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THE EFFECT OF A BOND-SITE INTERACTION ON THE GROUND-STATE INSTABILITIES OF THE ONE-DIMENSIONAL HUBBARD MODEL

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Бузату Ф.Д.
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Влияние межузельного взаимодействия
на нестабильности основного состояния
одномерной модели Хаббарда

В пертурбативном подходе анализируются нестабильности основного состояния для одномерной решеточной системы электронов с одноузельным (хаббардовским) и межузельным (прыжковым) взаимодействиями. Представлена фазовая диаграмма при нулевой температуре для различного заполнения зоны; притягивающее (отталкивающее) межузельное взаимодействие способствует возникновению сверхпроводящего состояния при низких концентрациях электронов (дырок). Обсуждается сравнение с точными результатами для модели Хаббарда и предыдущими работами для частных случаев.

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The Effect of a Bond-Site Interaction
on the Ground-State Instabilities
of the One-Dimensional Hubbard Model

The ground-state instabilities for a one-dimensional lattice system of electrons with on-site (Hubbard) and bond-site (hopping) interactions are analyzed in a perturbative approach. The zero temperature phase diagram at different band fillings is drawn; an attractive (repulsive) bond-site interaction favors the appearance of a superconductor state at low concentrations of electrons (holes). A comparison with the exact results for the Hubbard model and previous works for particular cases is also discussed.

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

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1. Introduction

The model considered in this work consists of the one-dimensional (1D) Hubbard Hamiltonian plus a bond-site interaction term X describing the coupling between a site electron and another residing on the adjacent bond,

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

where the Wannier representation was used; it is known as the (t, U, X) model and has been proposed [1] as relevant to quasi-1D materials with very screened electron-electron interactions like conducting polymers. In 2D, Hirsch [2] introduced the "hole superconductivity" using the same model (1). Exact results at $X = t$ [3, 4] indicate also the bond-site interaction as significant for a possible superconductor state.

We investigate in this paper the effect of the X term on the ground-state instabilities of the system in a perturbative approach. Starting from the Bloch representation of the (t, U, X) model

$$\mathcal{H} = \sum_{k;\sigma}\varepsilon(k)c^{\dagger}_{k,\sigma}c_{k,\sigma} + \frac{1}{2N}\sum_{k_1,\ldots,k_4;\sigma}\left\{U - 2\frac{X}{t}[\varepsilon(k_1) + \varepsilon(k_3)]\right\}\delta_{k_1\oplus k_2,k_3\oplus k_4}c^{\dagger}_{k_1,\sigma}c^{\dagger}_{k_2,-\sigma}c_{k_4,-\sigma}c_{k_3,\sigma}, \quad (2)$$

where

$$\varepsilon(k) = -2t\cos(ak) \quad (3)$$

(N denotes the number of sites and $\oplus$ – symbol stands for the usual addition operation and the reduction to the first Brillouin zone (BZ); we use also $\ominus$ with a similar meaning.) we solve the corresponding Bethe-Salpeter equation in the simplest approximation, both in the particle-particle and particle-hole channel. The poles of the solutions determine the transition 'temperatures' to an ordered state (CDW, SDW or SS); by comparing them one gets a ground state phase diagram (at $T = 0$) depending on the parameters U/t, X/t and the band filling factor n [5]. In the particular case of the Hubbard model we find a SDW state for $U > 0$ and a SS (CDW) phase for $U_c < U < 0$ ($U < U_c$). At $n = 1$ the X term brings no contribution; away from half filling, a rather small bond-site attraction (repulsion) determines the pairing of electrons (holes). An effective Hubbard constant can be introduced at low densities, explaining the occurrence of a superconductor phase around $X = t$ direction.

2. Bethe-Salpeter equation

The Bethe-Salpeter equations for particle-hole (ph) and particle-particle (pp) channel are both represented in Fig. 1; each of them decouples in three independent equations [6], two for the case when the total spin equals one – ${}^0\Gamma^-_{ph}$ (${}^0\Gamma^+_{pp}$) and ${}^1\Gamma_{ph}$ (${}^1\Gamma_{pp}$), corresponding to the projection of the total spin on the third axis $\sigma_z = 0$ and respectively $\sigma_z = \pm 1$, and one when the total spin is zero – ${}^0\Gamma^+_{ph}$ (${}^0\Gamma^-_{pp}$).

There are four kinds of instabilities usually studied in 1D systems. A *charge density wave* (CDW) can be defined as a collective excitation in the ph channel in the singlet state and such a phase appears as a complex pole of ${}^0\Gamma^+_{ph}$ in the total frequency variable Ω ; similar definitions can be done for the *spin density wave* (SDW), *singlet superconductivity* (SS) or *triplet superconductivity* (TS) instabilities. The relevant Γ–quantities in each case are

$$\begin{array}{lll} CDW & : & {}^0\Gamma^+_{ph} = \Gamma_2 + \Gamma_1 \\ SDW & : & {}^0\Gamma^-_{ph} = \Gamma_2 - \Gamma_1 \ (\sigma_z = 0) \ ; \ {}^1\Gamma_{ph} = \Gamma_3 \ (\sigma_z = \pm 1) \\ SS & : & {}^0\Gamma^-_{pp} = \Gamma_4 - \Gamma_5 \\ TS & : & {}^0\Gamma^+_{pp} = \Gamma_4 + \Gamma_5 \ (\sigma_z = 0) \ ; \ {}^1\Gamma_{pp} = \Gamma_6 \ (\sigma_z = \pm 1) \ , \end{array} \tag{4}$$

where Γ_1 to Γ_6 correspond to the six distinct choices of the spin variables, as can be seen in Fig. 2.

The Bethe-Salpeter equation is an exact equation, but we consider only its first approximation, when the exact Green function G is replaced by the free one G^0 and the irreducible part I (J) by Γ in the first perturbative order (proportional with the bare potential) :

$$G \simeq G^0 \ , \ \ I(J) \simeq \Gamma^{(1)}. \tag{5}$$

In this way we get the following approximate Bethe-Salpeter equation [7] :

$$\xi\Gamma(k,k';K,\Omega) = \frac{i}{2\pi}V(k,k';K) + \sum_{k''} V(k,k'';K)\mathcal{G}(k'';K,\Omega)\Gamma(k'',k';K,\Omega), \tag{6}$$

where Γ can be ${}^0\Gamma^+_{ph}$ (CDW) , ${}^0\Gamma^-_{ph} = {}^1\Gamma_{ph}$ (SDW) or ${}^0\Gamma^-_{pp}/2$ (SS) ; the TS case does not occur in our approximation. $K \in BZ$ denotes the total conserved momentum and the other quantities which appear in Eq. (6) are defined by

$$\xi = \begin{cases} -1 & CDW \\ 1 & SDW, SS \end{cases} \tag{7}$$

$$\mathcal{G}(k;K,\Omega) \ = \ \frac{i}{2\pi}\int_{-\infty}^{+\infty} d\omega \, G^0(k \oplus K/2, \omega + \Omega/2) \times \begin{cases} G^0(k \ominus K/2, \omega - \Omega/2) & CDW, SDW \\ G^0(K/2 \ominus k, \Omega/2 - \omega) & SS \end{cases} \tag{8}$$

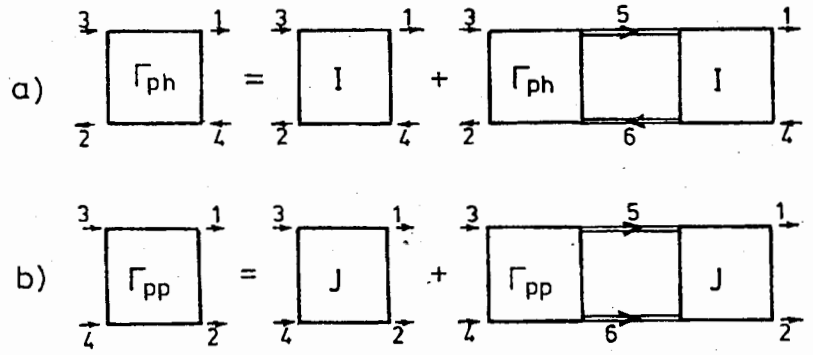


Figure 1. Bethe-Salpeter equation in: a) the particle-hole and b) the particle-particle channel.

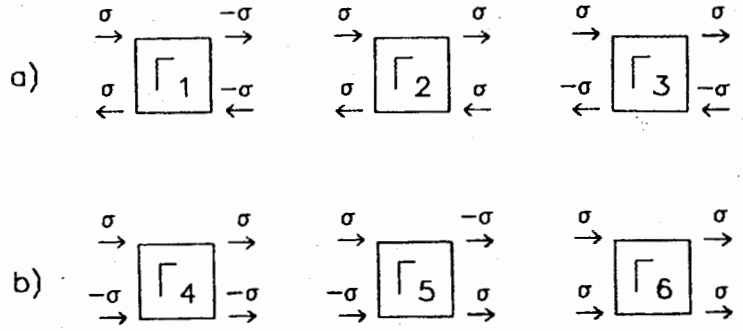


Figure 2. Choices of spin variables for Γ in: a) the particle-hole and b) the particle-particle channel.

$$V(k,k';K)=\frac{1}{N}\left\{U+4X_K\left[\cos(ak)+\cos(ak')\right]\right\}\quad,\quad X_K\equiv X\cos(aK/2). \tag{9}$$

Equation (6) can be solved analytically; its solution has the following structure, which can be guessed by iteration

$$\Gamma(k,k')\equiv\frac{i}{2\pi N}\left[\mathcal{U}+4\mathcal{X}_1\cos(ak)+4\mathcal{X}_2\cos(ak')+16\mathcal{X}_{1,2}\cos(ak)\cos(ak')\right]; \tag{10}$$

where the unknown quantities can be found from the matrix system

$$\widehat{M}\begin{pmatrix}\mathcal{U} & \mathcal{X}_2\\ \mathcal{X}_1 & \mathcal{X}_{1,2}\end{pmatrix}=\begin{pmatrix}U & X_K\\ X_K & 0\end{pmatrix} \tag{11}$$

with $\widehat{M}$ the 2×2 matrix

$$\widehat{M}\equiv\begin{pmatrix}\xi+c_0\dfrac{U}{t}+4c_1\dfrac{X_K}{t} & 4c_1\dfrac{U}{t}+16c_2\dfrac{X_K}{t}\\ c_0\dfrac{X_K}{t} & \xi+4c_1\dfrac{X_K}{t}\end{pmatrix} \tag{12}$$

and

$$c_j(K,\Omega)\equiv-\frac{t}{N}\sum_k\left[\cos(ak)\right]^j\mathcal{G}(k;K,\Omega)\quad,\quad j=0,1,2. \tag{13}$$

We are interested here only in the determinant D of the $\widehat{M}$ matrix :

$$D(K,\Omega)\equiv\det(\widehat{M})=1+\xi c_0\frac{U}{t}+8\xi c_1\frac{X_K}{t}+16(c_1^2-c_0c_2)\left(\frac{X_K}{t}\right)^2. \tag{14}$$

In the absence of the interactions $D=1$; as the interaction turns on, D can vanish indicating the occurrence of an instability in the ground state of the system.

Let us consider first the *ph* channel. The minimum energy at which an excitation can appear is zero and it happens when the total momentum K equals $k_F\oplus k_F$; this is the Peierls instability and reflects the degeneration which occurs in 1D systems: by exciting an electron from $-k_F$ to $+k_F$ you need zero energy. The Cooper instability occurs at $K=0$ and it is characteristic not only of 1D systems; the required excitation energy is $2\varepsilon_F$ and corresponds to adding or taking away two particles from the system. Consequently, we fix K at these values and look for the complex Γ-poles of the form

$$\Omega=E_{exc}+iT\quad,\quad E_{exc}=\begin{cases}0 & CDW,SDW \quad (K=k_F\oplus k_F).\\ 2\varepsilon_F & SS \qquad\qquad (K=0)\end{cases} \tag{15}$$

In this case, the determinant D takes the form

$$D=\mu+g_F\lambda\ln\left|\frac{\Omega_0}{T}\right|, \tag{16}$$

where

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

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

$$\Omega_0=8t\sin^2\left(\frac{\pi}{2}n\right)\begin{cases}\cos^{-1}\left(\frac{\pi}{2}n\right) & CDW,SDW\\ 1 & SS\end{cases} \tag{19}$$

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

g_F/t being the density of states at the Fermi level. From Eqs. (17) and (18) it can be observed that when $X=0$, μ and λ reduce to 1 and respectively to the Hubbard constant U .

3. Critical 'temperatures'

It follows that a transition to an ordered phase will occur for λ negative when the imaginary part of the total frequency has the BCS form

$$T_c=|\Omega_0|\exp\left(\frac{\mu}{g_F\lambda}\right)\quad,\quad\lambda<0. \tag{21}$$

T_c corresponds to the inverse of the relaxation time to the new ground-state or, by uncertainty principle, to the binding energy of the pairs; it can be interpreted also as transition temperature and it is well known that in a 1D system with short range forces there is no phase transition at any non-zero

temperature. However, following Gutfreund [8] (see also [9]), by comparing these transition 'temperatures' we can get a phase diagram at $T = 0$ which, at least for the $g-$ology case, is strikingly similar to that obtained from more sophisticated methods.

The dependence of critical 'temperatures' on the model parameters is presented in Figures 3 and 4. Due to the symmetry of Eq. (21) under the transformation $n \to 2 - n$, $X \to -X$, we can restrict to the case $n \leq 1$. The curves drawn in Fig. 3 correspond to the CDW instability; the same curves are obtained for SDW phase but with $U \to -U$, $X \to -X$. The SS case is considered in Fig. 4 where it can be seen that for a repulsive Hubbard interaction, the X term determines generally an increasing of the critical 'temperature'; there is also a maximum of T_c at $X = t$ for on-site attractions and small concentrations, which moves to the right as the density increases. We can observe also while the critical 'temperature' for density waves goes to infinite when $n \to 1$, it is limited under a certain value in the SS case.

4. Phase diagrams

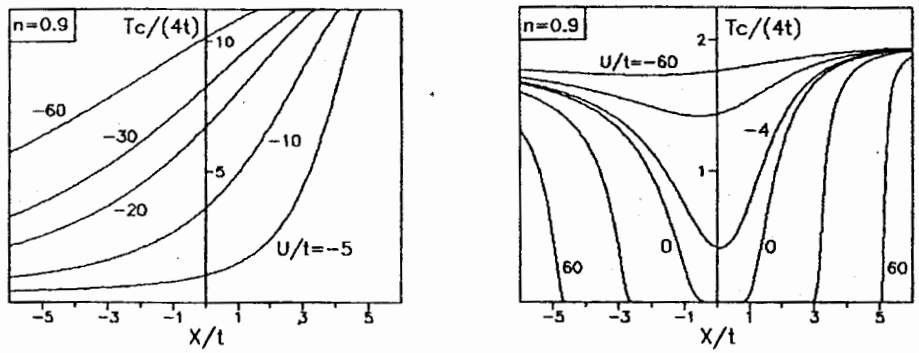
Having determined the critical 'temperatures', we can find the regions in the parameter space where the instabilities may occur. The result, typical to 1D systems, shows that there is no normal Fermi liquid behavior at any nonzero values of U and X. In the regions common to more instabilities, we choose that one with the highest T_c. In this way we get the phase diagram at $T = 0$ in a mean-field-type approximation.

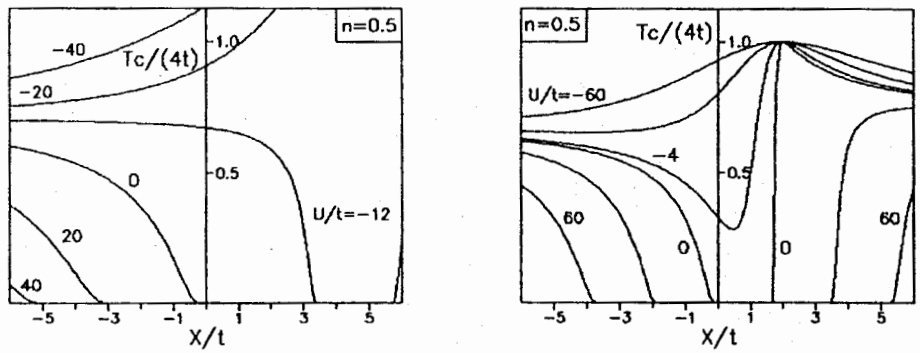
Let us consider first the case of the Hubbard model ($X = 0$); the corresponding phase diagram obtained in our approximation is presented in Fig. 5. For $U > 0$ we get only a $2k_F - SDW$ instability, consistent with the exact results [10] (which predict also a $4k_F - CDW$ instability). For $U < 0$ we find a critical value of the attraction

$$\frac{U_c}{t} = \frac{2\pi \sin(\frac{\pi}{2}n)}{\ln|\cos(\frac{\pi}{2}n)|} \qquad (22)$$

which separates a SS zone from a CDW one; technically, U_c comes from working with the exact dispersion law in the whole BZ, not only with its linearized version around the Fermi points. Earlier works indicate, for the attractive Hubbard model, a possible phase of "correlated" [11] or "localized" [12] Cooper pairs (a kind of a superposition of CDW and SS). At half filling it is clear that the ground-state is a CDW, as was pointed out by Shiba [13]; at other fillings, a SS state is expected in the small coupling regime [14, 15]. More recently, Bogoliubov and Korepin [16, 17] showed (using the asymptotic form of the correlation functions) that for $n < 1$ the ground state is SS.

Figure 3. Critical 'temperatures' for CDW instability. The same curves correspond to the SDW case but with $U \to -U$ and $X \to -X$.





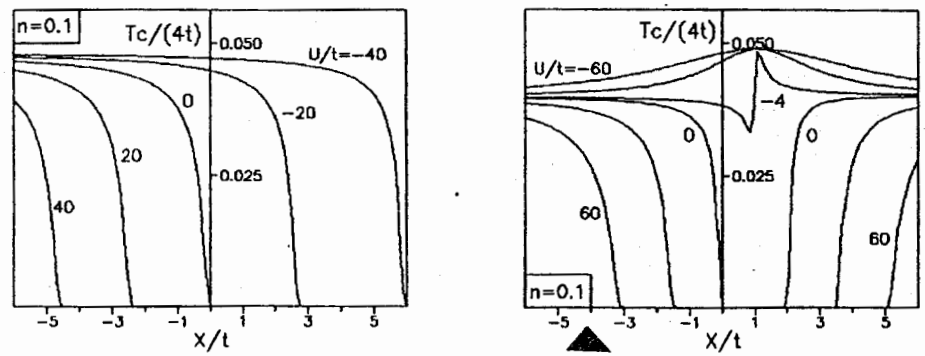


Figure 4. Critical 'temperatures' for SS instability. The unlabeled curves correspond to $U/t = \pm 20$.

Let us consider now the effect of the bond-site interaction. A few phase diagrams at different densities are presented in Fig. 6. At half filling the X term does not change the phase diagram of the Hubbard model, in agreement with other results (evaluation of the X term only at k_F [18] , exact diagonalization techniques [19] , valence bond calculations [20] or exact results for $X = t$ [21]). Going away from half filling, a SS zone appears between the SDW region and the CDW one. For densities lower than the quarter-filled case, the SS zone increases along $X = t$ direction for $U < 0$; a possible explanation is given in the next section.

For more realistic parameters of the model, the phase diagram looks like in Fig. 7; the only effect of the X term is the occurrence of a SS region at low densities (for $X < 0$) or for a band almost filled (for $X > 0$), the last case suggesting us the "hole superconductivity" mechanism proposed by Hirsch [2] in 2D (the bandwidth parameter for holes is $t-2X$ and thus the SS instability can appear at smaller values of X/U in comparison with the electron case).

5. Discussion

In accordance with our results, the effect of the X term (for reasonable parameters of the model) is more important away from half filling where it can determine the occurrence of a superconductor phase (even in the region where the bare potential is always positive: $|X|/U < 1/8$). This fact can be interpreted as an effect of low densities [22] : the effective value of the repulsive (on-site) interaction can become smaller than the attractive (bond-site) part due to the possibility of electrons to avoid each other by jumping on free neighbor sites. A quantitative estimation of this effective interaction can be determined as follows.

Once the Bethe-Salpeter equation in the *pp* channel solved, we can compute easily the ground-state energy of the (t, U, X) model in ladder approximation [23] . At low densities, where we expect this approximation gives good results, the X term can be included in an effective Hubbard constant which coincides with λ_{SS}/μ_{SS} given by Eqs. (17) and (18) :

$$U_{ef} = \frac{U + 8X - 4X^2/t}{(1 - X/t)^2}. \qquad (23)$$

The dependence of U_{ef} on X at different U values is drawn in Fig. 8. This effective on-site interaction takes negative values even for $U > 0$ and small X ; for $X = t$ it becomes infinite, determining a maximum of $T_c(SS)$ at low densities (and $U < 0$). In our opinion, the behavior of U_{ef} at $X = t$ can be connected with an important property of the (t, U, X) model [21, 24] :

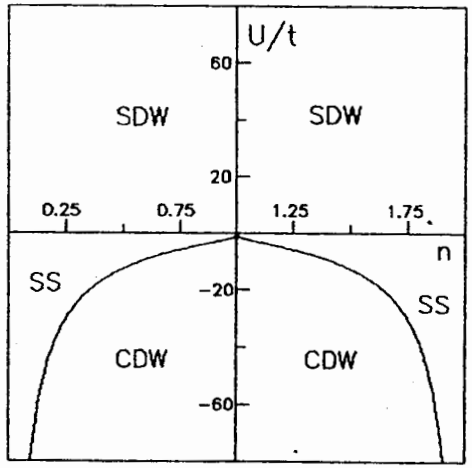


Figure 5. Phase diagram of the 1D Hubbard model in a mean-field-type approximation.

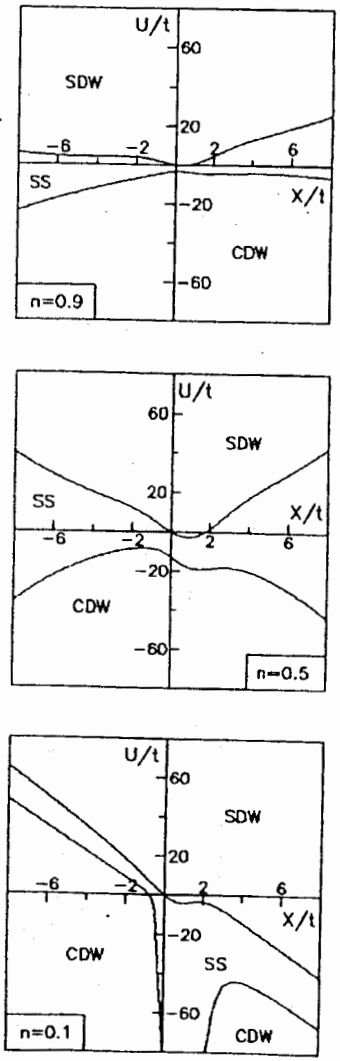


Figure 6. Phase diagrams for the 1D (t, U, X) model in a mean-field-type approximation. At half filling, a SDW phase appears in the upper half-plane and CDW in the lower one (as for the 1D Hubbard model).

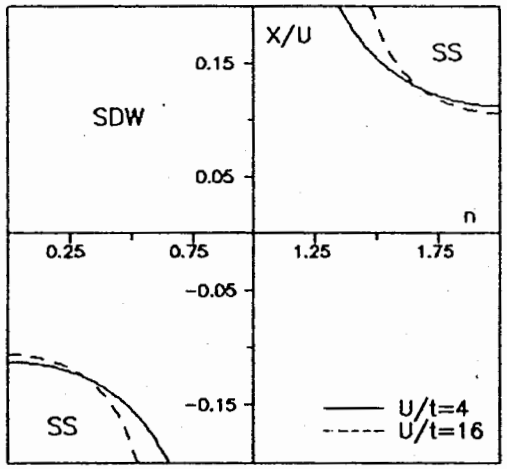


Figure 7. Phase diagram of the 1D (t, U, X) model for $|X| \ll U$ at two values of the on-site repulsion.

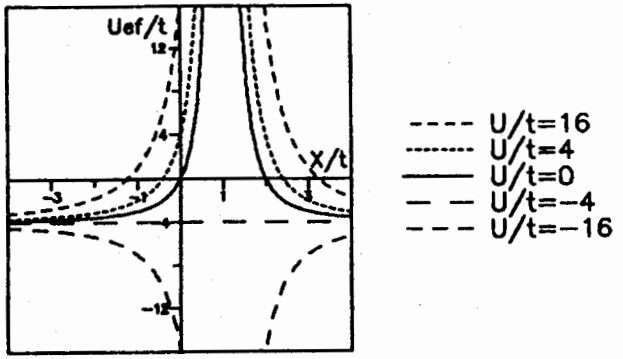


Figure 8. Effective on-site interaction for the 1D (t, U, X) model in the low density limit.

when $X = t$ the motion of electrons interfere in such a way that the number of double-occupied sites is conserved (exact results can be obtained in this particular case). As is well known, at low densities the main effects come from successive interactions of the same two electrons; but such an 'elementary' process breaks the symmetry mentioned above (excepting a very synchronized motion, physically not relevant). Let us suppose $U = 0$; due to the symmetry constraint, the electrons will avoid to stay on the same site and thus the number of double-occupied sites will be zero, as for the infinite repulsive Hubbard model. The picture does not change much for $U > 0$ or small attractions. However, for U less than a critical value ($-4t$ according to our estimations; such a value appears also as relevant in the exact results [3, 4]), the electrons will prefer to form only site-pairs, like in the infinite attractive Hubbard model.

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