Incommensurate and superconducting phases in an exactly solvable model

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An integrable lattice model of strongly interacted electrons with nearest-neighbor and next-nearest-neighbor hoppings is proposed and investigated. The exact ground-state phase diagram is calculated as a function of an on-site interaction, a value of the hopping integral between next-nearest-neighbor lattice sites and a band filling (the nearest-neighbor hopping integral is chosen equal to unity). The model describes incommensurate and superconducting phases which are realized simultaneously in a definite region of interaction parameters and a band filling. The long-distance asymptotics of the density-density and one-particle correlation functions are calculated in the incommensurate phase.

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We consider incommensurate and superconducting phases arising in quantum one-dimensional (1D) models of strongly correlated electrons with correlated hopping or the bond-charge interaction.[1] We propose a lattice integrable model, which describes the phenomenon of 1D incommensurability, and we show that the incommensurate and superconducting phases exist simultaneously. The modified anisotropic Heisenberg model exhibits a ferrimagnetic order, incommensurate with the lattice.[2] The chiral Potts integrable lattice model[3] demonstrates the phenomenon of incommensurability: in the incommensurate phase the ground-state momentum is not equal to zero, but in the commensurate phase it is equal to zero. Incommensurability in the one-dimensional sine-Gordon, U(1) Thirring and Wess-Zumino-Novikov-Witten models has been studied in Ref. 4.

The family of the models of strongly correlated electrons with a bond-charge interaction provides particularly simple examples of superconducting systems.[5,6,9] Phase diagrams as a function of an on-site interaction and the density of electrons have the similar forms: they find four phases, two of them exhibit off-diagonal long-range order (ODLRO). One of these phases is a superconducting phase; another is an insulator phase. The superconducting phase is realized if the value of an on-site interaction is less than the critical one. Other phases characterized by single occupied and empty lattice sites exist in the so-called $U\rightarrow\infty$ Hubbard state.

We consider a modification of a 1D model of strongly correlated electrons proposed and investigated in Refs. 6 and 7 The model Hamiltonian takes into account hoppings of single carriers between nearest-neighbor and next-nearest-neighbor lattice sites with arbitrary hopping integrals. The nearest-neighbor and next-nearest-neighbor hoppings are competing interactions forming an incommensurate phase. In terms of the Hubbard operators the Hamiltonian has the following form

$$\mathcal{H}=-t_1\sum_{\langle ij\rangle\sigma=\uparrow,\downarrow}(X_i^{\sigma 0}X_j^{0\sigma}+X_i^{\sigma 2}X_j^{2\sigma})-t_2\sum_{\langle\langle ij\rangle\rangle\sigma,\sigma'=\uparrow,\downarrow}\left[(X_i^{\sigma 0}X_j^{0\sigma}+X_i^{\sigma 2}X_j^{2\sigma})\left(1-\frac{3}{2}X_k^{\sigma'\sigma'}\right)-\frac{1}{2}X_k^{\sigma'\sigma}(X_i^{\sigma 0}X_j^{0\sigma'}+X_i^{\sigma' 2}X_j^{2\sigma})\right]+U\sum_{j=1}^{L}X_j^{22},\qquad(1)$$

where the Hubbard operators X_j^{ab} describe all possible configurations of electrons at given lattice site $j|a\rangle_j=X_j^{a0}|0\rangle(a=0,\uparrow,\downarrow,2)$; here, $|0\rangle$ denotes the Fock vacuum, $j=1,2,\ldots,L$, L is the total number of lattice sites, $\sigma\in\{\uparrow,\downarrow\}$ is the spin label, $\langle ij\rangle$ and $\langle\langle ij\rangle\rangle(i<k<j)$ denote neighboring and next-neighboring sites, respectively, and the hopping integrals t_1 and t_2 describe hoppings of electrons along the chain. The last term in Eq. (1) is the most important term for the Hubbard model; the on-site Coulomb repulsion U separates the energies of single- and two-electron states. We shall adopt for the chain periodic boundary conditions. The Hamiltonian $\mathcal{H}$ conserves not only the total number of electrons N and also the number of single electrons with spin σ, $N_{1\sigma}=\Sigma_{j=1}^{L}X_j^{\sigma\sigma}$, and the number of electron pairs, $N_2=\Sigma_{j=1}^{L}X_j^{22}$. In the case $t_2=0$ the Hamiltonian is reduced to that of Ref. 6. The kinetic terms of the Hamiltonian $\mathcal{H}$ (which are proportional to the hopping integrals t_1 and t_2) are an electron-hole invariant: indeed applying this transformation $X_j^{\sigma 0}\Rightarrow X_j^{-\sigma 2}, X_j^{2-\sigma}\Rightarrow X_j^{0\sigma}$, $X_j^{\sigma\sigma}\Rightarrow X_j^{-\sigma-\sigma}$, $X_j^{22}\Rightarrow X_j^{00}$ to Eq. (1) we obtain $\mathcal{H}(t_1,t_2,U)\Rightarrow\mathcal{H}(t_1,t_2,U)+U(L-N)$. Under the combined electron-hole symmetry $X_j^{\sigma 0}\Rightarrow(-1)^j X_j^{-\sigma 2}, X_j^{2-\sigma}\Rightarrow(-1)^j X_j^{0\sigma}$, $X_j^{\sigma\sigma}\Rightarrow X_j^{-\sigma-\sigma}$, $X_j^{00}\Rightarrow X_j^{22}$ the hopping integral t_1 changes the sign and the Coulomb interaction transforms to the similar form $\mathcal{H}(t_1,t_2,U)\Rightarrow\mathcal{H}(-t_1,t_2,U)+U(L-N)$. Hence we can restrict our consideration to the case $N\leqslant L$ and $t_1>0$. The Hamiltonian commutes with the spin and so-called η operators.[10]

We consider the 1D case which can be treated exactly. The model (1) is exactly solvable and the exact ground-state phase diagram may be presented. The behavior of single electrons is described in the framework of the Hubbard model with an infinite U. Below we present the exact solution of the model (1) obtained by the Bethe ansatz. The two-particle wave function for singlet $\Psi^s_{\sigma_1\sigma_2}(x_1,x_2)$ and triplet $\Psi^{tr}_{\sigma_1\sigma_2}(x_1,x_2)$ states of single electrons are similar, because they satisfy the conditions $\Psi^s_{\sigma_1\sigma_2}(x_1,x_2)=\Psi^{tr}_{\sigma_1\sigma_2}(x_1,x_2)=0$ at $x_1=x_2$: $\Psi^s_{\sigma_1\sigma_2}(x_1,x_2)=A^s_{12}[\exp(ik_1x_1+ik_2x_2)-\exp(ik_2x_1+ik_1x_2)]$, $\Psi^{tr}_{\sigma_1\sigma_2}(x_1,x_2)=A^{tr}_{12}[\exp(ik_1x_1+ik_2x_2)-\exp(ik_2x_1+ik_1x_2)]$ for $x_1<x_2$ and $\Psi^s_{\sigma_1\sigma_2}(x_1,x_2)$

$=A_{21}^{s}[\exp(ik_1x_1+ik_2x_2)-\exp(ik_2x_1+ik_1x_2)]$, $\Psi_{\sigma_1\sigma_2}^{tr}(x_1,x_2)$ $=-A_{21}^{tr}[\exp(ik_1x_1+ik_2x_2)-\exp(ik_2x_1+ik_1x_2)]$ for $x_1>x_2$; here, k_1,k_2 and x_1, x_2 are the momenta and coordinates of single carriers, and 1 and 2 are their spin indexes. The amplitudes $A_{12}^{s,tr}$ and $A_{21}^{s,tr}$ are related $A_{12}^{s}=-A_{21}^{s}$, $A_{12}^{tr}=A_{21}^{tr}$, which follow from the symmetry of the wave function. The similar solution for the two particle wave function has been used first by Wiegmann for an exactly solution of the Kondo problem.[11] The Bethe function takes a traditional form

$$\Psi_{\sigma_1,\sigma_2,\ldots,\sigma_N}(x_1,x_2,\ldots,x_N) = \sum_{\mathrm{P}} \mathrm{sgn(P)}A(P/Q)_{\sigma_1,\sigma_2,\ldots,\sigma_N}\exp\left(i\sum_{j=1}^{N} k_{Pj}x_{Qj}\right), \quad (2)$$

where the P summation extends over all the permutation of the momenta $\{k_j\}$, and $Q=\{Q_1,\ldots,Q_N\}$ is the permutation of the N particles such that coordinates satisfy $1\leqslant x_{Q1}\leqslant x_{Q2}\leqslant\cdots\leqslant x_{QN}\leqslant L$. The coefficients $A(P/Q)$ arising from the different permutations Q are connected via the spin permutation operator $P_{ij}\,A^{\cdots\sigma_i\sigma_j\cdots}_{\cdots Pi Pj\cdots}=P_{ij}\,A^{\cdots\sigma_j\sigma_i\cdots}_{\cdots Pj Pi\cdots}$.

The Bethe function is the eigenfunction of the Hamiltonian (1) for arbitrary hoppings of single carriers and the spectrum of system is given by

$$E(\{n^1\};N)=-2\sum_{l=1}^{\mathrm{L}}(t_1\cos k_l+t_2\cos 2k_l)n_l^1+UN_2, \quad (3)$$

where $\{n_l^1\}$ are the quantum number valued 0 or 1 that describes states of single carriers $N_1=\Sigma_{l=1}^{L}n_l^1$, the wave vectors $k_l=2\pi l/L$ $(l=1,2,\ldots,L)$. The model is reduced to the spinless fermionic one with the nearest- and next-nearest-neighbor hoppings. The ground state is obtained by minimizing the ground-state energy per site $\mathcal{E}=E/L$ for a fixed total density of electrons, $n=N/L$, clearly $n=n_1+2n_2$; here, $n_1=\Sigma_{\sigma=\uparrow,\downarrow}N_{1\sigma}/L$ is the density of single carriers, and $n_2=N_2/L$ is the density of electron pairs. We chose the hopping integral t_1 equal to unity. Then the coupling constants are dimesionless, and hereinafter $u=U/t_1$ and $\tau=t_2/t_1$. When the ratio τ is small enough the ground state coincides with the ground state of the model[6] and the spectrum of low-lying excitations is always the same. But when the ratio τ is sufficiently large new phases are appeared. We consider in detail some particular model exhibiting incommensurate behavior.

The spectrum of single-electron carriers $\varepsilon(k)$,

$$\varepsilon(k)=-2\cos k-2\tau\cos 2k, \quad (4)$$

depends on the ratio between the hopping integrals; in the case of a small interaction $|\tau|<\tau_c$ (here $\tau_c=1/4$), $\varepsilon(k)$ is a single-valued function of k (for positive k), and in the case of a strong interaction $|\tau|>\tau_c$, $\varepsilon(k)$ is a many-valued function of k. We have two or four Fermi momenta, depending on a band filling n_1, symmetrically arranged. Figure 1 illustrates this situation, when two planes separate the regions with two and four Fermi points. The Fermi momenta are asymmetrically arranged around the extremum $k=\pm Q$ $[Q=\arccos(-1/4\tau)]$. In the case of a strong interaction four Fermi momenta are realized at a small electron density $n_1<n_{1c}$ for $\tau<-\tau_c$ [here $n_{1c}=1/\pi\arccos(-1-1/2\tau)$] and at a high electron density $n_{2c}<n_1<1$ for $\tau>\tau_c$ [here $n_{2c}=1/\pi\arccos(1-1/2\tau)$]. In the first case the Fermi momenta are $k_{F1}=\pm(Q+p_1)$, $k_{F2}=\pm(Q-p_2)$ and $n_1=(p_1+p_2)/\pi$ if $n_1<n_{1c}$ or $k_{F1}=\pm(Q+p_1)$ and $n_1=k_{F1}/\pi$ if $n_1>n_{1c}$; in the second case these values are defined as $k_{F1}=\pm p_1$ and $n_1=k_{F1}/\pi$ if $n_1<n_{2c}$ and if $k_{F1}=\pm p_1$ and $k_{F2}=\pm p_2$ $(p_1<Q<p_2)$ and $n_1=1-(p_2-p_1)/\pi$ if $n_{2c}<n_1<1$ [with an additional constraint on the p_1 and p_2 values $\varepsilon(k_{F1})=\varepsilon(k_{F2})$]. The corresponding Fermi velocity $v_{F1,2}=v(k_{F1,2})$ is calculated according to Eq. (4) $v(k)=2\sin k+4\tau\sin 2k$, for the values of k defined above.

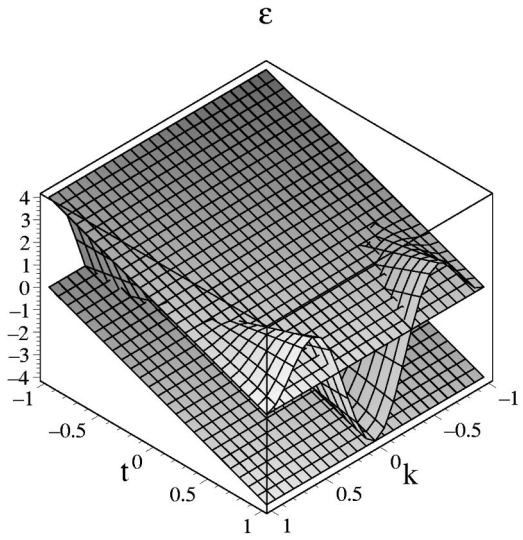

FIG. 1. The spectrum of single carriers $\varepsilon(k)$ as a function of τ and k. The incommensurate phase is realized, upper and lower planes detailed.

We have focused on the calculation of the exact ground-state phase diagram in the n-u-τ plane, as a rule $|t_2|<t_1$, and so we restrict our consideration to the case $|\tau|<1$. We find four different phases which will be discussed separately. The lower phase that arrangements below a lower plane (see Fig. 2) is characterized by $n_1=0$; electron pairs and empty sites are presented in the ground state. In this phase the ground state $|\Psi\rangle=(\eta^{\dagger})^{N/2}|0\rangle$ consists of the so-called η pairs,[10] where $\eta^{\dagger}=\Sigma_j\eta_j^{\dagger}$, $(\eta_j^{\dagger}=X_j^{20})$. At $u<4\tau+1/2\tau$ for $\tau<-\tau_c$, $u<-4(1+\tau)$ for $\tau>-\tau_c$ the ground state consists of only localized pairs with the density $n_2=n/2$ and empty sites. The pairs are static and in the absence of single electron states the ground state energy per site is simply $\mathcal{E}=un_2$. In a mixed phase the ground-state includes both finite densities of single electrons and electron pairs. Note that the pairs are not localized due to exchange between single- and double-electron states.[7,8] Both the mixed and lower phases have a finite ODLRO,[6] i.e., $\langle\eta_i^{\dagger}\eta_j\rangle\nrightarrow 0$ for $|i-j|\rightarrow\infty$. However, the lower phase is an insulator phase since pairs are localized in the absence of single-electron pairs. The mixed phase is a superconducting phase having normal metallic Drude weight.

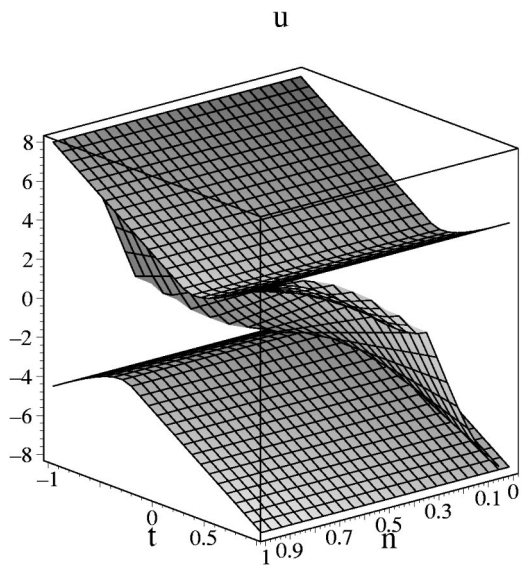

FIG. 2. Ground-state phase diagram as a function of $u=U/t_1$, $\tau=t_2/t_1$, and the total density n. The mixed phase is a bounded region between two planes.

An upper plane in Fig. 2 separates the ground state of the $U\to\infty$ Hubbard model and mixed phase. At $u>4(1-\tau)$ for $\tau<\tau_c$ and $u>4\tau+1/2\tau$ for $\tau>\tau_c$ the ground state is that of the $U\to\infty$ Hubbard model and consists of singly occupied and empty sites; the density of single carriers n_1 is equal to n. The $U\to\infty$ Hubbard phase is a metallic one excluding a half-filling. At a half-filling the system is an insulator with a gap $\Delta\varepsilon=u-u_{\max}$, where $u_{\max}=4(1-\tau)$ for $\tau<\tau_c$ and $u_{\max}=4\tau+1/2\tau$ for $\tau>\tau_c$. Both finite densities of single carriers $n_1>0$ and electron pairs $n_2>0$ (or $0<n_1<n$) are realized in the case of intermediate values of the interaction parameters u and τ and the total density of electrons, the so-called a mixed phase. Let us analyze different states of the mixed phase that are described by the stable solutions of n_1. There are three distinct regions of τ defined by the solutions of n_1. In the case of a small interaction $|\tau|<\tau_c$ and an arbitrary total density of electrons the minimum of the density of the ground-state energy

$$\mathcal{E}=-\frac{2}{\pi}\sin(\pi n_1)-\frac{\tau}{\pi}\sin(2\pi n_1)+\frac{1}{2}u(n-n_1)$$

corresponds to the solution of the equation.

$$u+4\cos(\pi n_1)+4\tau\cos(2\pi n_1)=0. \tag{5}$$

For $|\tau|<\tau_c$, Eq. (5) has only one nontrivial solution for the density of the single carriers,

$$n_1=\frac{1}{\pi}\arccos\left(-\frac{1}{4\tau}+\frac{1}{4\tau}\sqrt{1+8\tau^2-2u\tau}\right),$$

which takes place for $-4(1+\tau)<u<4(1-\tau)$. This solution survives in the case of the strong interaction also at $\tau<-\tau_c$, $n_1>n_{1c}$, and $\tau>\tau_c$, $n_1<n_{2c}$ for the same values of u. As we noted an usual situation with the two Fermi momenta in the spectrum of the single carriers is realized for the parameters considered above.

New solutions for n_1 corresponding to the minimum of $\mathcal{E}$,

$$\mathcal{E}=-\frac{2\tau}{\pi}\sin(\pi n_1)-\frac{1}{2\pi\tau}\cot\left(\frac{\pi n_1}{2}\right)+\frac{1}{2}u(n-n_1),$$

are obtained for a strong interaction at $\tau>\tau_c$, $n_{2c}<n_1<1$,

$$u+4\tau\cos(\pi n_1)-\frac{1}{\tau[1-\cos(\pi n_1)]}=0, \tag{6}$$

and at $\tau<-\tau_c$, $0<n_1<n_{1c}$,

$$-u+4\tau\cos(\pi n_1)+\frac{1}{\tau[1+\cos(\pi n_1)]}=0. \tag{7}$$

The last solution corresponds to the minimum of

$$\mathcal{E}=\frac{2\tau}{\pi}\sin(\pi n_1)+\frac{1}{2\pi\tau}\tan\left(\frac{\pi n_1}{2}\right)+\frac{1}{2}u(n-n_1).$$

The region $1\leqslant n\leqslant 2$ is the electron-hole transform of $0\leqslant n\leqslant 1$. By contrast with the case of a strong interaction, where the bandwidth $D(\tau)=2+4|\tau|+1/4|\tau|$ for $|\tau|>\tau_c$, the case of a small interaction is characterized a bandwidth which is independent of the value of the next-nearest hopping integral $D(\tau)=4$ for $|\tau|<\tau_c$. With respect to the model[6] we obtain two main effects, which are generated by the next-nearest hopping term: (i) the phase incommensurate with a lattice; (ii) it stabilizes the superconducting phase at a strong interaction. The superconducting phase exists in our model up to the value of $u_{\max}=4\tau+1/2\tau$ (for $\tau>\tau_c$), which corresponds to a point of the insulator-superconducting transition. This value depends on τ and is higher than all others of exactly solved models.[5,6,9] At a small interaction or $\tau<-\tau_c$ $u_{\max}$ is proportional to τ, namely, $u_{\max}=4-4\tau$. The large value of $u_{\max}$ provides a temperature stability of the superconducting phase.

The long-distance asymptotic of the one-particle correlation function $\langle X^{\sigma 0}(x)X^{0\sigma}(0)\rangle$ shows an oscillatory behavior at $T=0$ K in the incommensurate phase,

$$\langle X^{\sigma 0}(x)X^{0\sigma}(0)\rangle\simeq\frac{1}{x}\cos(\pi n_1 x/2)\times\cos\left[x\arccos\left(\frac{\cos Q}{\cos(\pi n_1/2)}\right)\right], \tag{8}$$

for $\tau<-\tau_c, 0<n_1<n_{1c}$, and

$$\langle X^{\sigma 0}(x)X^{0\sigma}(0)\rangle\simeq\frac{1}{x}\sin(\pi n_1 x/2)\times\cos\left[x\arccos\left(\frac{\cos Q}{\sin(\pi n_1/2)}\right)\right], \tag{9}$$

for $\tau>\tau_c, n_{2c}<n_1<1$; here, x is the coordinate.

Similarly, we obtain the leading term of the density-density correlation function

$$\langle X_1(x)X_1(0)\rangle \simeq \frac{1}{x^2}\cos(\pi n_1 x) + \frac{1}{x^2}\cos\left[x \arccos\left(\frac{\cos Q}{\cos(\pi n_1/2)}\right)\right] + \frac{2}{x^2}\cos(\pi n_1 x)\cos\left[x \arccos\left(\frac{\cos Q}{\cos(\pi n_1/2)}\right)\right], \tag{10}$$

for $\tau < -\tau_c, 0 < n_1 < n_{1c}$, and

$$\langle X_1(x)X_1(0)\rangle \simeq -\frac{1}{x^2}\cos(\pi n_1 x) + \frac{1}{x^2}\cos\left[x \arccos\left(\frac{\cos Q}{\sin(\pi n_1/2)}\right)\right] - \frac{2}{x^2}\cos(\pi n_1 x)\cos\left[x \arccos\left(\frac{\cos Q}{\sin(\pi n_1/2)}\right)\right], \tag{11}$$

for $\tau > \tau_c, n_{2c} < n_1 < 1$; here, $X_1 = \Sigma_\sigma X^{\sigma\sigma}$.

In the state with two Fermi momenta the long-distance asymptotics of these correlation functions are the similar to ones for spinless fermions:

$$\langle X^{\sigma 0}(x)X^{0\sigma}(0)\rangle \simeq \frac{1}{x}\cos(\pi n_1 x),$$

$$\langle X_1(x)X_1(0)\rangle \simeq \frac{1}{x^2}\cos(2\pi n_1 x).$$

Comparing these formulas we see the contrast between the asymptotics of the correlation functions in the incommensurate phase—the period of the oscillations depends on both the density of single carriers n_1 and vector Q.

In summary, a modified Hubbard model with an additional next-nearest-neighbor hoppings has been proposed and investigated. The exact ground-state phase diagram in the u-τ-n plane exhibits an unusual phase state in which the incommensurate state comes in a superconducting phase. It is shown that the incommensurate phase is realized for ratios of the next-nearest-neighbor hopping integral greater than some critical value $\tau_c = 1/4$ ($|t_2| > 1/4|t_1|$) in a defined region of the density of single carriers. The maximum critical value of on-site Coulomb repulsion $u_{\max}$ realized in the model is higher than all others in exactly solvable models.[6,9] A higher value of $u_{\max}$ enlarges the region of the coexistence of the incommensurate state in the superconducting phase. This phase has been illustrated by calculations of the asymptotics of the density-density and one-particle correlation functions. All correlation functions exhibit a power-law decay at $T = 0$ and oscillate. The period of the oscillations depends on the parameters of interaction.

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