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Low-Temperature Properties of the Hubbard Model

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Self-consistent equations corresponding to the single-loop approximation at an arbitrary relation between the Hubbard energy U and hop integral t have been obtained for the determination of the energy spectrum in the Hubbard model. The conditions of the insulator–metal transition, as well as the conditions for the transition from the paradielectric to antiferromagnetic state (spin-density wave), have been determined in the case of an exactly half-filled band.

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It was shown in Hubbard's classical work [1, 2] that the dielectric gap can disappear only owing to the scattering on fluctuations of the electron and spin densities. However, the magnitude of the corresponding fluctuations calculated from physical reasons corresponds to fluctuations of noninteracting localized electrons. Thus, Hubbard's results refer to the high-temperature limit. Fluctuations in the low-temperature limit are significantly suppressed owing to the presence of an energy gap. In this case, a transition to a metallic state occurs owing to effects of the kinematic interaction [3], leading to a decrease and subsequent disappearance of the energy gap. This phenomenon is studied in this work in the single-loop approximation.

Conditions of the appearance of antiferromagnetism for alternative two-sublattice systems can also be obtained in the single-loop approximation.

The Hubbard Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_t$ can be expressed in terms of X operators:

$$\hat{H}_0 = \sum_{\mathbf{r}} \left\{ (U - 2\mu)\hat{X}_{\mathbf{r}}^{2,2} - (\mu + \sigma)\hat{X}_{\mathbf{r}}^{\sigma,\sigma} \right\}, \tag{1}$$

$$\hat{H}_t = \sum_{\mathbf{r}_1, \mathbf{r}_2, \sigma} (\hat{X}_{\mathbf{r}_1}^{2,-\sigma} + \sigma\hat{X}_{\mathbf{r}_1}^{\sigma,0})(\hat{X}_{\mathbf{r}_2}^{-\sigma,2} + \sigma\hat{X}_{\mathbf{r}_2}^{0,\sigma}) t(\mathbf{r}_1 - \mathbf{r}_2).$$

Here and below, U is the Hubbard energy and μ is the chemical potential.

At a given projection of the spin σ, there are two independent transitions: from the empty state to single-particle state with the projection σ and from the single-particle state with the projection $-\sigma$ to two-particle state. Correspondingly, we introduce two end factors each equal to the sum of the occupation numbers of the final and initial states

$$f_1^\sigma = n_0 + n_1^\sigma, \quad f_2^\sigma = n_{11} + n_1^{-\sigma}, \tag{2}$$

which are related as $f_1^\sigma + f_2^\sigma = 1$.

The equations of the single-loop approximation are written in terms of the components of the inverse matrix:

$$\hat{G}_\omega^{-1}(\mathbf{p}) = \begin{pmatrix} E_1^\sigma - f_1^\sigma t_{\mathbf{p}} - \Sigma_{11}^\sigma & -f_1^\sigma \sigma t_{\mathbf{p}} - \Sigma_{12}^\sigma \\ -f_2^\sigma \sigma t_{\mathbf{p}} - \Sigma_{21}^\sigma & E_2^\sigma - f_2^\sigma t_{\mathbf{p}} - \Sigma_{22}^\sigma \end{pmatrix}. \tag{3}$$

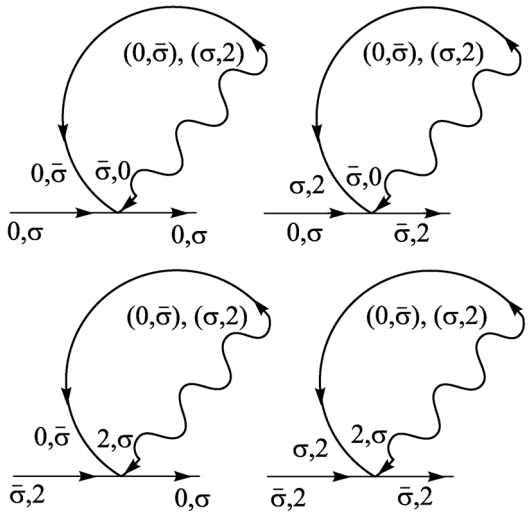

Fig. 1. Single-loop self-energy parts.

As is seen in Fig. 1, the off-diagonal self-energy functions of the single-loop approximation are expressed in terms of the diagonal functions as

$$\Sigma_{12}^{\sigma} = -\sigma\Sigma_{22}^{\sigma}, \quad \Sigma_{21}^{\sigma} = -\sigma\Sigma_{11}^{\sigma}. \tag{4}$$

Using these relations and the definition of diagonal matrix elements,

$$E_1^{\sigma} = i\omega + \mu + \sigma H, \quad E_2^{\sigma} = i\omega + \mu + \sigma H - U, \tag{5}$$

we obtain two Hubbard branches:

$$\xi_{\mathbf{p}}^{\pm} = \frac{S^{\sigma} + t_{\mathbf{p}}}{2} \pm \frac{1}{2}\sqrt{W_{\mathbf{p}}^{\sigma}} - \mu + \frac{U}{2} - \sigma H. \tag{6a}$$

Here,

$$W_{\mathbf{p}}^{\sigma} = (S^{\sigma} - t_{\mathbf{p}})^2 + U^2 - 2U[R^{\sigma} + t_{\mathbf{p}}(f_1^{\sigma} - f_2^{\sigma})], \tag{6b}$$

and, instead of the diagonal self-energy parts, we introduce the two quantities

$$S^{\sigma} = \Sigma_1^{\sigma} + \Sigma_2^{\sigma}, \quad R^{\sigma} = \Sigma_1^{\sigma} - \Sigma_2^{\sigma}. \tag{7}$$

Thus, the aim is to determine the relation between the average occupation numbers, temperature, and chemical potential, as well as to write two equations for the determination of self-energy parts $\Sigma_{1,2}^{\sigma}$.

Three desired relations are expressed in terms of two independent combinations of the single-particle Green's functions:

$$\begin{aligned} G_{-}^{\sigma}(\omega, \mathbf{p}) &= [G_{\omega}^{\sigma}(\mathbf{p})]_{1,1} + \sigma[G_{\omega}^{\sigma}(\mathbf{p})]_{2,1}, \\ G_{+}^{\sigma}(\omega, \mathbf{p}) &= \sigma[G_{\omega}^{\sigma}(\mathbf{p})]_{1,2} + [G_{\omega}^{\sigma}(\mathbf{p})]_{2,2}. \end{aligned} \tag{8}$$

In particular, using the definition of the average number of particles with a given projection σ, we obtain

$$\begin{aligned} n_{\sigma} &= \langle \hat{a}_{\sigma}^{+}\hat{a}_{\sigma}\rangle = n_{\mathrm{II}} + n_{\mathrm{I}}^{\sigma} = f_2^{-\sigma} \\ &= T\sum_{\mathbf{p},\omega}[G_{-}^{\sigma}(\omega, \mathbf{p})e^{i\omega\delta}f_1^{\sigma} + G_{+}^{\sigma}(\omega, \mathbf{p})e^{i\omega\delta}f_2^{\sigma}]. \end{aligned} \tag{9}$$

The equations for the determination of the self-energy parts are written similarly:

$$\begin{aligned} \Sigma_1^{\sigma} &= -T\sum_{\mathbf{p},\omega} t_{\mathbf{p}} G_{-}^{-\sigma}(\omega, \mathbf{p})e^{i\omega\delta}, \\ \Sigma_2^{\sigma} &= T\sum_{\mathbf{p},\omega} t_{\mathbf{p}} G_{+}^{-\sigma}(\omega, \mathbf{p})e^{i\omega\delta}. \end{aligned} \tag{10}$$

To sum over the complex frequencies $i\omega = i(2n + 1)\pi T$, we substitute an explicit expression for the single-particle Green's function into the right-hand sides of Eqs. (9) and (10), decompose into simple factors, and sum over complex frequencies.

The intermediate result has the form

$$T\sum_{\omega} G_{\nu}^{\sigma}(\omega, \mathbf{p})e^{i\omega\delta} = \sum_{\lambda = \pm} B_{\nu}^{\lambda}(\mathbf{p})n_{\mathrm{F}}(\xi_{\mathbf{p}}^{\lambda}), \tag{11}$$

where $n_{\mathrm{F}}(\epsilon)$ is the Fermi distribution and the coefficients $B_{\nu}^{\lambda}(\mathbf{p})$ are given by the expression

$$B_{\pm}^{(\lambda,\sigma)}(\mathbf{p}) = \frac{1}{2}\left[1 + \mathrm{sgn}(\lambda)\frac{t_{\mathbf{p}} - S^{\sigma} \pm U}{\sqrt{W_{\mathbf{p}}^{\sigma}}}\right]. \tag{12}$$

In terms of these two coefficients, the equation of state (9) and Eqs. (10) for the functions S^{σ} and R^{σ} are written in the form

$$\begin{aligned} n_{\sigma} &= f_2^{\sigma} \\ &= \sum_{\mathbf{p},\lambda}\{[B_{-}^{(\lambda,\sigma)}(\mathbf{p})f_1^{\sigma} + B_{+}^{(\lambda,\sigma)}(\mathbf{p})f_2^{\sigma}]n_{\mathrm{F}}(\xi_{\mathbf{p}}^{(\lambda,\sigma)})\}, \end{aligned} \tag{13}$$

$$S^{\sigma} = \sum_{\mathbf{p},\lambda}\{t_{\mathbf{p}}[B_{+}^{(\lambda,-\sigma)}(\mathbf{p}) - B_{-}^{(\lambda,-\sigma)}(\mathbf{p})]n_{\mathrm{F}}(\xi_{\mathbf{p}}^{(\lambda,-\sigma)})\}, \tag{14}$$

$$R^{\sigma} = -\sum_{\mathbf{p},\lambda'}\{t_{\mathbf{p}}[B_{+}^{(\lambda,-\sigma)}(\mathbf{p}) + B_{-}^{(\lambda,-\sigma)}(\mathbf{p})]n_{\mathrm{F}}(\xi_{\mathbf{p}}^{(\lambda,-\sigma)})\}. \tag{15}$$

Equations (14) and (15) generalize the Hubbard equations corresponding to the zero-loop approximation (Eq. (13) written at $S = R = 0$). The inclusion of single-loop corrections (14) and (15) results in significant changes both in the energy spectrum and in the magnetic properties appearing when an external magnetic field is switched on.[1]

If the lower Hubbard subband is half filled, then $\mu = U/2$ and the integration with respect to the momentum $\mathbf{p}$ occurs over the entire Brillouin zone. Under the assumption that the density of states $\rho(\epsilon) = \sum_{\mathbf{p}}\delta(\epsilon - t_{\mathbf{p}})$ is an even function of the energy ϵ, we obtain $S^{\sigma} = 0, f_1 = f_2 = 1/2$.

The excitation spectrum $\xi_{\mathbf{p}}^{\pm}$ is expressed in terms of the single-loop self-energy part R:

[1] Self-consistent equations (13)–(15) cannot be obtained within the dynamic mean field theory (DMFT) [4, 5] because the DMFT equations are based on the classical Fermi anticommutation relations. For this reason, the contribution corresponding to an electron loop shown in Fig. 1 is not taken into account.

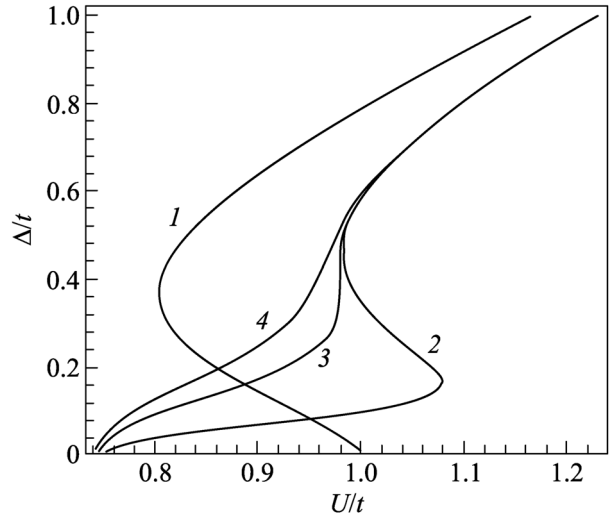

Fig. 2. Dielectric gap Δ/t versus the dimensionless Hubbard energy U/t ($\rho_0 = \theta(1-\epsilon^2)/2$, $n = 1$) for $T =$ (*1*) 0, (*2*) 0.01, (*3*) 0.04, and (*4*) 0.06.

$$R = \sum_{\mathbf{p}} \frac{t_{\mathbf{p}}^2}{\sqrt{t_{\mathbf{p}}^2 + \Delta^2}} [n_F(\xi_{\mathbf{p}}^-) - n_F(\xi_{\mathbf{p}}^+)]$$
$$= \int \rho_0(\epsilon) \frac{\epsilon^2}{\sqrt{\epsilon^2 + \Delta^2}} [n_F(\xi_\epsilon^-) - n_F(\xi_\epsilon^+)] d\epsilon, \quad (16)$$

where Δ is the dielectric gap, which is determined from the self-consistency condition

$$\xi_{\mathbf{p}}^{\pm} = \frac{t_{\mathbf{p}}}{2} \pm \frac{1}{2}\sqrt{t_{\mathbf{p}}^2 + \Delta^2}, \quad \Delta^2 = U^2 - 2UR. \quad (17a)$$

Here and below, the single-particle bare density of states is used:

$$\rho_0(\epsilon) = \sum_{\mathbf{p}} \delta(\epsilon - t_{\mathbf{p}}), \quad \xi_\epsilon^{\pm} = \frac{\epsilon}{2} \pm \frac{1}{2}\sqrt{\epsilon^2 + \Delta^2}. \quad (17b)$$

Thus, the single-loop approximation leads to a significant decrease in the correlation gap, which disappears under the condition $R = U/2$. Substituting this quantity into Eq. (16), we obtain the critical Hubbard energy below which the system is a metal:

$$U_c = 2\sum_{\mathbf{p}} |t_{\mathbf{p}}| = 2\int |\epsilon| \rho_0(\epsilon) d\epsilon. \quad (18)$$

The results of the calculations of the temperature dependence of Δ for the flat band model are shown in Fig. 2. In the region of ultimately low temperatures $T < T_c$, there is an ambiguous dependence $\Delta(U)$, which disappears at $T > 0.04$ (these results were obtained by the numerical renormalization group method [6, 7]).

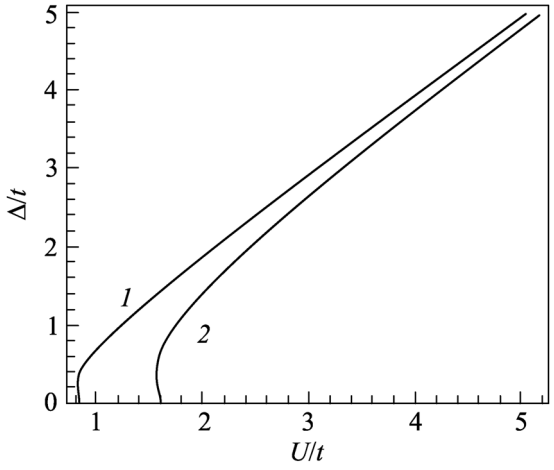

Fig. 3. Dielectric gap Δ/t versus the dimensionless Hubbard energy U/t ($T = 0$, $n = 1$). Lines *1* and *2* correspond to the semielliptic density of states and square lattice, respectively.

In the limit $T = 0$, the analytical expression for $U(\Delta)$ for a semielliptic density of states can be obtained: $\rho_0(\epsilon) = (4/\pi)\sqrt{1-\epsilon^2}$. At $T = 0$, Eq. (16) is represented in the form

$$R = R(\Delta) = \frac{4}{3\pi}\sqrt{1+\Delta^2}$$
$$\times \left[(1+2\Delta^2)\mathrm{E}\left(\frac{1}{\sqrt{1+\Delta^2}}\right) - 2\Delta^2 \mathrm{K}\left(\frac{1}{\sqrt{1+\Delta^2}}\right)\right]. \quad (19a)$$

Here and below, $\mathbf{K}(x)$ and $\mathbf{E}(x)$ are the complete elliptic integrals of the first and second kinds.

For the square lattice,

$$\rho_0(\epsilon) = \frac{2}{\pi^2}\mathrm{K}\left(\sqrt{1-\frac{\epsilon^2}{4}}\right) = \frac{8}{(|\epsilon|+2)\pi^2}\mathrm{K}\left(\frac{2-|\epsilon|}{2+|\epsilon|}\right), \quad (19b)$$

so that numerical integration is necessary:

$$R = R(\Delta) = \frac{8}{\pi^2}$$
$$\times \int_0^2 \frac{\epsilon^2}{(2+|\epsilon|)\sqrt{\epsilon^2+\Delta^2}} \mathrm{K}\left(\frac{2-|\epsilon|}{2+|\epsilon|}\right) d\epsilon. \quad (19c)$$

Thus, the dependence of the Hubbard energy U on the dielectric gap Δ (see Fig. 3) can be obtained in the explicit form

$$U = |R(\Delta)| + \sqrt{R^2(\Delta) + \Delta^2}. \quad (20)$$

Here, $\Delta = \sqrt{U^2 - 2UR}$ is the dielectric gap and all energy quantities are divided by the half-width $|t|$.

According to Fig. 3, the energy of the gap decreases with a decrease in the Hubbard energy U. Finally, it vanishes, which corresponds to an insulator–metal transition. The corresponding transition point calculated in [2] ($(U/t)_c = \sqrt{3}/2 \approx 0.866$) for the bare semielliptic density of states differs slightly from the value $(U/t)_c = 8/(3\pi) \approx 0.848$ obtained from Eq. (20).

The possibility of the appearance of the spin density wave in a two-sublattice crystal system will be considered below.

To determine the conditions for the appearance of the spin density wave, the spin magnetic susceptibility will be calculated. When a weak magnetic field depends on the coordinates, it is convenient to pass to the momentum representation: $\delta h_{\mathbf{r}} = \delta h_{\mathbf{q}} \exp(i\mathbf{qr})$. It is assumed that corrections to the electron density δn, to the end factors $\delta f_{1,2}$ ([8, 9]), and to the self-energy parts $\delta\Sigma_{1,2}$ ([10]) depend on the coordinates through the single Fourier component:

$$\begin{aligned}\delta n^{\sigma}_{\mathbf{r}} &= \delta f^{\sigma}_{1,\mathbf{r}} = -\delta f^{\sigma}_{2,\mathbf{r}} = \delta n^{\sigma}_{\mathbf{q}} \exp(i\mathbf{qr}) \\ &= \delta f^{\sigma}_1(\mathbf{q})\exp(i\mathbf{qr}) = -\delta f^{\sigma}_2(\mathbf{q})\exp(i\mathbf{qr}); \\ \delta\Sigma^{\sigma}_{1,\mathbf{r}} &= \delta\Sigma^{\sigma}_1(\mathbf{q})\exp(i\mathbf{qr}), \\ \delta\Sigma^{\sigma}_{2,\mathbf{r}} &= \delta\Sigma^{\sigma}_2(\mathbf{q})\exp(\mathbf{iqr}).\end{aligned} \tag{21}$$

An equation for the susceptibility $\chi_{\mathbf{q}}$ is obtained by varying the equation for the Green's function $G_{\omega}(\mathbf{p}, \mathbf{q})$, which is expressed in terms of the variation of the magnetic field $\mathbf{h}_{\mathbf{q}}$, end factor $f_{\mathbf{q}} = \delta f^{\sigma}_{1,\mathbf{r}} = -\delta f^{\sigma}_{2,\mathbf{r}}$, and single-loop self-energy parts $S_{\mathbf{q}} = \Sigma_{1,\mathbf{q}} + \Sigma_{2,\mathbf{q}}$ and $R_{\mathbf{q}} = \Sigma_{1,\mathbf{q}} - \Sigma_{2,\mathbf{q}}$:

$$\begin{aligned}\delta n^{\sigma}_{\mathbf{q}} &= \delta f^{\sigma}_{\mathbf{q}} T\sum_{\omega,\mathbf{p}}[G^{\sigma}_{-,\omega}(\mathbf{p}) - G^{\sigma}_{+,\omega}(\mathbf{p})] \\ &+ f^{\sigma}_1 T\sum_{\omega,\mathbf{p}}\delta G^{\sigma}_{-,\omega}(\mathbf{p},\mathbf{q}) + f^{\sigma}_2 T\sum_{\omega,\mathbf{p},\mathbf{q}}\delta G^{\sigma}_{+,\omega}(\mathbf{p},\mathbf{q}), \\ \delta S^{\sigma}_{\mathbf{q}} &= -T\sum_{\omega,\mathbf{p}} t_{\mathbf{p}}[\delta G^{-\sigma}_{-,\omega}(\mathbf{p},\mathbf{q}) - \delta G^{-\sigma}_{+,\omega}(\mathbf{p},\mathbf{q})], \\ \delta R^{\sigma}_{\mathbf{q}} &= -T\sum_{\omega,\mathbf{p}} t_{\mathrm{p}}[\delta G^{-\sigma}_{-,\omega}(\mathbf{p},\mathbf{q}) + \delta G^{-\sigma}_{+,\omega}(\mathbf{p},\mathbf{q})].\end{aligned} \tag{22}$$

The expressions for the Green's functions in the first sum in the first equation are determined by means of Eqs. (11) and (12). The variations of the Green's functions are determined in terms of the variation of the inverse function (3) with the use of the general formula

$$\delta\hat{G}^{\sigma}_{\omega}(\mathbf{p}) = -\hat{G}^{\sigma}_{\omega}(\mathbf{p})\delta\hat{G}^{-1}_{\sigma,\omega}(\mathbf{p},\mathbf{q})\hat{G}^{\sigma}_{\omega}(\mathbf{p}+\mathbf{q}). \tag{23}$$

Here, the Green's functions are calculated at zero magnetic field and the variation of the inverse Green's functions is determined using general formulas (3)–(5):

$$\delta\hat{G}^{-1}_{\sigma,\omega}(\mathbf{p},\mathbf{q}) = \begin{pmatrix} \sigma\delta h_{\mathbf{q}} - \delta f^{\sigma}_1(\mathbf{q})t_{\mathbf{p}+\mathbf{q}} - \delta\Sigma^{\sigma}_{11}(\mathbf{q}) & -\sigma\delta f^{\sigma}_1(\mathbf{q})t_{\mathbf{p}+\mathbf{q}} + \sigma\delta\Sigma^{\sigma}_{22}(\mathbf{q}) \\ -\sigma\delta f^{\sigma}_2(\mathbf{q})t_{\mathbf{p}+\mathbf{q}} + \sigma\delta\Sigma^{\sigma}_{11}(\mathbf{q}) & \sigma\delta h_{\mathbf{q}} - \delta f^{\sigma}_2(\mathbf{q})t_{\mathbf{p}+\mathbf{q}} - \delta\Sigma^{\sigma}_{22}(\mathbf{q}) \end{pmatrix}. \tag{24}$$

Below, it will be taken into account that all variations in our problem change sign at change in sign of the projection of the spin:

$$\delta f^{-\sigma}_k = -\delta f^{\sigma}_k, \quad \delta\Sigma^{-\sigma}_{11} = -\delta\Sigma^{\sigma}_{11}, \quad \delta\Sigma^{-\sigma}_{22} = -\delta\Sigma^{\sigma}_{22}. \tag{25}$$

Furthermore, according to the identity $f^{\sigma}_1 + f^{\sigma}_2 = 1$, $\delta f^{\sigma}_2 = -\delta f^{\sigma}_1$. Therefore, the aim is reduced to the solution of the system of equations

$$\begin{aligned} df &= F_f df^{\sigma}_1 + F_S dS + F_R dR + f' dh, \\ dS &= S_f df^{\sigma}_1 + S_S dS + S_R dR + S' dh, \\ dR &= R_f df^{\sigma}_1 + R_S dS + R_R dR + R' dh. \end{aligned} \tag{26}$$

Here, $\delta f_1 = \delta f^{+}_1$, $\delta S = \delta S^{+} = \delta\Sigma^{+}_{11} + \delta\Sigma^{+}_{22}$, and $\delta R = \delta R^{+} = \delta\Sigma^{+}_{11} - \delta\Sigma^{+}_{22}$.

The coefficients of Eqs. (26) are given by the expressions

$$\begin{aligned} F_f &= \sum_{\mathbf{p}} \frac{U}{\xi^{+}_{\mathbf{p}} - \xi^{-}_{\mathbf{p}}}[n_{\mathrm{F}}(\xi^{-}_{\mathbf{p}}) - n_{\mathrm{F}}(\xi^{+}_{\mathbf{p}})] \\ &+ T\sum_{\omega,\mathbf{p}} \frac{Ut_{\mathbf{p}+\mathbf{q}}(-E_2 f_1 - E_1 f_2 + S)}{W_{\omega}(\mathbf{p},\mathbf{q})}, \\ F_S &= T\sum_{\omega,\mathbf{p}} \frac{U(E_1 f_2 - E_2 f_1 - R)}{2W_{\omega}(\mathbf{p},\mathbf{q})}, \\ F_R &= T\sum_{\omega,\mathbf{p}} \frac{U(-E_2 f_1 - E_1 f_2 + S)}{2W_{\omega}(\mathbf{p},\mathbf{q})}; \end{aligned}$$

$$f' = T\sum_{\omega,\mathbf{p}}\Big\{-S^2+\frac{1}{2}[R+S(2-f_1+f_2)]E_1$$

$$+\frac{1}{2}[-R+S(2+f_1-f_2)]E_2-f_1E_2^2-f_2E_1^2\Big\}\frac{1}{W_\omega(\mathbf{p},\mathbf{q})};$$

$$S_f = T\sum_{\omega,\mathbf{p}}\frac{U^2t_\mathbf{p}t_{\mathbf{p}+\mathbf{q}}}{W_\omega(\mathbf{p},\mathbf{q})},$$

$$S_S = T\sum_{\omega,\mathbf{p}}\frac{Ut_\mathbf{p}(-E_1-E_2+2t_{\mathbf{p}+\mathbf{q}})}{2W_\omega(\mathbf{p},\mathbf{q})}, \qquad (27)$$

$$S_R = T\sum_{\omega,\mathbf{p}}\frac{U^2t_\mathbf{p}}{2W_\omega(\mathbf{p},\mathbf{q})},$$

$$S' = UT\sum_{\omega,\mathbf{p}}(E_1+E_2-t_{\mathbf{p}+\mathbf{q}}-S)\frac{t_\mathbf{p}}{W_\omega(\mathbf{p},\mathbf{q})};$$

$$R_f = T\sum_{\omega,\mathbf{p}}\frac{U(-E_1-E_2+2S)t_\mathbf{p}t_{\mathbf{p}+\mathbf{q}}}{W_\omega(\mathbf{p},\mathbf{q})},$$

$$R_S = T\sum_{\omega,\mathbf{p}}\frac{Ut_\mathbf{p}(U-2R-Ft_{\mathbf{p}+\mathbf{q}})}{2W_\omega(\mathbf{p},\mathbf{q})},$$

$$R_r = T\sum_{\omega,\mathbf{p}}\frac{Ut_\mathbf{p}(-E_1-E_2+2S)}{2W_\omega(\mathbf{p},\mathbf{q})},$$

$$R' = -T\sum_{\omega,\mathbf{p}}t_\mathbf{p}\{2S^2+[-2S-(f_1-f_2)t_{\mathbf{p}+\mathbf{q}}-R]E_1$$

$$+[-2S+(f_1-f_2)t_{\mathbf{p}+\mathbf{q}}+R]E_2+E_1^2+E_2^2\}\frac{1}{W_\omega(\mathbf{p},\mathbf{q})}.$$

Here, $U=E_1-E_2$, $\xi_\mathbf{p}^\pm$ are the energies in the upper and lower Hubbard subbands defined in Eqs. (6a) and (6b), respectively, and

$$W_\omega(\mathbf{p},\mathbf{q}) = (i\omega-\xi_\mathbf{p}^+)(i\omega-\xi_\mathbf{p}^-)$$
$$\times(i\omega-\xi_{\mathbf{p}+\mathbf{q}}^+)(i\omega-\xi_{\mathbf{p}+\mathbf{q}}^-).$$

In the case of the exactly half-filled band $n=1$, $\mu=-U/2$, $E_1=i\omega_n+U/2$, $E_2=i\omega_n-U/2$, $f_1=f_2=1/2$, and $S_0=0$ should be set in the equations. As a result, the coefficients determining the magnetic susceptibility have the form

$$F_f = \sum_\mathbf{p}\frac{U}{\sqrt{\Delta^2+t_\mathbf{p}^2}}[n_\mathrm{F}(\xi_\mathbf{p}^-)-n_\mathrm{F}(\xi_\mathbf{p}^+)],$$

$$F_S = T\sum_{\omega,\mathbf{p}}\frac{\Delta^2}{4W_\omega(\mathbf{p},\mathbf{q})}, \quad F_R = 0,$$

$$f' = T\sum_{\omega,\mathbf{p}}\frac{4\omega^2-\Delta^2}{4W_\omega(\mathbf{p},\mathbf{q})}; \qquad (28)$$

$$S_f = US_S, \quad S_S = -S' = UT\sum_{\omega,\mathbf{p}}\frac{t_\mathbf{p}t_{\mathbf{p}+\mathbf{q}}}{W_\omega(\mathbf{p},\mathbf{q})}, \quad S_R = 0,$$

$$R_f = R_S = R_r = R' = 0.$$

Here, the definition of the energy gap is used, $\Delta=\sqrt{U^2-2RU}$, in terms of which the energies in the upper and lower Hubbard subbands are expressed:

$$\xi_\mathbf{p}^\pm = \frac{1}{2}(\pm\sqrt{\Delta^2+t_\mathbf{p}^2}+t_\mathbf{p}).$$

The possibility of establishing antiferromagnetism (spin-density wave) in the case of a two-sublattice crystal system under the condition $t_{\mathbf{p}+\mathbf{Q}}=-t_\mathbf{p}$ (complete nesting) will be analyzed below. In this case, $W_\omega(\mathbf{p},\mathbf{Q})$ is an even function of the energy parameter ω:

$$W_\omega(\mathbf{p},\mathbf{Q}) = [\omega^2+(\xi_\mathbf{p}^+)^2][\omega^2+(\xi_\mathbf{p}^-)^2]. \qquad (29)$$

The coefficients determining the magnetic susceptibility at $\mathbf{q}=\mathbf{Q}$ have the form

$$F_f = \sum_\mathbf{p}\frac{U}{\sqrt{\Delta^2+t_\mathbf{p}^2}}[n_\mathrm{F}(\xi_\mathbf{p}^-)-n_\mathrm{F}(\xi_\mathbf{p}^+)],$$

$$F_S = T\sum_{\omega,\mathbf{p}}\frac{\Delta^2}{4W\omega(\mathbf{p},\mathbf{Q})}, \quad F_R = 0,$$

$$f' = T\sum_{\omega,\mathbf{p}}\frac{4\omega^2-U^2}{4W_\omega(\mathbf{p},\mathbf{Q})}; \qquad (30)$$

$$S_f = US_S, \quad S_S = -S' = -UT\sum_{\omega,\mathbf{p}}\frac{t_\mathbf{p}^2}{W_\omega(\mathbf{p},\mathbf{Q})}, \quad S_R = 0,$$

$$R_f = R_S = R_r = R' = 0.$$

Since the momentum dependence of the right-hand sides in Eqs. (30) appears only in the hop integral $t_\mathbf{p}$, it is convenient to introduce the bare density of states

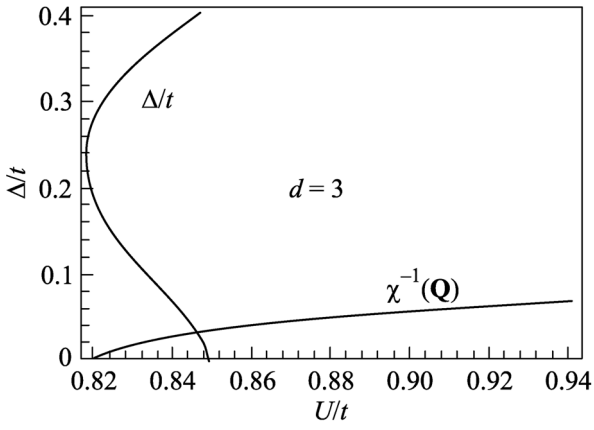

Fig. 4. Dielectric gap Δ/t and inverse antiferromagnetic susceptibility $\chi(\mathbf{Q})^{-1}$ for the semielliptic density of states.

$\rho(\epsilon) = \sum_{\mathbf{p}} \delta(\epsilon - t_{\mathbf{p}})$. If $\rho(\epsilon) = \rho(-\epsilon)$, Eqs. (30) become

$$F_f = \int \rho(\epsilon) \frac{U}{\sqrt{\epsilon^2 + \Delta^2}} [n_F(\xi_\epsilon^-) - n_F(\xi_\epsilon^+)] d\epsilon,$$

$$F_S = A_0(T)\frac{\Delta^2}{4}, \quad F_R = 0,$$

$$f' = A_2(T) - A_0(T)\frac{\Delta^2}{4}, \tag{31}$$

$$S_f = US_S, \quad S_S = -S' = -UD_s, \quad S_R = 0,$$

$$R_f = R_S = R_r = R' = 0,$$

where

$$A_k = T\sum_\omega \int \rho(\epsilon) \frac{\omega^k}{V_\omega(\epsilon)} d\epsilon,$$

$$V_\omega(\epsilon) = [\omega^2 + (\xi_\epsilon^+)^2][\omega^2 + (\xi_\epsilon^-)^2],$$

$$D_s = T\sum_\omega \int \rho(\epsilon) \frac{\epsilon^2}{V_\omega(\epsilon)} d\epsilon, \tag{32}$$

$$\xi_\epsilon^\pm = \frac{1}{2}[\epsilon \pm \sqrt{\Delta^2 + \epsilon^2}].$$

According to Eqs. (32), the antiferromagnetic correction at any temperature is $\delta R = 0$. The remaining system of equations has the form

$$df_1 = F_f df_1 + F_S dS + f' dh,$$
$$dS = S_f df_1 + S_S dS + S' dh. \tag{33}$$

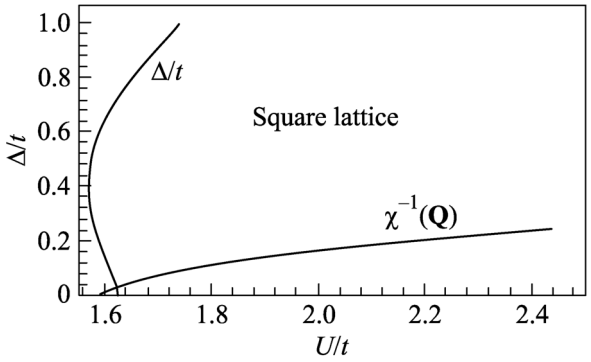

Fig. 5. Dielectric gap Δ/t and inverse antiferromagnetic susceptibility $\chi(\mathbf{Q})^{-1}$ for the square lattice.

The coefficients in these equations at $T = 0$ are

$$F_f = UA, \quad F_S(0) = \frac{A}{2}, \quad f' = 0,$$

$$A = \int \rho(\epsilon) \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} d\epsilon,$$

$$S_f(0) = US_S(0), \quad S_S(0) = S'(0) = -2\frac{U^2}{\Delta^2}R, \tag{34}$$

$$R = \int \rho(\epsilon) \frac{\epsilon^2}{\sqrt{\epsilon^2 + \Delta^2}} d\epsilon.$$

The substitution of these coefficients into the system of equations (33) makes it possible to obtain the inverse magnetic susceptibility:

$$\chi^{-1} = \left(2\frac{df_1}{dh}\right)^{-1}$$
$$= \frac{\Delta^2}{4AUR}\left(1 - UA + 2R\frac{U}{\Delta^2} - AR\frac{U^2}{\Delta^2}\right). \tag{35}$$

Thus, the condition of the appearance of antiferromagnetism at $T = 0$ is modified to the form

$$1 - UA + 2R\frac{U}{\Delta^2} - AR\frac{U^2}{\Delta^2} = 0. \tag{36}$$

The Hubbard energy U is related to the dielectric gap Δ as

$$U = U(\Delta) = R(\Delta) + \sqrt{R(\Delta)^2 + \Delta^2}. \tag{37}$$

All other coefficients entering into Eq. (35) can be similarly expressed in terms of the parameter Δ: $A(\Delta)$ and $R(\Delta)$.

The substitution of these functions into condition (36) makes it possible to determine the critical value $U_{af}/t \le 1$ that corresponds to the appearance of the spin density wave (see Fig. 4).

According to Figs. 4 and 5, antiferromagnetic ordering occurs in the dielectric phase in a close vicinity of the point of transition from the dielectric to metallic phase.

Thus, not only the point of transition from the dielectric to metallic state but also the point of appearance of the antiferromagnetic order parameter with the use of Eq. (36) can be determined in the single-loop approximation.

The calculations in the single-loop approximation provide the general conclusion that a metal–insulator phase transition can be detected in the simplest S-electron Hubbard model for the exactly half-filled band. In this case, antiferromagnetic ordering (spin density wave) at $T = 0$ exists in the entire metallic region ($t > U_c$).

The physical reason for a decrease in the dielectric gap should be attributed to the so-called kinematic interaction, which is attractive at a high electron density ($n > 2/3$) [10].

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