48, 1184 (1965) [Sov. Phys. JETP 21, 790 (1965)].
[8]E. G. Maksimov and O. A. Pankratov, Fiz. Tverd. Tela (Leningrad) 16, 874 (1974) [Sov. Phys. Solid State 16, 561 (1974)].
[9]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polyav statisticheskoĭ fizike (Quantum Field Theoretical Methods in Statistical Physics), Fizmatgiz, 1962 [Pergamon, 1965].
[10]L. D. Landau and E. M. Lifshitz, Statisticheskaya fizika (Statistical Physics), Nauka, 1964 [Pergamon, 1971].
[11]Yu. V. Kopaev, Fiz. Tverd. Tela (Leningrad) 12, 3 (1970) [Sov. Phys. Solid State 12, 1 (1970)].
[12]D. G. Andrianov, N. B. Brandt, E. R. Ioon, V. I. Fistul', and C. M. Chudinov, Pis'ma Zh. Eksp. Teor. Fiz. 17, 494 (1973) [JETP Lett. 17, 356 (1973)].
[13]L. P. Strakhov, Fiz. Tverd. Tela (Leningrad) Tela 11, 3067 (1969) [Sov. Phys. Solid State 11, 2492 (1970)].

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Susceptibility of inhomogeneous quasi-one-dimensional Fermi systems with repulsion

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Quasi-one-dimensional Fermi systems with repulsion are considered. The effect of impurities is studied in those cases in which these structures are one-dimensional antiferromagnets. It is found that the impurities lead to a logarithmic or fractional-power increase in the susceptibility at low temperatures. The power in the temperature dependence of the susceptibility does not depend on the impurities and is determined by the interaction between the electrons. It is shown that phase transitions that do not alter the one-dimensional character of the spin interactions or impede this increase in the susceptibility are possible.

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1. INTRODUCTION

At the present time there is no doubt that many of the highly conducting quasi-one-dimensional complexes of TCNQ are metals at high temperatures. The question of the state of these substances at low temperatures is, however, more complicated. One of the possible states is the antiferromagnetic state which can arise if the conduction electrons form a Fermi system with repulsion. Such systems have been studied previously in a particular case in the Hubbard model.[1–3] At low temperatures the magnetic susceptibility remains finite and the specific heat depends linearly on the temperature. In this work it is shown that the defects that can be present in the system strongly affect the magnetic properties and make possible a logarithmic or power increase of the susceptibility as the temperature is lowered. The temperature dependence of the specific heat remains linear.

The interaction of electrons from different strands does not alter the behavior of the susceptibility at low temperatures, even though it can lead to a phase transition at finite temperatures. Hopping from strand to strand can have a substantial influence.

2. INFLUENCE OF INHOMOGENEITIES ON THE SPIN CORRELATION FUNCTIONS

We shall consider a system of parallel conducting strands. We assume that the probability of electron hops from strand to strand is small. We also assume that the interaction of electrons from different strands is small. There are reasons to believe that even strong interaction of electrons from different strands, which can lead to a phase transition, has little effect on the spin correlation functions. However, we shall speak of this later. In this section we assume the strands to be isolated. We write the Hamiltonian of one strand in the form

$$\hat{H}=-\sum_{i\neq j} T_{ij}^{\alpha,\alpha'} a_{i\alpha}^{+} a_{j\alpha'} + \frac{1}{2}\sum_{i,j,\alpha,\alpha'} V_{ij} a_{i\alpha}^{+} a_{j\alpha'}^{+} a_{j\alpha'} a_{i\alpha} - \mu \sum_{i,\alpha} a_{i\alpha}^{+} a_{i\alpha} - \mathbf{H}\sum_{i} \mathbf{S}_i, \tag{1}$$

where $a_{i\alpha}^{+}(a_{i\alpha})$ are the creation (annihilation) operators for electrons with spin α at site i, $T_{ij}^{\alpha\alpha'}$ are the overlap integrals, μ is the chemical potential, and

$$\mathbf{S}=\sum_{\alpha,\beta} \boldsymbol{\sigma}_{\alpha\beta} a_{\alpha}^{+} a_{\beta}, \tag{2}$$

where $\boldsymbol{\sigma}$ is the vector whose components are the Pauli matrices.

The impurities lead to the result that the quantities T_{ij} and V_{ij} do not depend only on the difference $i-j$, and also to the fact that the transition amplitude $T_{ij}^{\alpha\alpha'}$ is a matrix.

We shall assume that the parameters of the Hamiltonian (1) are such that in the absence of impurities the system is a one-dimensional antiferromagnet. Such a case occurs in, e.g., the Hubbard model with a half-filled band.[1] The model considered by Ovchinnikov,[4] with a quarter-filled band and sufficiently strong nonlocal repulsion, also describes a one-dimensional antiferromagnet. In the absence of impurities the susceptibility of such systems remains finite. Below we shall

be interested in the magnetic susceptibility of systems with impurities.

By means of the usual relation, the susceptibility χ is expressed in terms of the spin correlation function $K(x, \tau)$:

$$\chi=\int_{-\infty}^{\infty}\int_{0}^{1/T}K(x,\tau)\,dx\,d\tau, \tag{3}$$
$$K(x,\tau)=\overline{\langle T_\tau \mathbf{S}(0,0)\mathbf{S}(x,\tau)\rangle},$$

where T_τ is the time-ordering operator. The bar denotes averaging over the impurities.

In the general case, taking the impurities into account is very complicated. Therefore, we shall consider a certain particular case in which the influence of the impurities can be studied to completion. Such a case is the Hubbard model with a half-filled band and strong repulsion, with impurities that flip the spins.

Thus, we let

$$V_{ij}=V\delta_{ij}, \quad T_{ij}^{\alpha,\alpha'}=T_i^{\alpha,\alpha'}\delta(|i-j|-1). \tag{4}$$

Assuming that $V\gg T_i^{\alpha\alpha'}$ and expanding in the parameter $T_i^{\alpha\alpha'}/V$, we transform the Hamiltonian (1) to the form

$$\hat{H}=\frac{1}{V}\sum_{\alpha,\alpha'}T_i^{\alpha\alpha'}T_i^{*\beta\beta'}a_{i\alpha}^{+}a_{i+1,\alpha'}a_{i+1,\beta'}^{+}a_{i\beta}-\mathbf{H}\sum_i \mathbf{S}_i. \tag{5}$$

Strong repulsion leads to suppression of the density fluctuations. In this case the density operator $\sum_\alpha a_{i\alpha}^{+}a_{i\alpha}$ can be regarded as a number. Only the spin interactions are important. By expressing the one-electron operators in (5) in terms of the spin operators by formula (2), we can reduce the Hamiltonian (5) to a Heisenberg Hamiltonian with impurities:

$$\hat{H}=J\sum_i(\mathbf{S}_i U_{i+1}\mathbf{S}_{i+1})-\mathbf{H}\sum_i \mathbf{S}_i. \tag{6}$$

In formula (6), U_{i+1} is an operator that acts on the spins and depends on the label i. In the general case the operator U_{i+1} is arbitrary and terms linear in S_i can be present in the Hamiltonian (6) even in the absence of a field.

Below we shall consider the case of spin-orbit scattering:

$$|T_i^{++}|=|T_i^{--}|=T_i^{(0)}, \quad T_i^{+-}=T_i^{-+}=T_i^{(1)},$$
$$T_i^{++}T_i^{*(1)}+T_i^{(1)}T_i^{*--}=0, \quad (T_i^{(0)})^2+|T_i|^2=J^2V/2, \tag{7}$$

where J does not depend on the coordinates. We can convince ourselves that fulfillment of the conditions (7) leads to the result that we are considering impurities whose action reduces merely to rotation of the spin vector at each point through its own angle. Here the operators U_{i+1} in (6) are orthogonal. In the following we shall not need the explicit expression for U_{i+1} in terms of the amplitudes $T_i^{\alpha\alpha'}$.

To calculate the correlator (3) in zero magnetic field we shall change to new operators $\mathbf{C}_i$, by the formulas

$$\mathbf{C}_i=\prod_{k=-\infty}^{i}U_k\mathbf{S}_i. \tag{8}$$

Using the orthogonality of the operators U_k, we can verify that the operators $\mathbf{C}_i$ satisfy the usual spin commutation relations. Substituting the expression (8) into formulas (2) and (7), we obtain

$$K(x,\tau)=\left\langle T_\tau \mathbf{C}(0,0)\left[\prod_{k=x}^{0}U_k^{-1}\right],\mathbf{C}(x,\tau)\right\rangle, \tag{9}$$

$$\hat{H}=J_0\sum_i \mathbf{C}_i\mathbf{C}_{i+1}. \tag{10}$$

In the expression (9),

$$C(x,\tau)=e^{\hat{H}\tau}C_x e^{-\hat{H}\tau}. \tag{11}$$

The angle brackets in (9) denote averaging with the Hamiltonian (10). The formulas (9), (10) and (11) show that, in the model under consideration, the averaging over the impurities and the thermodynamic averaging are separable in the calculation of the correlator $K(x, \tau)$.

If the impurities at different points are also independent, the average of the product of operators U_k^{-1} is equal to the product of the averages:

$$\overline{\prod_{k=x}^{0}U_k^{-1}}=\prod_{k=x}^{0}\overline{U_k^{-1}}. \tag{12}$$

We write the action of the rotation operator U_k^{-1} on an arbitrary vector $\mathbf{X}$ in the form

$$U_k^{-1}\mathbf{X}=\mathbf{X}\cos\varphi_U+\mathbf{n}_U|\mathbf{X}|\sin\varphi_U, \tag{13}$$

where φ_U is the rotation angle and $\mathbf{n}_U$ is a unit vector lying in the plane perpendicular to the vector $\mathbf{X}$.

Let the probability $W(\varphi_U)$ of a rotation through the angle φ_U have the Gaussian form

$$W(\varphi_U)=\exp(-\varphi^2 l)/\pi l. \tag{14}$$

We consider the case $l\gg 1$. Performing the averaging in (13) with the distribution (14) with $l\gg 1$, we obtain

$$\overline{U_k^{-1}}=1-1/l\approx e^{-1/l}. \tag{14a}$$

Substituting (14a) into (12) and (9), we express the correlation function $K(x, \tau)$ of the Heisenberg model with impurities in terms of the correlation function $K_0(x, t)$ of the Heisenberg model without impurities:

$$K(x,\tau)=\exp(-|x|/l)K_0(x,\tau), \tag{15}$$
$$K_0(x,\tau)=\langle T_\tau \mathbf{C}(0,0),\mathbf{C}(x,\tau)\rangle. \tag{16}$$

In the general case too, when the impurities are arbitrary and the system is described by the Hamiltonian (1), we may assume that the spin correlation function $K(x, \tau)$ of the inhomogeneous model with $l\gg 1$ is connected with the correlation function $K_0(x, \tau)$ of the homogeneous model by the relation (15). In this case the quantity l is related in some complicated way to the parameters of the Hamiltonian (1). Below we shall not be

interested in this dependence, but shall study the consequence of a finite value of l.

Thus, a knowledge of the spin correlation function of the homogeneous system enables us to calculate the susceptibility of the inhomogeneous system by means of formulas (2) and (15).

3. CALCULATION OF THE SUSCEPTIBILITY

The simplest model with repulsion in which antiferromagnetic ordering is possible is the Hubbard model with repulsion and a half-filled band. The spin correlation function $K_0(x, \tau)$ of this model is calculated in the Appendix ((A.7a)). For small fields $H \ll T$, using formulas (3), (15), (A.7a) and (A.8) we write the susceptibility in the form of the integral

$$\chi=\frac{AT}{v_s}\int_0^\infty\int_0^{1/T}\cos\pi x\exp(-|x|/l)\,\mathrm{sh}^{-1/2}[\pi T(x/v_s+i\tau)]\,\mathrm{sh}^{-1/2}[\pi T(x/v_s-i\tau)]\,dx\,d\tau, \tag{17}$$

where v_s is the velocity of the gapless excitations (see the Appendix). At sufficiently high temperatures $T \gg v_s/1$, values of $x, v_s\tau \sim 0$ are important in the integral. In this region the susceptibility depends weakly on the temperature and is close to the susceptibility of the homogeneous system.

More interesting is the case of low temperatures $T \ll v_s/1$. Calculating the integral in (17) for this relationship between the parameters, we obtain

$$\chi=\frac{2A}{v_s l\pi^3}\ln\frac{v_s}{Tl}. \tag{18}$$

Formula (18) shows that the susceptibility grows logarithmically with decrease of temperature in the Hubbard model with defects.

In the Hubbard model with repulsion and a half-filled band the ground state is nonconducting, and antiferromagnetic ordering of the spins exists over short distances. The form of the spin correlation function (A.7a) is due to the fact that spin waves play the principal role in the formation of the singularities. If the repulsion is not local, the system can be a dielectric even when there is an odd number of electrons per site,[4] and the spins form an antiferromagnetic structure. In the general case it is not just a doubling of the period that can occur. An increase of the period by an integer factor is possible.

The effect of long-wavelength excitations on the pair correlation function and density-density function was investigated in[5]. It was found that the principal role in the formation of the singularities of the correlation functions is played by just such excitations. The other excitations lead only to changes of factors. In this case, the calculation of, e.g., the pair correlation function $\Pi(x, \tau)$ reduced to calculation of the average

$$\Pi(x, \tau)\sim\langle\exp\{i\varphi(x, \tau)-i\varphi(0, 0)\}\rangle \tag{19}$$

with the free-energy functional $F[\varphi]$:

$$F[\varphi]=\varkappa\int[\dot\varphi^2+v_s^2(\nabla\varphi)^2]\,dx\,d\tau, \tag{20}$$

where $\varkappa$ is the compressibility. After calculations in (19), the following expression for the quantity $\Pi(x, \tau)$ was obtained:

$$\Pi(x, \tau)=A\left(\frac{T}{v_s}\right)^{\beta}\mathrm{sh}^{-\beta/2}\left[\pi T\left(\frac{x}{v_s}+i\tau\right)\right]\mathrm{sh}^{-\beta/2}\left[\pi T\left(\frac{x}{v_s}-i\tau\right)\right], \tag{21}$$

where

$$\beta=(2\pi\varkappa v_s)^{-1}.$$

In the same spirit we can calculate the spin correlation function $K_0(x, \tau)$ of an arbitrary one-dimensional antiferromagnet without impurities, if long-wavelength spin excitations exist in it. We represent the function $K_0(x, \tau)$ in the form

$$K_0(x, \tau)=\tfrac{1}{2}\langle T_\tau S^-(0, 0)S^+(x, \tau)\rangle, \tag{22}$$
$$S^+=S_x+iS_y,\quad S^-=S_x-iS_y.$$

As previously,[5] we assume that the calculation in (22) reduces to calculation of the average (19) with the free-energy functional (20). In this case $\varphi(x, \tau)$ represents the phase of the vector S^+, and in place of the compressibility we have the magnetic susceptibility. If this is so, the expression for the correlation function $K_0(x, \tau)$ has the form

$$K_0(x, \tau)=A\cos p_0 x\left(\frac{T}{v_s}\right)^{\alpha}\mathrm{sh}^{-\alpha/2}\left[\pi T\left(\frac{x}{v_s}+i\tau\right)\right]\mathrm{sh}^{-\alpha/2}\left[\pi T\left(\frac{x}{v_s}-i\tau\right)\right], \tag{23}$$

$$\alpha=(2\pi\chi_0 v_s)^{-1}. \tag{23a}$$

In the Hubbard model, $p_0=\pi$, and the susceptibility χ_0 is connected with the velocity v_s of the excitations by the relation[6]

$$\chi_0=(2\pi v_s)^{-1}. \tag{24}$$

Substituting (24) into (23a) and (23), we convince ourselves that the expression (23) for $K_0(x, \tau)$ coincides with the expressions (A.7a), (A.8). Thus, we may expect that in an arbitrary one-dimensional antiferromagnet without impurities the correlation function has the form (23). Here the index α is not necessarily equal to unity.

Substituting the expression (23) for the correlator $K_0(x, \tau)$ into formulas (3), (15) and calculating the integral in (3), we obtain the following formula for the susceptibility χ of the system with impurities, for $T \ll v_s/l$, $H \ll T$, $\alpha < 1$:

$$\chi=AB\left(\frac{1-\alpha}{2}, \frac{1-\alpha}{2}\right)\left(\frac{T}{2v_s}\right)^{\alpha-1}\Big/\,2\pi l v_s p_0^2, \tag{25}$$

where $B(x, y)$ is Euler's beta-function. If $T \gg v_s/l$ or $\alpha > 1$, the susceptibility depends weakly on the temperature.

The formulas (18) and (25) show that impurities can lead to a logarithmic or fractional-power increase of the susceptibility.

4. THE SPECIFIC HEAT

We shall consider the specific heat of a homogeneous antiferromagnet at low temperatures. Suppose that impurities are absent. In this case the specific heat is known in the Heisenberg model and in the XY-model. In these models it depends linearly on the temperature. Apparently, the existence of gapless long-wavelength spin excitations leads to a dependence of the same form. To check this statement we shall calculate the specific heat using the long-wavelength excitations. Assuming such excitations to be bosons, we obtain

$$C=\frac{\partial E}{\partial T}=\frac{\partial}{\partial T}\int_{-\infty}^{\infty}\frac{v_s|k|}{\exp(v_s|k|/T)-1}\frac{dk}{2\pi}. \tag{26}$$

Calculating the integral in (26) and differentiating with respect to T, we find the specific heat

$$C=2\zeta(2)T/\pi v_s, \tag{27}$$

where $\zeta(x)$ is the Riemann zeta-function.

In the XY-model the specific heat can also be calculated directly by going over to spinless fermions. The specific heat of such fermions is equal to

$$C=2\frac{\partial}{\partial T}\int_{-\infty}^{\infty}\frac{v_0|k|}{\exp(v_0|k|/T)+1}\frac{dk}{2\pi}, \tag{28}$$

where v_0 is the velocity at the Fermi surface.

Using the equality of v_0 and v_s, we convince ourselves that the specific heats calculated from formulas (26) and (28) have the same value (27). In the Heisenberg model there exist numerical calculations[2,3] showing that the specific heat C and susceptibility χ_0 are connected by the relation

$$C\approx 7\chi_0 T. \tag{29}$$

By expressing v_s in terms of χ_0 in formula (27) by means of the relation (24), we obtain the formula (29). The effect of impurities is easily taken into account in the Heisenberg model (6), (7) with spin-flipping impurities. In this case the Hamiltonian with impurities is reduced by the operator replacement to the Heisenberg Hamiltonian (10) without impurities, and the specific heat has the form (27), as before.

We may suppose that the specific heat at low temperatures is also determined by formula (27) in more complicated antiferromagnetic systems, provided that $l\gg 1$. In this case, only the coefficient in the linear temperature dependence of the specific heat depends on the form of the interaction and on the impurities.

5. PHASE TRANSITIONS IN QUASI-ONE-DIMENSIONAL SYSTEMS WITH REPULSION

Above, we have studied purely one-dimensional systems, in which phase transitions cannot occur. The interaction of electrons from different strands and electron hops from strand to strand can lead to the appearance of phase transitions at finite temperatures. Nevertheless, below the transition point too, it is possible that the spin interactions have a one-dimensional character and that, consequently, all the results obtained above are applicable.

For definiteness we shall consider a one-dimensional system of electrons with infinite repulsion at one center and finite repulsion at neighboring centers. Let the band be quarter-filled, so that there is one electron to two sites. It was shown by Ovchinnokov[4] that for sufficiently strong repulsion at neighboring sites the ground state of such a system becomes dielectric, and alternation of the electron density occurs, with period equal to twice the distance between sites. The spin structure in this case is antiferromagnetic.

If the temperature is finite, fluctuational displacement of a small piece through a distance equal to the distance between sites is possible. Such fluctuations lead to disappearance of the long-range order in the arrangement of the electrons. The density-density correlator $P(x)$ of such a system has the form[7]

$$P(x)=\cos\pi x\exp(-|x|/r_c). \tag{30}$$

In formula (30) the correlation length r_c is equal to

$$r_c=\tfrac{1}{2}\exp(U_0/T), \tag{31}$$

where U_0 is the energy of the boundary between the small pieces.

The interaction of electrons from different strands can be taken into account in the self-consistent field approximation, as was done in[5,8]. Then for the transition temperature we obtain the equation

$$1=Vr_c(T_c)/T, \tag{32}$$

where $V=\min V(k_\perp)$; $V(k_\perp)$ is the Fourier component of the interaction between different strands. Solving Eq. (32) for $V\ll U_0$, we obtain

$$T=\frac{U_0}{\ln(U_0/V)}. \tag{33}$$

Below T_c the system is dielectric. Formula (33) was obtained under the assumption that U_0 for $T\sim T_c$ depends weakly on the temperature. If $\ln(U_0/V)$ is not very large, this is not so. In the case when the energy functional $F[\Delta]$ of one chain can be written in the form of a Ginzburg–Landau energy with a real order parameter Δ, instead of (33) we have[9]

$$T_c\approx\tfrac{1}{4}T_{c0}, \tag{34}$$

where T_{c0} is the Ginzburg–Landau transition temperature. The phase transition described occurs because of the density-density interaction of different strands, which cannot alter the one-dimensional character of the spin interactions. Therefore, such a transition does not affect the results obtained for purely one-dimensional spin systems.

The situation changes if electron hops from strand to strand are present. We write the total Hamiltonian of

the system in the form

$$\hat{H}=\sum_i \hat{H}_i+\sum_{i,j} W_{ij}\int \mathbf{S}_i(x)\mathbf{S}_j(x)\,dx. \tag{35}$$

Here H_i is the Hamiltonian of one strand and W_{ij} is the amplitude of the interaction of a spin on strand i with a spin on strand j and is proportional to the square of the one-electron hopping amplitude. The interaction of spins from different strands leads to the result that the system becomes a three-dimensional antiferromagnet at low temperatures. Determining the transition temperature T_c by means of the self-consistent field method, we obtain

$$T_c\approx W^{1/(2-\alpha)},\quad W=\sum_j W_{ij}. \tag{36}$$

In this case the results obtained in the preceding sections for a one-dimensional spin system cease to be applicable below the transition point determined by formula (36).

6. CONCLUSION

Quasi-one-dimensional Fermi systems with repulsion have been considered above. It was assumed that this repulsion leads to dielectric ordering at low temperatures. There exist numerous experimental indications that the highly conducting complexes of TCNQ with asymmetric cations (NMP–TCNQ, Q_n–$(TCNQ)_2$, etc.) are such systems.[10,11] These substances are characterized by the complete equivalence of the TCNQ molecules in the chain, and this, apparently, is the reason for the fact that these compounds display metallic properties at high temperatures. At the same time, the asymmetry of the cations in these complexes introduces basic disorder into the crystal lattice. Therefore, in such substances we can expect an increase of the susceptibility in accordance with formulas (18), (25).

The growth of the susceptibility has been observed experimentally in NMP–TCNQ, Q_n–$(TCNQ)_2$ and Ad–$(TCNQ)_2$.[11] The measurements showed that in a broad temperature range 0.1–10 K the susceptibility is described by formula (25), in which each substance has its own index α. Bulaevskiĭ *et al.*[11] also assumed that the increase of the susceptibility is caused by disorder of the lattice. In their opinion, however, the law of this increase is determined by the probability that the exchange integral at any particular point vanishes. In this case the law of the increase would depend strongly on the form and degree of the disorder. Such a dependence has not been detected experimentally.[11] Clearly, this is evidence in favor of the model proposed in the present work.

The situation with the specific heat is more complicated. According to the measurements of[10,12,13] at low temperatures ($2<T<5$ K), the specific heat depends linearly on the temperature, in agreement with the conclusion reached in Sec. 4. At the same time the authors of[14] assert that the specific heat is proportional to a fractional power of the temperature. Further experiments at lower temperatures could clarify the situation.

Specific-heat measurements at higher temperatures[15] have made it possible to detect a phase transition at 7.2 K in NMP–TCNQ and at 14 K in Q_n–$(TCNQ)_2$. The susceptibility varies weakly at the phase-transition point, indicating that this transition is nonmagnetic. The increase of the susceptibility below the transition point is possible only for a one-dimensional spin interaction. All this is evidence that a transition to a dielectric, with the one-dimensional antiferromagnetic ordering described in the preceding section, occurs.

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APPENDIX

We shall calculate the spin correlation functions in the Hubbard model with repulsion and a half-filled band. The Hamiltonian of this model has the form

$$\hat{H}=-T_0\sum_{i,\alpha} a_{i\alpha}^{+}(a_{i+1,\alpha}+a_{i-1,\alpha})+V\sum_{i,\alpha} a_{i\alpha}^{+}a_{i,-\alpha}^{+}a_{i,-\alpha}a_{i\alpha}-\frac{V}{2}\sum_{i,\alpha} a_{i\alpha}^{+}a_{i\alpha}. \tag{A.1}$$

To calculate the correlation functions K_z and $\tilde{K}$, equal to

$$K_z(x,\tau)=\langle S_z(0,0)S_z(x,\tau)\rangle, \tag{A.2}$$
$$\tilde{K}(x,\tau)=\langle S^{+}(0,0)S^{-}(x,\tau)\rangle; \tag{A.3}$$
$$\mathbf{S}(i,\tau)=\sum_{\alpha,\beta}\sigma_{\alpha\beta}a_{i\alpha}^{+}(\tau)a_{i\beta}(\tau),$$

we go over to operators creating ($c_{i\alpha}^{+}(\tau)$) and annihilating ($c_{i\alpha}$) new fermions:

$$a_{j+}=c_{j+},\quad a_{j-}=e^{-i\pi j}c_{j-}^{+},$$
$$a_{j+}^{+}=c_{j+}^{+},\quad a_{j-}^{+}=e^{i\pi j}c_{j-}. \tag{A.4}$$

In the new operators the Hamiltonian (A.1) goes over into a Hubbard Hamiltonian with attraction[16]:

$$\hat{H}=-T_0\sum_{i} c_{i\alpha}^{+}(c_{i+1,\alpha}+c_{i-1,\alpha})-V\sum_{i,\alpha} c_{i,\alpha}^{+}c_{i,-\alpha}^{+}c_{i,-\alpha}c_{i\alpha}+\frac{V}{2}\sum_{i,\alpha} c_{i,\alpha}^{+}c_{i\alpha}. \tag{A.5}$$

Then,

$$K_z(x,\tau)=\sum_{\alpha,\beta}\langle c_{0,\alpha}^{+}(0)c_{0,\alpha}(0)c_{x,\beta}^{+}(\tau)c_{x\beta}(\tau)\rangle.$$
$$\tilde{K}(x,\tau)=\cos\pi x\langle c_{0,+}^{+}(0)c_{0,-}^{+}(0)c_{x,-}(\tau)c_{x,+}(\tau)\rangle. \tag{A.6}$$

We see that, in the c-operators, the spin correlation functions go over into the pair correlation function and the density-density function. Such functions were calculated earlier with the aid of a hypothesis about the role of the sound excitations.[5] On the basis of the results of this paper we obtain

$$K_z(x,\tau)=A(T/v_s)^{1/\alpha}\cos\pi x\,\mathrm{sh}^{-1/2\alpha}[\pi T(x/v_s+i\tau)]\,\mathrm{sh}^{-1/2\alpha}[\pi T(x/v_s-i\tau)]. \tag{A.7a}$$
$$\tilde{K}(x,\tau)=B(T/v_s)^{\alpha}\cos\pi x\,\mathrm{sh}^{-\alpha/2}[\pi T(x/v_s+i\tau)]\,\mathrm{sh}^{-\alpha/2}[\pi T(x/v_s-i\tau)]. \tag{A.7b}$$

where A, B and α are quantities that depend on the interaction, and v_s is the velocity of the gapless excitations. It is assumed that the temperature is much smaller than the magnitude of the gap.

Using the isotropy in spin space, we find the values

$$\alpha=1, \quad B/A=2. \tag{A.8}$$

We note that for $T_0 \ll V$ the Hubbard model with repulsion and a half-filled band is equivalent to the Heisenberg model for an antiferromagnet.

[1]E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).
[2]J. C. Bonner and M. E. Fisher, Phys. Rev. 135, A640 (1964).
[3]R. B. Griffiths, Phys. Rev. 133, A768 (1964).
[4]A. A. Ovchinnikov, Zh. Eksp. Teor. Fiz. 64, 342 (1973) [Sov. Phys. JETP 37, 176 (1973)].
[5]K. B. Efetov and A. I. Larkin, Zh. Eksp. Teor. Fiz. 69, 764 (1975) [Sov. Phys. JETP 42, 390 (1975)].
[6]M. Takahashi, Progr. Theor. Phys. 43, 1619 (1970); 42, 1098 (1969); 43, 860(E) (1970).
[7]V. G. Vaks, A. I. Larkin and S. A. Pikin, Zh. Eksp. Teor. Fiz. 51, 361 (1966) [Sov. Phys. JETP 24, 240 (1967)].
[8]K. B. Efetov and A. I. Larkin, Zh. Eksp. Teor. Fiz. 66, 2290 (1974) [Sov. Phys. JETP 39, 1129 (1974)].
[9]P. A. Lee, T. M. Rice and P. W. Anderson, Phys. Rev. Lett. 31, 462 (1973).
[10]A. J. Epstein, S. Etemad, A. F. Garito and A. J. Heeger, Phys. Rev. B5, 952 (1972).
[11]L. N. Bulaevskiĭ, A. V. Zvarykina, Yu. S. Karimov, R. B. Lyubovskiĭ and I. F. Shchegolev, Zh. Eksp. Teor. Fiz. 62, 725 (1972) [Sov. Phys. JETP 35, 384 (1972)].
[12]P. Delhaes, F. Aly and P. Dupuis, Sol. State Commun. 12, 1099 (1973).
[13]S. Etemad, A. F. Garito and A. J. Heeger, Phys. Lett. 40A, 45 (1972).
[14]L. N. Bulaevskiĭ, A. A. Gusseĭnov, O. N. Eremenko, V. N. Topnikov and I. F. Schegoiev, Fiz. Tverd. Tela (Leningrad) 17, 781 (1975) [Sov. Phys. Solid State 17, 498].
[15]F. F. Igoshin, A. P. Kir'yanov, V. N. Topnikov and I. F. Shchegolev, Zh. Eksp. Teor. Fiz. 68, 1203 (1975) [Sov. Phys. JETP 41, 597].
[16]H. Shiba, Progr. Theor. Phys. 48, 2171 (1972).

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On the possibility of controlling surface phenomena by means of laser radiation

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Processes that can be induced by laser radiation on a surface with adsorbed atoms or molecules are considered. The radiation can alter the desorption, increase the surface diffusion, and influence the heterogeneous catalysis in a selective manner (i.e. act on certain types of atoms). Desorption of atoms due to laser irradiation can be used, among other things, to determine the sites of various atomic groups on the surface of the adsorbent. In order to photograph the surface with sufficiently high resolution, a method for obtaining holograms of the adsorbent is proposed, using collimated atomic beams instead of coherent light.

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INTRODUCTION

Many recent papers have reported the use of laser radiation for selective excitation of vibrational and electronic levels in atoms and molecules.[1–5] Selective excitation uncovers new possibilities of acting on chemical reactions, makes possible mass separation of atoms,[3–5] etc. In the overwhelming number of the considered cases, the laser radiation acts on a homogeneous medium, and for a number of reasons this medium is chosen to be a gas.

In this article we consider the action of laser radiation on heterogeneous systems. We are interested in the new possibilities and effects that may be provided by the presence of the phase-separation surfaces in this case. These include: selective action on the processes of desorption of atoms and molecules adsorbed on a surface with ensuing change of the concentration, mass separation of the atoms via selective desorption (laser chromatography), the effect on the surface diffusion, the change of the catalytic properties of the adsorbents, information on the composition and location of the active groups present on the adsorbent surface (in principle one can hope even to decode the "mosaic" of the molecular groups on the surface of biological objects such as cells, etc.).

Some of these questions have already been considered earlier,[6,7] namely resonant buildup in an adsorption potential with the aid of a set of frequencies, as well as detachment of atoms from a surface. In particular, the possibility was considered of generating hypersound by matched oscillations of the adsorbed atoms in the potential of the wall.[6,7] The possibility of selective heterogeneous separation of vibrationally-excited molecules was considered in[8], but in this variant the selective excitation of the vibrational levels by the laser beam was produced not on the surface but in the volume.

1. ACTION OF LASER ON ADSORBATE. ESTIMATES OF THE PROBABILITIES OF EXCITATION AND DESORPTION UNDER THE INFLUENCE OF LASER RADIATION

Depending on the frequency, the mechanisms whereby laser radiation acts on adsorbed particles can be quite different—infrared radiation is capable of inducing par-