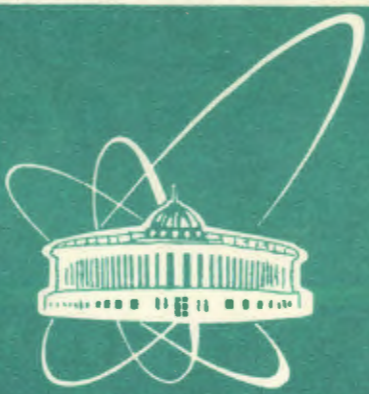

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1*D* (t,U,X)-MODEL: GROUND STATE PHASE DIAGRAM IN A MEAN-FIELD TYPE APPROXIMATION

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I Introduction

The $(t, U, X)-$model has been introduced [1] in order to describe the properties of quasi-1D materials with a highly screened interelectronic potential, like conducting polymers. The Hamiltonian corresponding to this model

$$H = -t\sum_{i,\sigma}(c^{+}_{i+1,\sigma}c_{i,\sigma} + H.c.) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} + X\sum_{i,\sigma}(c^{+}_{i+1,\sigma}c_{i,\sigma} + H.c.)(n_{i,-\sigma} + n_{i+1,-\sigma}) \quad (1)$$

contains, besides the one-electron part in the tight binding approximation (with t the bandwidth parameter), the on-site (or Hubbard) interaction U and a bond-site (or hopping) term X which accounts for the interaction between a site-electron and another residing on the adjacent bond; $c^{+}_{i,\sigma}\,(c_{i,\sigma})$ are the usual Fermi creation (annihilation) operators in the Wannier representation. In the case of a completely screened electron-electron potential ($\delta-$function type), X/U is a small quantity of the same order of magnitude as the overlap $S \ll 1$ between the atomic orbitals, all the other nearest-neighbor interaction parameters being of order S^2 and thus negligible in the tight binding picture [1, 2].

For $X = 0$ rel.(1) reduces to the Hubbard model, solved by "Bethe ansatz" many years ago [3] and whose properties such as the correlation functions have been intensively studied in the later time, for both attractive [4, 5] and repulsive [6]–[13] case. The effect of the X term on the various instabilities of the system is less known; at half-filling it seems not to play a considerable role [14]– [17], but how the picture changes with the band filling was not investigated, in our knowledge, until now. On the other hand, in the 2D case, the contribution of the X term was proposed to explain the "hole superconductivity" mechanism [18, 19]; in a definite range of the parameters (determined below), a similar effect can be seen in 1D too.

A possible approach in studying the 1D systems[1] is the perturbation theory[2]. In spite of the difficulties encountered in the 1D case, especially due to the divergences in the bare particle-particle and particle-hole diagrams, it can offer nevertheless a qualitative description of the model [22]. In the framework of the 1D Fermi gas model (or, "g-ology"), the perturbational expansion can

[1] For an excellent review of recent results and different approaches to the theory of correlated Fermions in one dimension, see Ref. [20].

[2] A pioneering contribution to this field is the work of Bychkov *et al.* [21].

be improved by the renormalization group technique [23], the exact solvable models providing a good test for such approximate results.

The aim of this paper is to determine, using the (zero temperature) Green function formalism in the Bloch representation, the occurrence of the possible instabilities in the ground state of the 1D $(t,U,X)-$model. This can be done by finding the poles of the vertex function Γ which obeys the Bethe-Salpeter equation; by setting the irreducible vertex part equal to the bare interaction and using the 'free' expression for the single-particle propagators, this equation can be solved. In such a way, which amounts to making a mean-field type approximation, one finds a transition to an ordered state at a finite frequency (or equivalently, temperature), in contradiction with the well known fact that there is no phase transition in an 1D system with short range forces [24]. However, by comparing these mean-field 'transition temperatures' one gets [25, 26] a phase diagram which, in the case of the 1D "g-ology", is strikingly similar to that obtained from more rigorous treatments.

II The vertex equation

The Hamiltonian (1) can be rewritten in the Bloch representation as

$$H=\sum_{k,\sigma}\varepsilon(k)c^{+}_{k,\sigma}c_{k,\sigma}+\frac{1}{2N}\sum_{k_1,\ldots,k_4,\sigma}V_{k_3,k_4,k_2,k_1}c^{+}_{k_3,\sigma}c^{+}_{k_4,-\sigma}c_{k_2,-\sigma}c_{k_1,\sigma} \qquad (2)$$

where

$$\varepsilon(k)=-2t\cos(ak),\quad t>0 \qquad (3)$$

$$V_{k_3,k_4,k_2,k_1}=V(k_1,k_3)\,\delta(k_1+k_2,k_3+k_4) \qquad (4)$$

with

$$V(k_1,k_3)=U-2X\left[\frac{\varepsilon(k_1)}{t}+\frac{\varepsilon(k_3)}{t}\right] \qquad (5)$$

The $k-$sums in (2) run over the first Brillouin zone $BZ=\left(-\frac{\pi}{a},\frac{\pi}{a}\right]$, a is the lattice constant and N the number of lattice sites; the $\delta-$function in (4) assures the momentum conservation up to a reciprocal lattice vector.

Let us consider now the vertex function Γ which describes the scattering of electrons and can reflect the instabilities of the system; it obeys the Bethe-Salpeter equation [27], diagramatically pictured in Fig.1, where $I(J)$ is the irreducible part of Γ in the particle-hole (particle-particle) channel and the double line denotes the exact one-particle propagator G. There are six distinct

choices for spin variables in Γ, as shown in Fig.2; we denoted them by Γ_l $(l=1,6)$. A singularity in Γ indicates the onset of an instability to an ordered phase and there are four types of ordering usually studied in an 1D system: *charge density wave* (CDW) and *spin density wave* (SDW) in the particle-hole channel, *singlet superconductivity* (SS) and *triplet superconductivity* (TS) in the particle-particle channel. The relevant vertex functions corresponding to each of them are:

$$\begin{array}{ll} CDW: & \Gamma_1+\Gamma_2 \\ SDW: & \Gamma_1-\Gamma_2 \text{ (longitudinal)};\ \Gamma_3 \text{ (transverse)} \\ SS: & \Gamma_4+\Gamma_5 \\ TS: & \Gamma_4-\Gamma_5\ (S_z=0);\ \Gamma_6\ (S_z=\pm 1) \end{array}$$

where S_z denotes the value of the total spin projection on the third axe.

In our above mentioned approximation

$$I(J)\simeq V,\ G\simeq G_0 \qquad (6)$$

the TS phase will not occur ($\Gamma_4=\Gamma_5,\Gamma_6=0$); the other three vertex functions $\Gamma_{CDW}\equiv\Gamma_1+\Gamma_2$, $\Gamma_{SDW}\equiv\Gamma_3$ [3] and $\Gamma_{SS}\equiv\Gamma_4$ can be determined from the following equation

$$\xi\Gamma(k_1,k_3;K,\Omega)=V(k_1,k_3)+\frac{a}{2\pi}\int_{BZ}dk\,V(k_1,k)\,\mathcal{G}(k;K,\Omega)\,\Gamma(k,k_3;K,\Omega) \qquad (7)$$

where $K(\Omega)$ is the conserved total momentum (frequency),

$$\xi=\begin{cases}1 & SDW,SS\\ -1 & CDW\end{cases} \qquad (8)$$

$$\mathcal{G}(k;K,\Omega)=\frac{i}{2\pi}\int_{-\infty}^{+\infty}d\omega\,G_0(k,\omega)\times\begin{cases}G_0(\overline{k-K},\omega-\Omega) & CDW,SDW\\ G_0(\overline{K-k},\Omega-\omega) & SS\end{cases} \qquad (9)$$

the overline denoting the corresponding reduced vector in the BZ; the 'free' propagator G_0 has the usual form

$$G_0(k,\omega)=\frac{\theta(|k|-k_F)}{\omega-\epsilon(k)+i\eta}+\frac{\theta(k_F-|k|)}{\omega-\epsilon(k)-i\eta}\ ,\quad k\in BZ,\ \eta\geq 0 \qquad (10)$$

[3] The longitudinal and transverse components of the spin density should be equal in the disordered phase; in determining the transition to the ordered phase, we chose for convenience Γ_3.

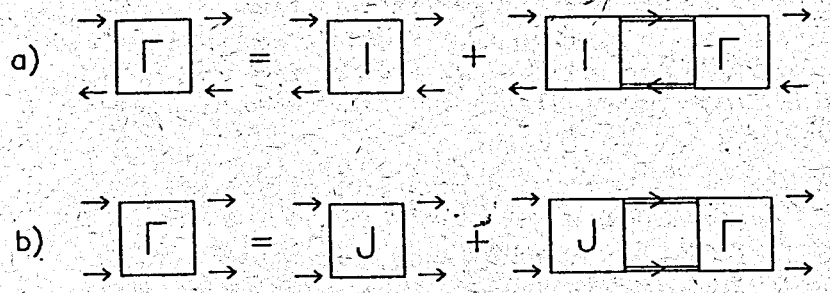

Figure 1: The Bethe-Salpeter equation for: a) particle-hole b) particle-particle channel.

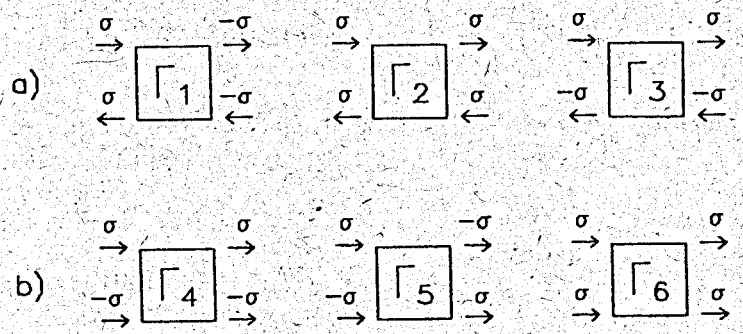

Figure 2: The choices of spin variables for Γ in: a) particle-hole b) particle-particle channel.

with θ the step function and

$$\epsilon(k) = \varepsilon(k) - \varepsilon(k_F) \tag{11}$$

the excitation energy.

The equation (7), with V given by (5), can be solved by iteration; it has a solution of the form

$$\Gamma(k_1, k_3) = \mathcal{U} - 2\mathcal{X}_1 \frac{\varepsilon(k_1)}{t} - 2\mathcal{X}_3 \frac{\varepsilon(k_3)}{t} - 4\mathcal{X}_{13} \frac{\varepsilon(k_1)\varepsilon(k_3)}{t^2} \tag{12}$$

where $\mathcal{U}$, $\mathcal{X}_1$, $\mathcal{X}_3$ and $\mathcal{X}_{13}$ depend on K and Ω and can be found, after replacing (12) in (7), by identification; the result is the following algebraic system:

$$\hat{M} \begin{pmatrix} \mathcal{U} & \mathcal{X}_3 \\ \mathcal{X}_1 & \mathcal{X}_{13} \end{pmatrix} = \begin{pmatrix} U & X \\ X & 0 \end{pmatrix} \tag{13}$$

where $\hat{M}$ is the 2×2 matrix

$$\hat{M} = \begin{pmatrix} \xi + c_0 \frac{U}{t} + 4c_1 \frac{X}{t} & 4c_1 \frac{U}{t} + 16c_2 \frac{X}{t} \\ c_0 \frac{X}{t} & \xi + 4c_1 \frac{X}{t} \end{pmatrix} \tag{14}$$

and

$$c_j(K, \Omega) = -\frac{at}{2\pi} \int_{BZ} dk \left[-\frac{\varepsilon(k)}{2t} \right]^j \mathcal{G}(k; K, \Omega) \quad , \quad j = 0, 1, 2 \tag{15}$$

The quantity which we are interested in is $D \equiv \det(\hat{M})$. If $D \neq 0$, the relations (12)–(15) define a solution of the vertex equation (7). In the non-interacting case ($U = X = 0$), $D = 1$. As the interaction turns on, D can vanishes; in this case, the transposed homogeneous equation corresponding to (7) or (13) gets its first nonzero solution, Γ has a pole, and an instability of the ground state is coming out [27]. The transition points to the ordered phase are therefore determined by the condition $D = 0$.

The coefficients $c_j(K, \Omega)$ can be calculated from rel.(3), (9), (10) and (15); c_0 is actually (up to a factor $\pm t$) the contribution of the elementary particle-particle (Δ_0) or particle-hole (Π_0) diagrams and the others two (for $j = 1$ or 2) can be also expressed in terms of these quantities. All of them are singular in the static limit ($\Omega \to 0$) at $|\overline{K}| = 2k_F$ (CDW, SDW) or $|\overline{K}| = 0$ (SS); in this case the real part of $\det(\hat{M})$ has the following form:

$$D \simeq \mu + g\lambda \ln \left| \frac{4tE}{\Omega} \right| \quad , \quad \Omega \ll 4t \tag{16}$$

where

$$\mu = \begin{cases} \left[1-(1-n)\dfrac{X}{t}\right]^2 & SS \\ \left[1 \pm \dfrac{\ln|\cos(\frac{\pi}{2}n)|}{\pi\tan(\frac{\pi}{2}n)}\dfrac{X}{t}\right]^2 & CDW \\ & SDW \end{cases} \tag{17}$$

$$\lambda = \begin{cases} \dfrac{U}{t} + 8\cos\left(\dfrac{\pi}{2}n\right)\dfrac{X}{t} - \\ \dfrac{8}{\pi}\left[\sin\left(\dfrac{\pi}{2}n\right) + \dfrac{\pi}{2}(1-n)\cos\left(\dfrac{\pi}{2}n\right)\right]\left(\dfrac{X}{t}\right)^2 & SS \\ \pm\dfrac{1}{2}\left[\dfrac{U}{t} + 8\cos\left(\dfrac{\pi}{2}n\right)\dfrac{X}{t}\right] + \\ \dfrac{4}{\pi}\sin\left(\dfrac{\pi}{2}n\right)\left[\cos(\pi n) + \dfrac{\ln|\cos(\frac{\pi}{2}n)|}{\tan^2(\frac{\pi}{2}n)}\right]\left(\dfrac{X}{t}\right)^2 & CDW \\ & SDW \end{cases} \tag{18}$$

$$E = 2\sin^2\left(\frac{\pi}{2}n\right)\begin{cases} 1 & SS \\ \cos^{-1}(\frac{\pi}{2}n) & CDW, SDW \end{cases} \tag{19}$$

$$g = \left[2\pi\sin\left(\frac{\pi}{2}n\right)\right]^{-1} \tag{20}$$

g/t being the density of states at the Fermi level and n the band filling factor ($ak_F = \dfrac{\pi}{2}n, n = 0 \div 2$).

III The phase diagram

It follows from rel.(16) that a transition to an ordered phase will appear for $\lambda < 0$ at a finite frequency or temperature (in adimensional units)

$$T_c = |E|\exp\left(\frac{\mu}{g\lambda}\right) \tag{21}$$

which is the mean-field type 'transition temperature' given by our approximation (6). If one now asks in what regions of the $(X/t, U/t)$–plane is one of these 'transition temperatures' higher than all the others (at a given density) one gets the pictures from Fig.3.

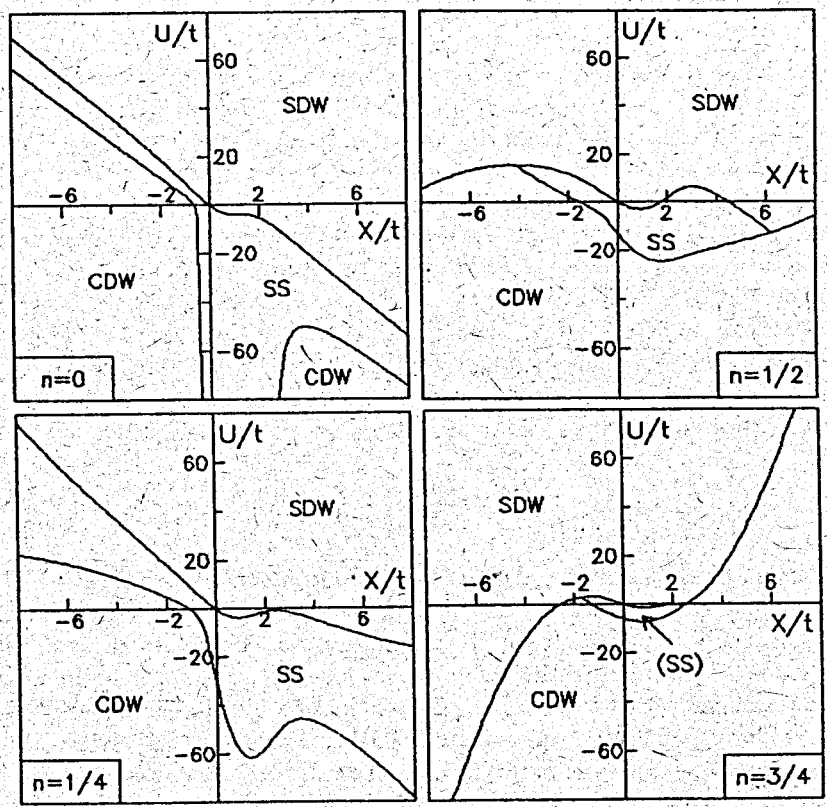

Figure 3: The ground state phase diagram of the 1D (t, U, X)–model at various densities; at half-filling, a SDW phase appears in the upper half-plane and CDW in the lower one (the X term has no effect on the phase diagram of the Hubbard model).

In drawing the phase diagram at various densities, we may take $n \leq 1$; the pictures corresponding to $n > 1$ can be obtained by using the symmetry of rel.(21) under the transformation

$$n \to 2 - n \ , \ X \to -X \tag{22}$$

which is of course a consequence of how the bond-site interaction term changes under a particle-hole transformation: although the X term breaks the charge conjugation symmetry of the Hamiltonian (1)[15, 16], its symmetric part under this transformation simply renormalizes the bandwidth parameter[17], only the antisymmetric one 'surviving' as a two-particle interaction.

Let us consider first the case of the Hubbard model ($X = 0$). For $U > 0$ a SDW with the wave vector $2k_F$ is formed, in agreement with the mean-field results for the 1D Fermi gas model when all the coupling constants g_i $(i = 1, 4)$ are equal (see for example [18, 23, 24]); the charge dynamics as well as other interesting properties of the repulsive Hubbard model [6]-[13] are not available in this poor approximation. For $U < 0$, unlike the "g-ology" prediction (a SS phase), our calculation determines a critical value of the attraction

$$\frac{U_c}{t} = \frac{2\pi \sin(\frac{\pi}{2}n)}{\ln|\cos(\frac{\pi}{2}n)|} \tag{23}$$

which separates a dominant SS phase ($U > U_c$) from a CDW phase ($U < U_c$); this is a direct consequence of working with the exact dispersion law (3) in the whole BZ, not only with its linearized expression around the Fermi points. Our result is consistent with earlier works which indicate a phase of "correlated" [28] or "localized" Cooper pairs (a superposition of CDW and SS) [29]: from rel.(23) follows that the ground state is a CDW at half-filling, as it was pointed out by Shiba [30]; at other densities, a superconductor state is favored in the weak coupling regime [22, 31]. More recently, Bogoliubov and Korepin [4, 5] showed that for $n < 1$ the CDW correlator decays faster with the distance than the correlator of pairs of fields in the singlet state, and thus the Cooper pairs are formed in the attractive Hubbard model.

In our mean-field type approximation, at half-filling the X term does not affect the phase diagram of the Hubbard model, as other results indicate too. By taking into account only the interactions at the Fermi surface, there is no coupling between the bond and site charge densities for $n = 1$ (see rel.(5)) [14]; however, in a linearized version of the Hamiltonian (2), the $k-$dependence of the bond-site interaction cannot be neglected *a priori* and a evaluation of the X term in the Boson representation [15] gives rise to an Umklapp scattering which enhances slightly the dimerization in an extended model of polyacetylene. The effect of the off-diagonal Coulomb interactions on the ground state of

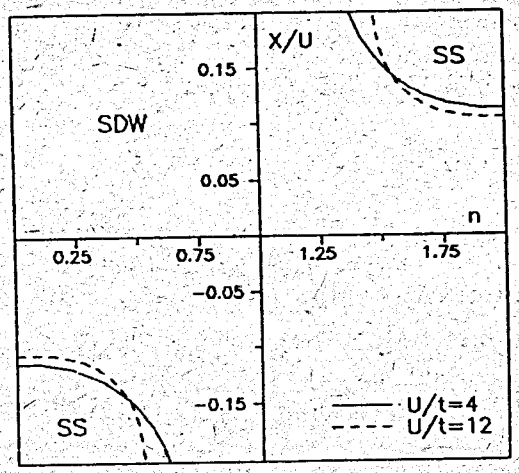

Figure 4: The phase diagram of the 1D $(t, U, X)-$model for $|X| \ll U \sim 4t$.

a general 1D "Peierls-Hubbard" model at half-filling was extensively analyzed by Campbell *et al.* [16]; using a combination of Lanczos exact diagonalizations with phase randomization techniques, they found that, even for intermediate coupling, the X term determines merely a renormalization of the bandwidth parameter. Valence bond calculations for the 1D $(t, U, X)-$model [17] indicate also only a weak dependence of correlation functions on X/U, with no effect on the ground state phase diagram of the Hubbard model.

Going away from the half-filling, an increasing SS zone appears and a rearrangement of the CDW and SDW domains, as can be seen in the right side pictures of Fig.3. For densities below a quarter filled band, the SS zone seems to grow along two directions: $X = t$ (for $U < 0$) and $U \simeq -8X \cos(\frac{\pi}{2}n)$, the region around the last one becoming narrower for $n < 0.2$.

For more realistic parameters of the model ($|X| \ll U \sim 4t$), the phase diagram looks like in Fig.4, where the curve separating the SS and SDW regions depends slightly on U/t. The occurrence of a SS instability, even in the region where the bare potential V given by rel.(5) is always positive ($|X|/U < 0.125$), can be interpreted as follows: at low densities, a bond-site attraction favors successive interactions between the same two electrons; if the on-site repulsion is not too large ($U < 10\ |X|$, according to Fig.4) the attractive part of the potential can become more effective than the repulsive one and the electrons will be localized in pairs. By increasing the density, the average distance between the pairs decreases, an electron can find an other 'partner' and the picture breaks down, the bond-site attraction determining

now a delocalization of electrons. A similar effect has a bond-site repulsion in the case of a band almost full, suggesting us the "hole superconductivity" mechanism proposed by Hirsh [18, 19] in 2D.

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