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GROUND-STATE INSTABILITIES IN THE ONE-DIMENSIONAL PENSON—KOLB—HUBBARD MODEL

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Неустойчивости основного состояния одномерной модели Пенсона—Колба—Хаббарда

Исследуются различные виды неустойчивости (*CDW*, *SDW*, *SS*) в одномерной модели Хаббарда с взаимодействием, отвечающим одновременному перескоку пары электронов. При этом используется приближенное уравнение Бете—Солпитера. Исследование проводится для произвольной электронной плотности и любых значений модельных параметров. При отсутствии одноузельного взаимодействия, в соответствии с недавно полученными результатами, не обнаруживается перевода при половинном заполнении для любого конечного отрицательного параметра, отвечающего одновременному перескоку пары электронов. В нашем вычислении предполагается, что модель Пенсона—Колба (t, W) с $|W/t| < \pi/\sin k_F$ качественно ведет себя как модель Хаббарда (t, U). Представлены фазовые диаграммы модели Пенсона—Колба—Хаббарда (t, U, W) при различных плотностях.

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Ground-State Instabilities in the One-Dimensional Penson—Kolb—Hubbard Model

Different kinds of instabilities (*CDW*, *SDW*, *SS*) in the 1D Hubbard model with pair-hopping interaction are investigated using and 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 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.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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1 Introduction

The studies of the one-dimensional models of correlated electronic systems can be a primary source to understand the occurence of the high temperature superconductivity in materials which physics 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 which 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 which may lead to the insulating phase of the cuprates.

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

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

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 1D; a spin-gap transition at half filling for $W < 0$ has been the subject of some controversy [2, 3, 4, 5]. Recently, some variantes of the PKH model were solved by 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 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 occurence of instabilities in the ground-state of the PKH model in the same manner [9] as it was done 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 Γ 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.

2 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

$$\chi(k,\omega) = -i \int dt\, e^{i\omega t} \, < T\{\mathcal{D}(k,t)\mathcal{D}^{\dagger}(k,0)\} > \tag{2}$$

where T is the usual chronological operator and $\mathcal{D}(k,t)$ is a density operator. The brackets indicate an average in the ground-state (for zero-temperature case) or a statistical average (for finite-temperature case). If $\mathcal{D}(k,t)$ is a charge-density operator, the corresponding susceptibily Γ_{CDW} will test the *charge density wave* (CDW) instability; in a similar way can be defined the susceptibilities relevant to the other kinds of instabilities: Γ_{SDW} for *spin density wave* (SDW), Γ_{SS} for *singlet superconductivity* (SS) and Γ_{TS} for *triplet superconductivity* (TS). The correspondence between these quantities and the components of the vertex function can be found in Refs. [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:

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

where Γ can be any of the quantities Γ_{CDW}, Γ_{SDW} or Γ_{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 (Ω) denotes the transfer momentum (frequency) in the particle-hole (ph) channel and the total momentum (frequency) in the particle-particle (pp) channel,

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

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

where the addition or subtraction of the k-vectors are defined modulo 2π (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 expresion

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

where N denotes the number of sites in the chain.

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

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

with

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

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

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

where $\widehat{M}$ is the 3×3 matrix

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

and

$$\begin{cases} g = \dfrac{1}{N}\sum_q \mathcal{G}(q;K,\Omega) \\[2ex] c_n = \dfrac{1}{N}\sum_q (\cos q)^n\, \mathcal{G}(q;K,\Omega)\ ,\ \ n = 1,2 \\[2ex] s_n = \dfrac{1}{N}\sum_q (\sin q)^n\, \mathcal{G}(q;K,\Omega)\ ,\ \ n = 1,2 \\[2ex] p = \dfrac{1}{N}\sum_q \sin q \cos q\, \mathcal{G}(q;K,\Omega) \end{cases} \tag{11}$$

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

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

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

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

where E_{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 $\mid T/\Omega_0 \mid \ll 1$. 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

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

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

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

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

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

ρ_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 μ/λ is negative (for each case: CDW, SDW or SS); when more than one instability can occur in a given region, we decide for the phase which 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 λ/μ never becomes infinite.

3 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 $n_c > \frac{2}{\pi} Arccos(e^{-2}) \simeq 0.914$ and a CDW phase for $n > n_c$; the critical density n_c tends to one 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 analysed 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 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 $w_c \doteq 0$. In our calculation the only transition which occurs at half filling (in the investigated range) is for $w = 0$.

4 Phase diagrams for the PKH model

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

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

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 the superconducting phase can not appear when $u + 2w > 0$; this is due to the form of the bare potential $V(K)$, given by Eq. (6) in the *pp* 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 SDW or (and) CDW phase still remain. The SS region decreases by increasing the density; it disappears for $n = 1$. 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 big values of u and w they found a sequence $SDW \to CDW \to SS$ in passing from $u > -w$ to $u < -w$; this one can be also observed in our results from Fig. 2.

5 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 mean-field-type approximation predicts results 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 which 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 extend this fact can be related or not with 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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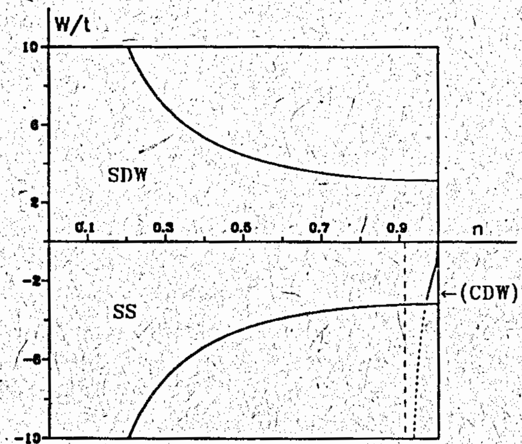

Figure 1. Ground-state phase diagram of the 1D Penson-Kolb model in a mean-field-type approximation. Here and in the next figures the unlabeled (empty) parts correspond to regions beyond the validity limits of the used approximations.

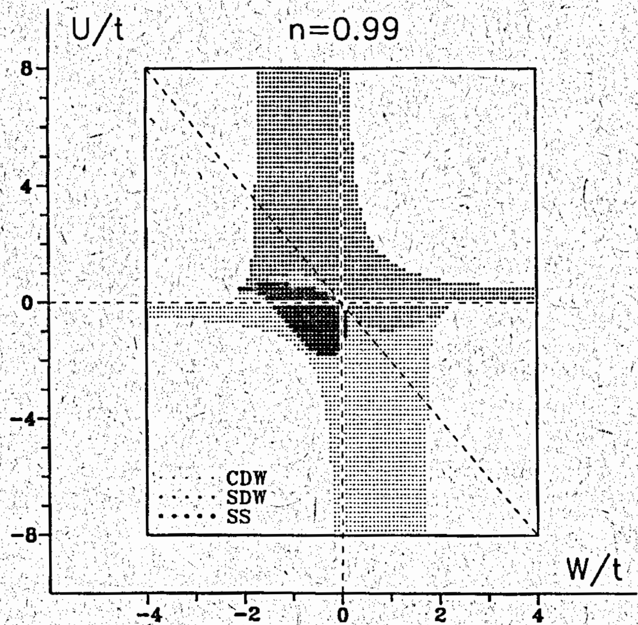

Figure 2. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model near half filling.

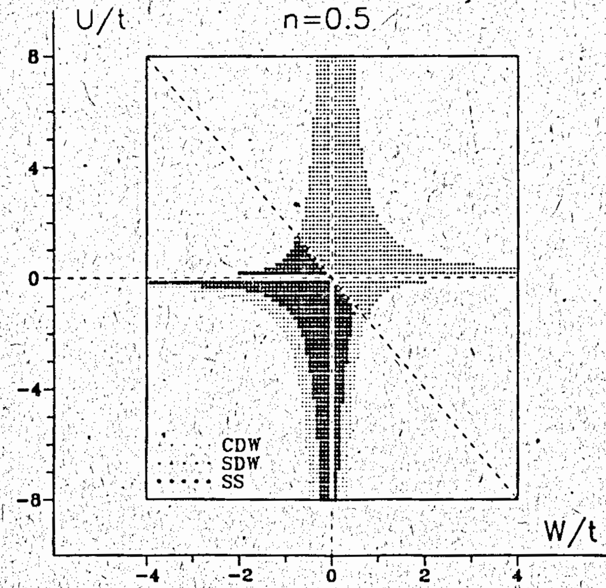

Figure 3. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model in the quarter filled case.

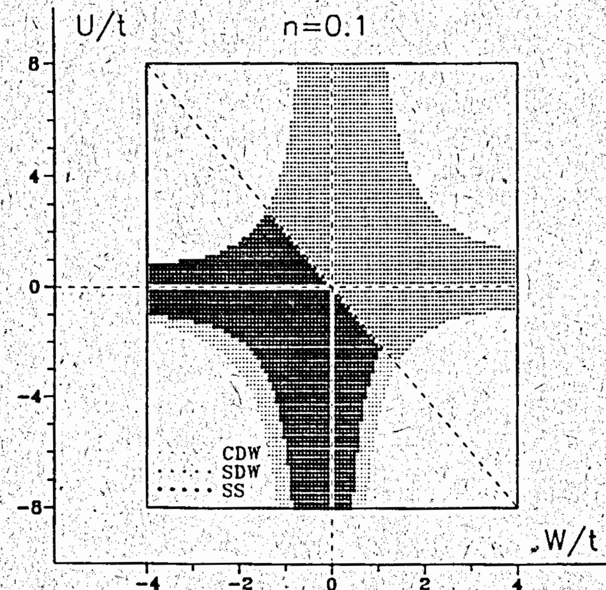

Figure 4. Ground-state phase diagram of the 1D Penson-Kolb-Hubbard model at low density.

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