# Ground-state instabilities in the one-dimensional Penson-Kolb-Hubbard model

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Different kinds of instabilities (charge-density wave, spin-density wave, singlet superconductivity) in the one-dimensional Hubbard model with pair-hopping interaction are investigated using an approximate Bethe-Salpeter equation. The study is performed at any density of electrons and for arbitrary values of the model parameters. In the absence of the on-site interaction, no transition occurs at half-filling for any finite negative pair-hopping parameter, in agreement with recent results; our calculation suggests that the Penson-Kolb model $(t,W)$ with $|W/t|<\pi/\sin k_F$ behaves qualitatively like the Hubbard model $(t,U)$. Phase diagrams of the Penson-Kolb-Hubbard model $(t,U,W)$ at various densities are presented.

## I. INTRODUCTION

The studies of the one-dimensional (1D) models of correlated electronic systems can be a primary source for understanding the occurrence of the high-temperature superconductivity in materials the physics of which is mainly two dimensional. In these high-$T_c$ superconductors the ''Cooper pairs'' are extremely small with coherence lengths comparable with the size of the unit cell. Various mechanisms can lead to this local pairing.[1] In this paper we consider a model that can be relevant to the high-$T_c$ superconductivity because it contains not only such a local pairing but also an on-site electron-electron repulsion, interaction that may lead to the insulating phase of the cuprates.

The Hamiltonian of the Penson-Kolb-Hubbard (PKH) model is[2]

$$\mathscr{H}=-t\sum_{i,\sigma}\ (c^{\dagger}_{i+1,\sigma}c_{i,\sigma}+\text{H.c.})+U\sum_{i}\ n_{i,\uparrow}n_{i,\downarrow}$$
$$+W\sum_{i}\ (c^{\dagger}_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i+1,\downarrow}c_{i+1,\uparrow}+\text{H.c.}), \qquad (1)$$

where we have used the standard notation for fermion operators: $c^{\dagger}_{i,\sigma}(c_{i,\sigma})$ creates (destroys) an electron of spin $\sigma=\uparrow,\downarrow$ on the lattice site $i$ and $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$. In the absence of the on-site interaction term $U$, the Hamiltonian (1) reduces to the Penson-Kolb (PK) model[3] where the competition between the single and pair hopping of electrons can lead to interesting effects in one dimension; a spin-gap transition at half-filling for $W<0$ has been the subject of some controversy.[2–5] Recently, some variants of the PKH model were solved by the Bethe ansatz method,[6,7] where the single-particle hopping term is modified to include interaction effects: the jumping of an electron to an empty site differs from that corresponding to an occupied one.[8] But the integrability of such a model is possible only under some restrictions on the interaction parameters. Consequently, it remains interesting to have results depending on all parameters of the model and in a wide range. That is why we will consider both positive and negative values for $U$ and $W$ $(t>0)$ in Eq. (1) and arbitrary density; however, our results for the ground state phase diagram are valid in a definite range of parameters determined below.

We investigate the possible occurrence of instabilities in the ground state of the PKH model in the same manner[9] as for the 1D $(t,U,X)$ model:[10] within the (zero-temperature) Green-function formalism in the Bloch representation, the instabilities are signaled by the poles of the vertex function $\Gamma$, which obeys the Bethe-Salpeter equation. We solve this equation in the approximation when the irreducible vertex part is just the bare potential and the single-particle propagator has the ''free'' expression. The imaginary part of the poles (in the total frequency variable), interpreted as the inverse of the relaxation time to a new ground state, gives us the regions in the parameters space where the instabilities can occur; in the regions common to more instabilities we choose that phase with the shortest relaxation time.

## II. BETHE-SALPETER EQUATION

To understand what kinds of instabilities can occur in the system, one can investigate the generalized susceptibilities. It is assumed that we start from a phase where there is no order parameter, and study the density-density fluctuations. When the generalized susceptibility is singular, it is an indication that a spontaneous distortion or ordering can occur in the system.

The general form of the susceptibility is

$$\chi(k,\omega)=-i\int dt e^{i\omega t}\langle T\{\mathscr{D}(k,t)\mathscr{D}^{\dagger}(k,0)\}\rangle \qquad (2)$$

where $T$ is the usual chronological operator and $\mathscr{D}(k,t)$ is a density operator. The brackets indicate an average in the ground state (for the zero-temperature case) or a statistical average (for the finite-temperature case). If $\mathscr{D}(k,t)$ is a charge-density operator, the corresponding susceptibility $\Gamma_{\text{CDW}}$ will test the *charge-density-wave* (CDW) instability; in a similar way the susceptibilities relevant to the other kinds of instabilities can be defined: $\Gamma_{\text{SDW}}$ for *spin-density wave* (SDW), $\Gamma_{\text{SS}}$ for *singlet superconductivity* (SS), and $\Gamma_{\text{TS}}$ for

 

*triplet superconductivity* (TS). The correspondence between these quantities and the components of the vertex function can be found in Ref. 9.

The generalized susceptibilities are two-particle Green functions and they obey the Bethe-Salpeter equation. In the simplest approximation, where only the bare interaction is considered for the irreducible vertex part and the one-particle propagator $G$ is replaced by the free one $G^0$, it can be written as

$$\xi\Gamma(k,k';K,\Omega)=\frac{i}{2\pi}V(k,k';K) + \sum_{k''} V(k,k'';K)\mathcal{G}(k'';K,\Omega) \times\Gamma(k'',k';K,\Omega) \tag{3}$$

where $\Gamma$ can be any of the quantities $\Gamma_{\mathrm{CDW}}$, $\Gamma_{\mathrm{SDW}}$, or $\Gamma_{\mathrm{SS}}$; the TS case does not occur in this approximation because the interaction in the Hamiltonian (1) is only between electrons with opposite spin. $K$ ($\Omega$) denotes the transfer momentum (frequency) in the particle-hole ($ph$) channel and the total momentum (frequency) in the particle-particle ($pp$) channel,

$$\xi=\begin{cases} -1, & \text{CDW} \\ 1, & \text{SDW, SS.} \end{cases} \tag{4}$$

$$\mathcal{G}(k;K,\Omega)=\frac{i}{2\pi}\int_{-\infty}^{+\infty} d\omega G^0(k+K/2,\omega+\Omega/2) \times\begin{cases} G^0(k-K/2,\omega-\Omega/2), & \text{CDW, SDW} \\ G^0(K/2-k,\Omega/2-\omega), & \text{SS,} \end{cases} \tag{5}$$

where the addition or subtraction of the $k$ vectors are defined modulo $2\pi$ (the lattice constant is considered one). $V$ in Eq. (3) comes from the interaction part of the Hamiltonian (1) in the Bloch representation and has the expression

$$V(k,k';K)=\frac{1}{N}\begin{cases} U+2W\cos(k+k'), & \text{CDW, SDW} \\ U+2W\cos(K), & \text{SS,} \end{cases} \tag{6}$$

where $N$ denotes the number of sites in the chain.

For the $ph$ channel, Eq. (3) admits a solution of the form

$$\Gamma=\frac{i}{2\pi N}\hat{E}^T(k)\hat{X}(K,\Omega)\hat{E}(k') \tag{7}$$

with

$$\hat{E}(k)=\begin{pmatrix} 1 \\ \cos k \\ \sin k \end{pmatrix}, \hat{X}(K,\Omega)=\begin{pmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{pmatrix}, \tag{8}$$

where $\hat{E}^T$ means the transposed matrix of $\hat{E}$. The unknown coefficients $X_{ij}(K,\Omega)$ are determined from the following algebraic system:

$$\hat{M}\hat{X}=\begin{pmatrix} U & 0 & 0 \\ 0 & -2W & 0 \\ 0 & 0 & -2W \end{pmatrix}, \tag{9}$$

where $\hat{M}$ is the $3\times3$ matrix

$$\hat{M}\equiv\begin{pmatrix} \xi-gU & -c_1U & -s_1U \\ -2c_1W & \xi-2c_2W & -2pW \\ 2s_1W & 2pW & \xi+2s_2W \end{pmatrix} \tag{10}$$

and

$$\begin{aligned} g&=\frac{1}{N}\sum_q \mathcal{G}(q;K,\Omega) \\ c_n&=\frac{1}{N}\sum_q (\cos q)^n\mathcal{G}(q;K,\Omega), \quad n=1,2 \\ s_n&=\frac{1}{N}\sum_q (\sin q)^n\mathcal{G}(q;K,\Omega), \quad n=1,2 \\ p&=\frac{1}{N}\sum_q \sin q\cos q\,\mathcal{G}(q;K,\Omega)\ . \end{aligned} \tag{11}$$

Since for the SS case $V(k,k';K)\equiv V(K)$, the solution of the Eq. (3) in the $pp$ channel reads immediately

$$\Gamma_{\mathrm{SS}}=\frac{i}{2\pi N}\frac{V(K)}{1-V(K)g(K,\Omega)}. \tag{12}$$

An instability in the ground state of the system occurs when the determinant $D$ of the $\hat{M}$ matrix vanishes for the first time starting from the noninteracting case, indicating that the $X_{ij}$ diverge and consequently $\Gamma$ diverges. Following Ref. 9, we look for the $\Gamma$ poles of the form

$$\Omega=E_{\mathrm{exc}}+iT, \quad E_{\mathrm{exc}}=\begin{cases} 0, & \text{CDW, SDW} \quad (K=2k_F) \\ 2\varepsilon_F, & \text{SS} \quad (K=0), \end{cases} \tag{13}$$

where $E_{\mathrm{exc}}$ is the excitation energy to provide the system to undergo a phase transition; $T$ is the inverse of the relaxation time of the unstable ground state and can be also regarded as a "temperature"; $k_F=\pi n/2$ is the Fermi momentum ($n$ being the density of electrons) and $\varepsilon_F=-2t\cos k_F$. In this case, the determinant $D$ has the form

$$D\simeq\mu+\rho_F\lambda\ln\left|\frac{\Omega_0}{T}\right|, \tag{14}$$

which is valid for $|T/\Omega_0|\ll1$. This condition is similar to the BCS theory, where only the excitations of electrons around the Fermi level (with energies much less than the Debye energy) are taken into account. We will use the expression (14) to find the solutions of the equation $D=0$ for $|T/\Omega_0|<1$ and we expect the results to be reliable at least for not too big values of $|\lambda/\mu|$, which plays the role of the coupling constant.

The parameters in Eq. (14) are given by

$$\mu=\begin{cases}\pm 1+\dfrac{2}{\pi}(\sin k_F)w\pm\dfrac{w^2}{\pi^2}\pm\dfrac{1}{2\pi^2}\dfrac{k_F^2-\ln^2|\cos k_F|}{\sin^2 k_F}\,uw, & \text{SDW}\\ +\dfrac{1}{2\pi^3\sin k_F}\left(\dfrac{2k_F}{\tan k_F}\ln|\cos k_F|+k_F^2-\ln^2|\cos k_F|\right)uw^2, & \text{CDW}\\ 1, \quad \text{SS},\end{cases} \tag{15}$$

$$\lambda=\begin{cases}-\dfrac{1}{2}\left[u+2w\pm\dfrac{2}{\pi}\left(\sin k_F+\dfrac{\ln|\cos k_F|}{\sin k_F}\right)uw\pm\dfrac{2}{\pi}(\sin k_F)w^2, \right. & \text{SDW}\\ \left.+\dfrac{1}{\pi^2}\left(1-2\,\dfrac{k_F}{\tan k_F}+\dfrac{k_F^2}{\sin^2 k_F}+2\ln|\cos k_F|\right)uw^2\right], & \text{CDW}\\ u+2w, \quad \text{SS},\end{cases} \tag{16}$$

where $u\equiv U/t$, $w\equiv W/t$ ;

$$\Omega_0=8t\sin^2 k_F\begin{cases}(\cos k_F)^{-1}, & \text{CDW, SDW}\\ 1, & \text{SS},\end{cases} \tag{17}$$

$$\rho_F=(2\pi\sin k_F)^{-1}, \tag{18}$$

$\rho_F/t$ being the density of states at the Fermi level.

It follows that a transition to an ordered phase will occur at the critical ''temperature''

$$T_c=|\Omega_0|\exp\left(\frac{\mu}{\rho_F\lambda}\right), \tag{19}$$

with $\mu/\lambda<0$ (so that $|T_c/\Omega_o|<1$). In order to get the phase diagram for the Hamiltonian (1), we determine at first the regions in the $(w,u)$ space where the quantity $\mu/\lambda$ is negative (for each case: CDW, SDW, or SS); when more than one instability occurs in a given region, we decide for the phase that is held first, i.e., with the shortest relaxation time (or equivalently, with the biggest critical ''temperature'' $T_c$). We restrict our considerations to that region of the $(w,u)$ space containing the origin $u=w=0$ and where $\lambda/\mu$ never becomes infinite.

## III. PHASE DIAGRAM OF THE PK MODEL

For $U=0$ the Hamiltonian (1) reduces to the PK model.[3] By comparing the various critical ''temperatures'' (for CDW, SDW, and SS) we get the phase diagram plotted in Fig. 1: the investigated region is $|w|\sin k_F<\pi$ following from the condition $|T_c/\Omega_0|<1$, as discussed above. For $w>0$ we get only a SDW. For $w<0$ there is a SS phase for densities less than a critical one $n_c>(2/\pi)\arccos(e^{-2})\simeq 0.914$ and a CDW phase for $n>n_c$; the critical density $n_c$ tends to 1 as $n\to 1$. According to our calculations, at half-filling the system is in a SDW state for $w>0$ and in a CDW phase for $w<0$. Let us remark that at half-filling the condition $|T_c/\Omega_0|=1$ (when the effective coupling constant becomes infinite) determines the limits $w=\pm\pi$. It is interesting to note that close to our limit $w=-\pi$, around the value $w\simeq -3.5$, Sikkema and Affleck[5] found a phase-separation transition; in our approach, the existence of such a transition can be in principle analyzed by calculating the compressibility in the homogeneous phase.[12]

Since at $w=0$ the electrons move freely and at large negative $w$ the ground state contains only doubly occupied and empty sites, it was argued[3] that there should be a ''pairing transition'' at some negative $w_c$. Exact diagonalizations on chains up to 12 sites[2,3] have shown that at half-filling this transition occurs around $w_c\simeq -1.4$; but conformal field methods[4] and renormalization-group studies[5] have shown that $w_c=0$. In our calculation the only transition that occurs at half-filling (in the investigated range) is for $w=0$.

## IV. PHASE DIAGRAMS FOR THE PKH MODEL

In the limit of half-filling $(n\to 1)$ we found a SDW-CDW transition along the curve

$$u=-2w\left[1-\frac{w^2}{1+(1-1/\pi^2)w^2}\right], \tag{20}$$

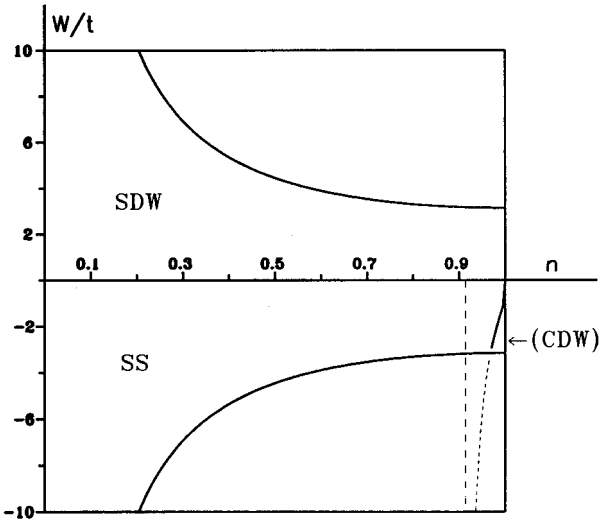


FIG. 1. Ground-state phase diagram of the 1D Penson-Kolb model in a mean-field-type approximation. Here and in the next figures the unlabeled (empty) parts correspond to regions beyond the validity limits of the used approximations.

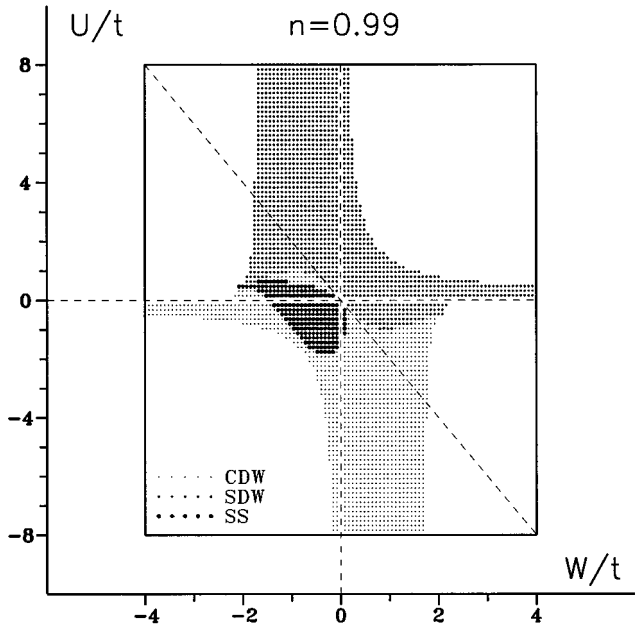


FIG. 2. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model near half-filling.

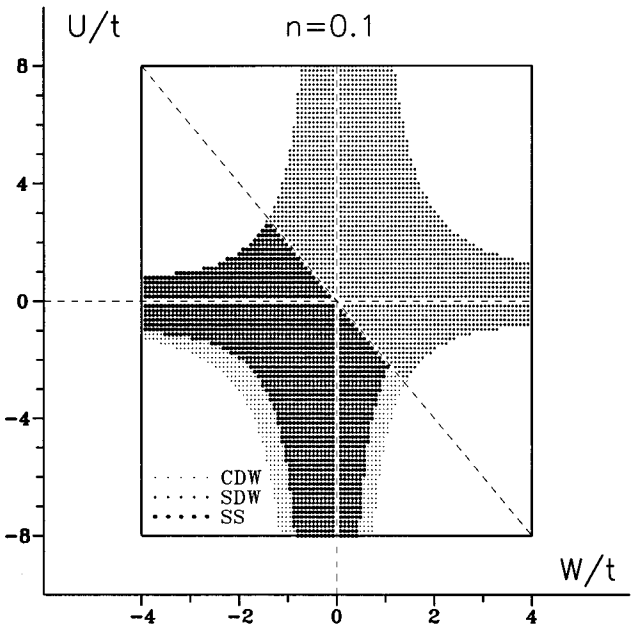


FIG. 4. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model at low density.

in agreement with the prediction of Hui and Doniach,[2] who found such a transition for $u,|w|\ll 1$ along the line $u\simeq -2w$. The obtained phase diagrams at various densities are presented in Figs. 2–4. The first remark is that the superconducting phase cannot appear when $u+2w>0$; this is due to the form of the bare potential $V(K)$, given by Eq. (6) in the particle-particle channel, which becomes repulsive in that region. However, it follows from Figs. 2–4 that we do not get systematically a SS phase for $V(K)<0$; some regions of the SDW and/or CDW phase still remain. The SS region decreases by increasing the density; it disappears for $n=1$. Technically, this fact comes mainly from the expression of $\Omega_0$, given by Eq. (17): it grows indefinitely as $n\rightarrow 1$ in the particle-hole channel, determining an increasing of the critical ''temperatures'' for the density-wave instabilities and thus a suppression of the SS phase. Let us note that near half-filling our phase diagram is qualitatively in agreement with that obtained by Hui and Doniach,[2] who studied the same model with $u>0$ and $w<0$ using exact diagonalization for samples of up to 12 sites. For example, for rather large values of $u$ and $w$ they found a sequence SDW $\rightarrow$ CDW $\rightarrow$ SS in passing from $u>-w$ to $u<-w$; this one can be also observed in our results from Fig. 2.

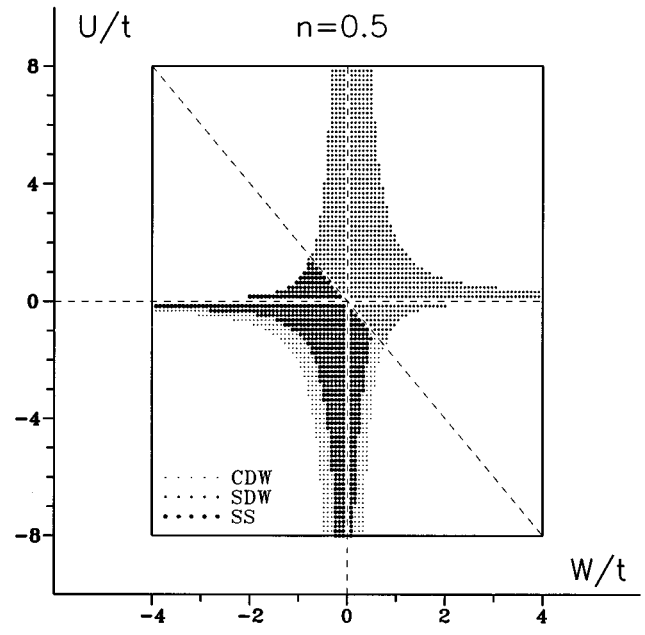


FIG. 3. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model in the quarter-filled case.

## V. CONCLUSIONS

In this paper we have presented phase diagrams for the PKH model at arbitrary densities of electrons and for moderate values of the parameters $W/t$ and $U/t$. Our results, obtained by using the simplest approximation of the Bethe-Salpeter equation in both particle-particle and particle-hole channels, are consistent with other works done at half-filling. In the particular case of the PK model ($U=0$) we have found for $|W|/t<\pi/\sin k_F$ a phase diagram similar to that corresponding to the Hubbard model in the same approximation;[9] at half filling, the only transition that occurs is a SDW-CDW at $W=0$. However, beyond the limits $|W|/t=\pi/\sin k_F$ indicated by our approach, we expect a qualitative change in the ground state of the PK model. To what extent or whether or not, this fact can be related to the phase separation transition found by Sikkema and Affleck[5] at $W/t\simeq -3.5$ near half-filling is a subject for further investigations.

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