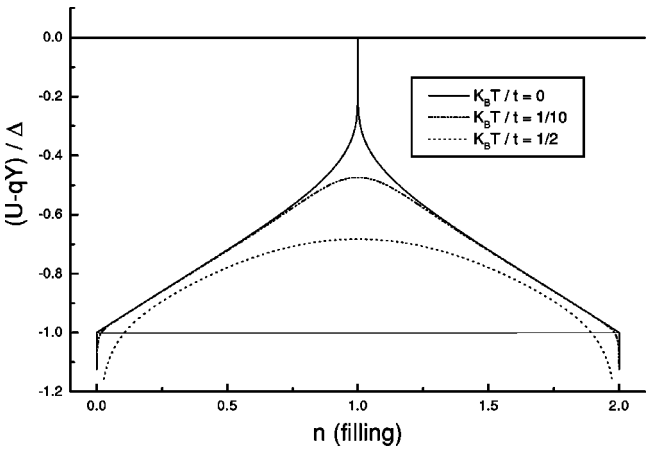

FIG. 2. Phase diagram of the π phase in $d=2$; the critical value $\tilde{U}_c$ of the effective attraction $\tilde{U} = U - qY$ is plotted versus the filling for some values of the temperature T. At a given T the π phase exists for $\tilde{U} \leqslant \tilde{U}_c$; here $\Delta = 8t$ is the bandwidth and $q=4$ is the number of nearest neighbors. The values of $\tilde{U}$ are negative because the pair hopping term renormalizes the Coulomb repulsion U to a negative regime. The curves are centered around half-filling; at $T=0$ a filling independent region exists for $\tilde{U} \leqslant -\Delta$, like in AAS and EKS models (see Fig. 1).

As noticed in Sec. II, besides the parametric form (5) and (6), in this case we can also deal with one closed form; indeed, since $\epsilon_{\mathbf{k}} = -\epsilon_{\pi-\mathbf{k}}$, $R_{\mathbf{k}}$ is independent of $\mathbf{k}$, and thus Eq. (7) holds. By substituting $\bar{\mu}$ into $R_{\mathbf{k}}$, and then $R_{\mathbf{k}}$ into Eq. (5), we obtain from Eq. (6) the critical equation

$$\frac{1}{(2\pi)^d}\int_B d\mathbf{k}\sum_{s=\pm 1}\frac{s}{2}\tanh\left[\beta\frac{t\epsilon_{\mathbf{k}} + s\tilde{U}_c\delta(n)/2}{2}\right] = \delta(n), \quad (8)$$

where $\delta(n) = 1 - n$ is the ''doping.''

Since Eq. (8) is invariant under the transformation $\delta(n) \rightarrow -\delta(n)$, it is easily seen that $\tilde{U}_c$ is symmetric with respect to the value at half-filling ($n=1$). The critical curves in $d=2$ and $d=3$ are plotted in Figs. 2 and 3 respectively, where use has been made of the density of states $g^{(d)}(\epsilon)$ [with normalization $(2\pi)^{-d}d\mathbf{k} = d\epsilon g^{(d)}(\epsilon)$] which is known in literature for $d=2,3$.

For the sake of consistency with our approximation, we have plotted the region of the phase diagram where the values of $\tilde{U}$ do not exceed the bandwidth $\Delta = 4td$.

Notice the different behavior of $\tilde{U}_c$ in the two cases, in particular for low temperatures. Indeed in $d=2$ we have a very sharp, cuspidlike shape at half-filling, while in $d=3$ a ''plateau'' is obtained, meaning that the effective interaction threshold is almost independent of the density of electrons in the lattice for a rather wide range of n. This effect is due to the quite different behavior of the density of states $g^{(2)}$ and $g^{(3)}$. Indeed using the parametric form it is possible to show that at low T's the shape of $\tilde{U}_c$ in the neighborhood of half-filling is governed by the behavior of $g^{(d)}$ around $\epsilon = 0$. In fact, inserting Eq. (7) into Eq. (8), and making use of the density of states $g^{(d)}(\epsilon)$, it is possible to deduce that

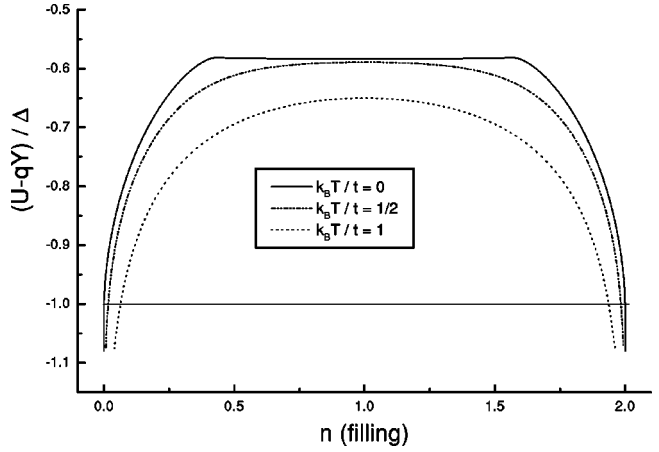

FIG. 3. Phase diagram of the π phase in $d=3; \Delta=12t$ is the bandwidth and $q=6$ is the number of nearest neighbors. With respect to the case $d=2$ (see Fig. 2) the curves have a plateau around half-filling; indeed at $T=0$ the highest values of $\tilde{U}_c$ are reached at the symmetric values $n\sim 0.4$ and $n\sim 1.6$. As the temperature is increased, the η_π pairs start breaking up and the extension of the π phase reduces.

$$\tilde{U}_c(n=1) = -\left(\int_{-\epsilon_{\max}}^{+\epsilon_{\max}} g^{(d)}(\epsilon) p_\beta(\epsilon) \right)^{-1}, \tag{9}$$

where $p_\beta(\epsilon) = \beta t/4 \cosh^{-2}(\beta t/2\epsilon)$. This holds for *any* temperature T. In particular when $T\to 0$ Eq. (9) yields

$$\tilde{U}_c(n=1) = -\frac{1}{g^{(d)}(0)}. \tag{10}$$

Now, since $g^{(3)}$ is almost constant around $\epsilon=0$, when $T\sim 0$ Eq. (8) gives

$$1-n \approx \int_{-|\bar{\mu}|}^{+|\bar{\mu}|} g^{(3)}(\epsilon) \approx -2\bar{\mu} g^{(3)}(\epsilon)|_{\epsilon=0}, \tag{11}$$

and using Eq. (7) we obtain that $\tilde{U}_c$ is actually independent of n [indeed $g^{(3)}(0)=0.1427$ and so $1/0.1427=7.0078$ which is just the value of $\tilde{U}$ around half-filling when $T=0$]. It can also be proved that at $T=0$ the plateau is slightly concave, so that the highest value of $\tilde{U}_c$ is actually reached away from half-filling, at the symmetric values $n\sim 0.4$ and $n\sim 1.6$.

IV. THE NEXT-NEAREST-NEIGHBORS CONTRIBUTION

Let us now turn to the case when in the Hamiltonian (3) a next-nearest-neighbors contribution is included in the hopping term, which therefore becomes

$$-t \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \sum_\sigma c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} - \alpha t \sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle} \sum_\sigma c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma}. \tag{12}$$

The latter term breaks the particle-hole $c^\dagger_{\mathbf{j}} \to e^{i\boldsymbol{\pi}\cdot\mathbf{j}} c_{\mathbf{j}}$ symmetry of the model. The dispersion relation reads now $\epsilon_{\mathbf{k}} = \Sigma_{i=1}^d 2\cos k_i + \alpha \Sigma_{i<j\leq d} 4 \cos k_i \cos k_j$. As observed at the end of Sec. II, the symmetry $\epsilon_{\mathbf{k}} = -\epsilon_{\boldsymbol{\pi}-\mathbf{k}}$ does not hold anymore. This yields both mathematical and physical new features. In particular, the equation for the critical surface has to be given only in the parametric form (5) and (6), $\bar{\mu}$ being the parameter.

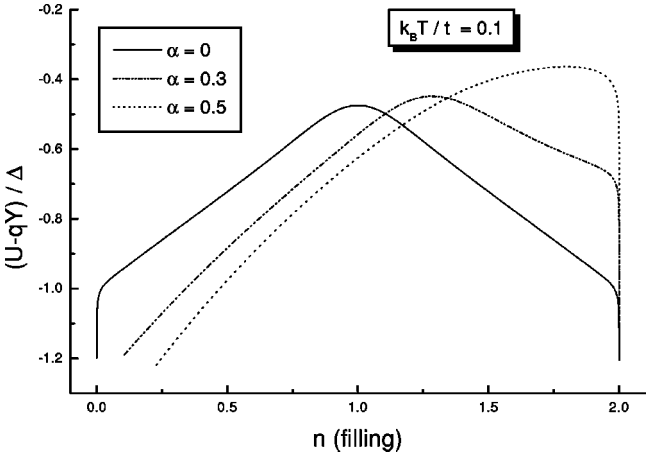

FIG. 4. The π phase diagram in $d=2$ for different values of the next-nearest-neighbors hopping amplitude α at the temperature $k_B T/t = 0.1$. Notice that when α is increased the superconducting region rises up towards less negative values of the $\tilde{U}=U-qY$, and its maximum is reached at a $n_{\max}$ which moves away from half-filling. This means that, at a given temperature, the next-nearest-neighbors interaction reduces the effective attraction $\tilde{U}$, yielding an increase of the highest reachable critical temperature (see also Fig. 6).

We are here interested in the case $d=2$. In this case the density of states reads

$$g^{(2)}_\alpha(\epsilon) = \frac{1}{2\pi^2\sqrt{1+\alpha\epsilon}} K\left(\frac{1-(\epsilon/4-\alpha)^2}{1+\alpha\epsilon} \right), \tag{13}$$

where α is assumed to be $|\alpha|\leq 1/2$, since the next-nearest-neighbors term is expected to be small with respect to the nearest-neighbors one. For $\alpha=0$ we recover the usual form. Notice that for $\alpha\neq 0$ the function $g^{(2)}_\alpha$ is not even in ϵ; indeed we have $g^{(2)}_\alpha(-\epsilon) = g^{(2)}_{-\alpha}(\epsilon)$. Thus the critical curve $\tilde{U}_c$ vs n acquires an asymmetric form, the highest value of $\tilde{U}$ falling now at a $n_{\max}\neq 1$, as shown in Fig. 4. Moreover, at a given temperature T, such a maximum of the critical curve is shifted upward with respect to the curve of the case $\alpha=0$. This means that at a given T, the effect of the next-nearest-neighbors term is to *reduce* the ''optimal'' effective attraction $\tilde{U}$. In turn, this implies at a given $\tilde{U}$ the *raising* of the highest critical temperature reachable by doping the system.

We have also studied how $n_{\max}$ depends on α. The relation is almost linear for $|\alpha|\leq 0.4$, while it displays a sudden increase of slope around $|\alpha|\sim 0.45$; in Fig. 5 we have extended the curve to the range $0\leq|\alpha|\leq 1$ (which could be still acceptable in principle) to show how $n_{\max}$ approaches the limiting values $n=0$ or $n=2$. Notice that the curve is odd in α; this is because the parametric Eqs. (5) and (6) are invariant under the transformation $\bar{\mu}\to -\bar{\mu}; \alpha\to -\alpha; \tilde{U}\to\tilde{U}$, and therefore one can show, in agreement with Ref. 16, that $T_c(\tilde{U},n;\alpha) = T_c(\tilde{U},2-n;-\alpha)$. It is possible to see that the curve depends very weakly on the temperature T.

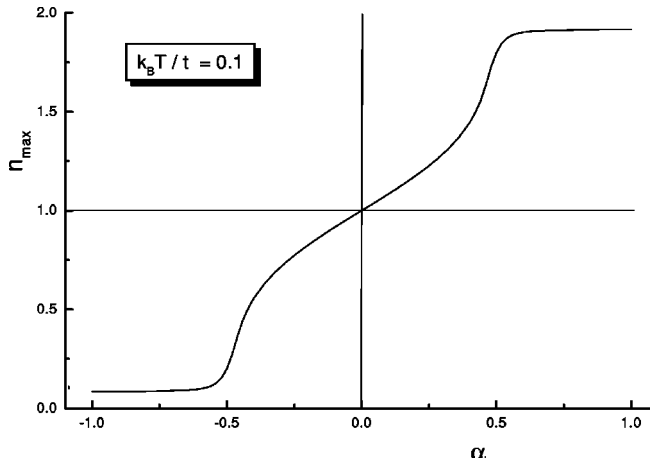

FIG. 5. The behavior of $n_{\max}$ (i.e., the point of maximum for the curves of Fig. 4) as a function of the next-nearest-neighbors parameter α, at temperature $k_BT/t=0.1$. The curve is odd. Notice that for $|\alpha|\leqslant 0.4$ the behavior is almost linear; as $|\alpha|$ is further increased, $n_{\max}$ approaches 0 or 2, as one can also see in Fig. 4. This behavior of $n_{\max}$ depends very weakly on the temperature T.

Finally, we have plotted the phase diagram of T_c vs n at fixed α, shown in Fig. 6. We can observe that the next-nearest-neighbors term has mainly two effects. First it shifts away from half-filling the range of values of n at which the superconducting phase exists; this suggests that the system has to be doped in order to observe a superconducting behavior. Secondly, it raises the highest reachable critical temperature with respect to the case where only a nearest neighbors interaction is considered. Having in mind the phenomenology of high-T_c materials, this study supports the idea that the actual microscopic Hamiltonian should be particle-hole *not*-invariant.

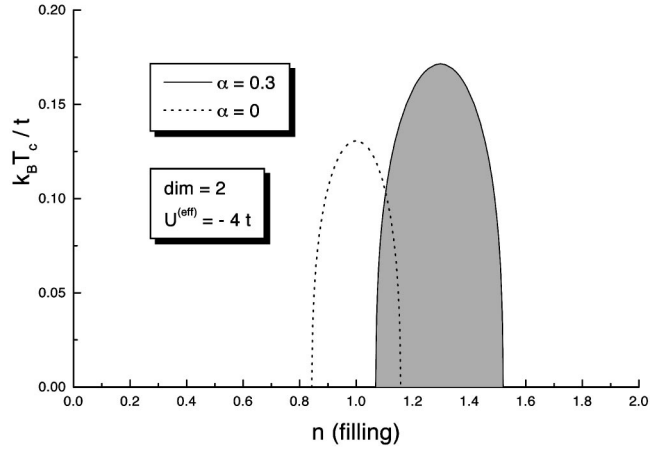

FIG. 6. The critical temperature versus the filling in $d=2$, for a given value $\tilde{U}=-4t$ of the effective attraction. Here α is the parameter of the term of *next-nearest-neighbors* (NNN) hopping, which breaks the particle-hole symmetry of the model. With respect to the case $\alpha=0$, the NNN term yields both the increase of the highest critical temperature and the displacement away from half-filling of the superconducting π phase. In fact the highest T_c is reached at $n\sim 1.3$.

V. DISCUSSION AND CONCLUSIONS

The phase diagrams obtained within the Hartree scheme can be given a more precise physical interpretation by comparing them with the 1D exact results known for some very specific cases. Strictly speaking, such a comparison is only possible for $T=0$, since the phase diagram of these integrable models is not known at $T\neq 0$. In so doing, we observe that at zero temperature our results in Fig. 2 and Fig. 3 have the same structure as those in Fig. 1. One can recognize three distinct regions in the phase space. The first one is characterized by filling independent π phase. By reducing the effective attraction $\tilde{U}$, one enters a second region in which the existence of the π phase depends on the actual filling. Finally, above the critical curve the π phase disappears.

Thus, the comparison with the exactly solved 1D cases, lead us to interpret the filling independent region as the phase in which all particles are paired in η_π pairs (2). This is in agreement with known result in $d>1$.[3] The second region should be characterized by simultaneous presence of paired, unpaired electrons and empty sites, whereas in the third one no paired electrons could move.

Switching on the temperature, thermal fluctuations are expected to break pairs. The dependence on the temperature of our phase diagrams supports this idea. Actually for a given filling n, the greater becomes T, the greater must be the magnitude of the effective attractive interaction $\tilde{U}$ in order to keep the η_π pairs bound together. In fact in Figs. 2 and 3 the curves of higher T's lay below the lower T's ones (this result can be proved rigorously). It is worth recalling that, thanks to the presence of the pair-hopping term, an effective attractive interaction $\tilde{U}$ is consistent with a positive value of the Coulomb interaction U. Hence the present Hartree treatment of the thermodynamics of the PKH model yields a structured filling dependent superconducting phase even in presence of repulsive on site Coulomb interaction between electrons. At fixed temperature, the actual border of such π phase could be eventually modified around half-filling due to the competition with antiferromagnetic order. Finally, we stress that the phase diagram in Fig. 6 —obtained by including the next-nearest-neighbors hopping term—exhibits appealing features: for $\alpha\neq 0$ the optimal doping of the superconducting region is at $n_{\max}\neq 1$, and the critical temperature is enhanced. Moreover, with respect to the results reported in Ref. 16 on the attractive Hubbard model, our figure shows that even at $T=0$ the superconducting phase exists only for an appropriate range of filling values, *not* including half-filling. We emphasize that the whole curve of the critical temperature vs filling (6) actually reminds the one obtained for high-T_c materials.

The study of the influence that particle-hole nonsymmetric terms in the Hamiltonian have on the features of the phase diagram has been worked out in 2D, the conduction in high-T_c superconducting materials typically taking place along the cuprate planes. As the Hartree approach is more accurate the higher is the dimension, dealing with a 3D and *anisotropic* order parameter would possibly be more reliable. Work is in progress along these lines. At the same time, since the results obtained here are encouraging, a numerical study of the temperature behavior of the present model in $d=2$ would be probative.

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