

Correlation effects in metal–dielectric transitions in nonideal systems

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Ordered nonideal systems are studied near the singular point where the electronic density of states vanishes and there occurs in self-consistent field theory a dielectric–metal transition accompanied at $T = 0$ by a 3/2-order phase transition. It is shown that the correlation effects can be taken into account with the aid of the ε -expansion method for the case in which the number of dimensions is close to four. The indicated method allows the determination of all the critical exponents in the low-frequency gapless and high-frequency regions; the asymptotic form of the density-of-states “tail” is found in the dielectric region.

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INTRODUCTION

It became clear after the discovery of gapless superconductivity¹ that, in a nonideal system, the phase transition point where the gap (G) appears does to, generally speaking, coincide with the point where the order parameter Δ appears. A similar situation was found in the exciton-dielectric model with impurities,² in the Hubbard model,³ as well as in the model of the disordered binary solid solution.⁴

It is shown in Refs. 1 and 2 that the transition into the gapless state is connected with the appearance of a complex self-energy part $i\tilde{\omega}$ that, together with the anomalous self-energy part $\tilde{\Delta}$, satisfies the following system of equations:

$$\tilde{\omega} = \omega + \tilde{\omega}/2\tau_1(\tilde{\Delta}^2 + \tilde{\omega}^2)^{1/2}, \quad \tilde{\Delta} = \Delta + \tilde{\Delta}/2\tau_2(\tilde{\Delta}^2 + \tilde{\omega}^2)^{1/2}. \quad (1)$$

For a superconductor, $\tau_1^{-1} - \tau_2^{-1} = 2\tau_s^{-1}$ is the reciprocal time characterizing the relaxation with spin flip; for the exciton dielectric $-\tau_2 = \tau_1$ is the characteristic time of the relaxation without spin flip; $\omega = (2n + 1)\pi T$ is the Matsubara frequency, which, after the analytic continuation $i\omega \rightarrow \omega + i\delta$, determined the energy ω as measured from the Fermi level.

Expanding Eq. (1) in powers of $\tilde{\omega}/\tilde{\Delta}$, we obtain the nonlinear equation

$$\tilde{\omega}\tau + b\tilde{\omega}^3 = \omega, \quad (2)$$

which is similar to the self-consistency condition for the order parameter in the theory of second-order phase transitions. Here $\tau = 1 - (\tau_1^{-1} - \tau_2^{-1})(2\Delta)^{-1}$ is a quantity that determines the proximity to the transition point in the gapless state in terms of the impurity density, which is assumed to be sufficiently low.

It is shown in Ref. 5 that the system of equations (1) is valid in the nonideal Hubbard model as well if the quantity Δ is assumed to be the antiferromagnetic order parameter and $\tau_1 = -\tau_2$, as in the theory of the excitonic dielectric. In Ref. 6 it is shown that the expansion (2) is applicable also to the ordinary ideal Hubbard model, but for temperatures higher than the Néel temperature. In this case τ is a dimensionless quantity determining the proximity in terms of pressure to the critical point of the transition from the paraelectric into the parametallic state.

In the nonsymmetric models, when the expansion (1) contains a term quadratic in $i\tilde{\omega}$, we can always perform a linear transformation, and then choose the chemical potential such that as $\omega \rightarrow 0$ the self-consistency condition in the new variables has the canonical form (2). The positive coefficient b , which is, in order of magnitude, equal to the reciprocal of the square of the characteristic energy, is assumed for simplicity to be equal to unity below. In the gapless (metallic) phase, where $\tau < 0$ as $\omega \rightarrow 0$,

$$\tilde{\omega}(0+) = |\tau|^{1/2}. \quad (3)$$

If, on the other hand, $|\omega| \gg \tau^{3/2}$, then

$$\tilde{\omega} = \omega^{1/2}. \quad (4)$$

In the gap-containing (dielectric) phase, where $\tau > 0$, $\tilde{\omega}(0) = 0$, it is not difficult to determine the frequency $i\omega$ at which a nonzero complex solution $i\tilde{\omega}$ first appears, which is equivalent to the appearance of the dielectric gap

$$G = 2(\tau/3)^{1/2}. \quad (5)$$

Similarly, we can investigate the singularities of all the thermodynamic and kinetic quantities near the critical point of the transition into the metallic state (the M transition). An elementary analysis by the self-consistent field method⁷ shows that the density of electronic states, the diffusion coefficient, and the reciprocal of the square of the screening distance are proportional to $\tilde{\omega}(0+)$, so that all these quantities go to zero according to a square-root law.

The permittivity exhibits strong spatial dispersion over distances of the order of the correlation length R_c (see below). It becomes infinite at large distances, i.e., for $qR_c \ll 1$:

$$\varepsilon(q \rightarrow 0) \propto \tau^{-1/2}. \quad (6)$$

As shown in Refs. 5 and 8, the singular part of the energy of the metallic phase at $T = 0$ is given by the integral

$$-\tau \int \tilde{\omega}^2 d\omega, \quad (7)$$

so that we find with the aid of Eq. (1) that

$$\Delta E \propto \tau \tilde{\omega}^3 (\partial\omega/\partial\tilde{\omega}) \propto |\tau|^{7/2}. \quad (8)$$

In all the enumerated models, the static conductivity σ near the transition point and at $T = 0$ is proportional to $\tilde{\omega}(0+)$; therefore,

$$\sigma \propto \tilde{\omega}^2 \propto |\tau|. \quad (9)$$

In the limit $\omega \rightarrow 0$, the correlation length can be expressed in terms of the ratio of mean-square velocity to the order parameter (3) (see Ref. 5):

$$R_c^2 = \left(\frac{\partial \epsilon}{\partial p} \right)^2 / \tilde{\omega}^2(0+). \quad (10)$$

In the ideal Hubbard model (at $T > T_N$) and for the binary solid solution, the mean kinetic energy $\epsilon(\mathbf{p})$ has the same order of magnitude as the quantity $b^{-1/2}$, so that the correlation length becomes large only near the transition point. In the nonideal Hubbard model, in an excitonic dielectric, and in a superconductor, where the self-consistency conditions have the form (1), the quantity $b^{1/2}$ is of the order of the mean characteristic time of the relaxation without spin flip. For this reason, even at points far from the transition point, the correlation length in these models is large compared to the mean interelectron distance, so that Eq. (2) possesses quite a broad region of applicability.

It is quite clear that, as in the localization theory,⁹ the quantity $\tilde{\omega}(0+)$ has the meaning of an order parameter. For this reason, it is natural to attempt to construct a theory of the M transition in the region of strong correlations, in analogy to the fluctuation theory of second-order phase transitions. In this case we cannot hope for a complete physical analogy, if only because the order parameter is complex and there are no grounds for assuming that identical critical phenomena occur on both sides of the transition point.

In the first section we compute the correlation function corresponding to the critical vibrations. In the second section we show that the correction to four-vertex part, as computed with the aid of perturbation theory, has different signs in the dielectric and metallic phases. This suggests that, in the dielectric phase, in which the interaction of the critical vibrations is attractive, we have inhomogeneous localization of the states in that region of energies where the gap computed in the self-consistent field theory exists. This is the subject of the fifth section. The main results obtained in the third and fourth sections pertain to the metallic phase, in which repulsion of the critical vibrations occurs. In these sections we write out equations possessing the properties of scale invariance, from which we are able to obtain the thermodynamic critical exponents for $d = 4 - \epsilon$ ($\epsilon \ll 1$) dimensions.

1. CRITICAL VIBRATIONS AND THE CORRELATION FUNCTION

Let us consider the singularities of the two-particle vertex part in the case of zero energy transfer and low total momentum or small momentum transfer. In $d > 2$ dimensions we can limit ourselves in both cases to a simple ladder summation, as shown in Fig. 1. The broken lines represent scattering on the static fluctuations-impurities,^{1,2} composition fluctuations,⁴ or spin fluctuations.³ The continuous

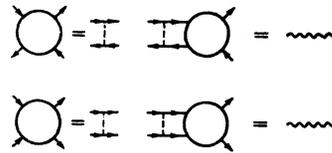


FIG. 1. Equations for the critical vibrations in the self-consistent field approximation.

lines represent "impurity"-averaged ω -, $\tilde{\omega}$ -, and $\tilde{\Delta}$ -dependent electron Green functions.

In the simplest case of an excitonic dielectric, the irreducible part, corresponding to a given spin component, of the Green function has two components, which correspond to momenta differing by half a reciprocal-lattice vector:

$$G^{-1} = \begin{pmatrix} i\tilde{\omega} - \xi_p & \tilde{\Delta} \\ \tilde{\Delta} & i\tilde{\omega} + \xi_p \end{pmatrix}. \quad (11)$$

For the nonideal Hubbard model, the Green function has the same form, but the second state differs from the first state not only in momentum, but also in the sign of the spin component.

In the ideal Hubbard model the irreducible Green function corresponding to the paraphase also has, for a given spin projection, two components corresponding to different electronic transitions. In the ordered phase, where anomalous averages occur, the irreducible Green function has 4 components, but below we shall not need its explicit form. The Green function for the superconductor differs only in sign from (11). In this case the second component differs from the first not only in the spin projection, but also in the direction of the momentum. For this reason in the case of the superconductor the equations depicted in Fig. 1 should be replaced by one equation in which it is not necessary to indicate the direction of the electronic lines.

It is shown in Ref. 5 that, in the ideal Hubbard model, for equal frequencies ω and small momentum transfers q , the two-particle Green function depicted in Fig. 1 satisfies the following equation:

$$(m + q^2 R^2) D_*(q) = \lambda. \quad (12)$$

Here R and λ are the correlation length (10) for $|\tau| = 1$ and the amplitude of the scattering on the impurities; below we shall, for simplicity, assume these quantities to be equal to unity. The expansion of the quantity m in powers of $\tilde{\omega}$ has the same form as in the theory of phase transitions:

$$m = \tau + 3b\tilde{\omega}^2. \quad (13)$$

For frequencies $\omega \ll b^{-1/2}$ the quantity $\tilde{\omega}$ is determined with the aid of Eq. (2).

Exactly the same equation is satisfied by the correlation function for low total momenta. A similar situation obtains also for the exciton dielectric if we write the equation for the correlation function with the use of the Green function (11). In all cases critical properties are possessed by those vertex parts in which the two left or two right end points have identical quantum numbers with respect to which the electron Green function is irreducible.

In the low-temperature region, where the M transition in the Hubbard model occurs in the ordered phase, the critical properties are possessed by the two-particle amplitudes having identical spin components. In the most complicated case, namely, for a superconductor with paramagnetic impurities, the critical quantities are the four diagonal components, which differ in the direction of the momentum or spin. Thus, the critical correlation function corresponds entirely to a definite superposition of two-particle electron states.

It is important to note that the two-particle vertex part has a singularity in the case of a low sum frequency as well. In the gapless phase this singularity has a diffusion character, and determines the anomalous properties of the kinetic coefficients. But it is not difficult to show¹⁰ that, for $d > 2$, the influence of the diffusion modes is greatly suppressed because of the disappearance of the nonlinear diffusional interactions in the region of long wavelengths.

2. INTERACTION OF THE CRITICAL VIBRATIONS

To compute the vertex part corresponding to the scattering of the critical vibrations, we use a self-consistent-field-type perturbation theory, in which it is necessary to take into account the simplest irreducible diagrams containing the smallest number of integrations. As a first approximation, let us perform the averaging of the electronic tetragon, discarding in the process the intersecting diagrams, as shown in Fig. 2. A similar computation is carried out in Ref. 10 for the interaction of the diffusion modes and in Ref. 1 for a superconductor.

As noted in the preceding section, to the critical vibrations correspond pairs of electron lines with equal single-particle quantum numbers, each of the components entering with the same weight. For this reason, each polygon to which pairs of critical electron lines come up is proportional to the trace of those groups of electron Green functions which form a critical mode. For zero frequency transfer we must, in the case (of interest to us) of scattering by static impurities, over those momenta of the electron Green functions which form closed polygons. Using as the simplest example the exciton Green function (11) and the self-consistency conditions (1), we easily see that, after the integration over the momenta, the diagram (a) can be explained in even powers of $\bar{\omega}$, and in the zeroth approximation, makes a negative contribution ($-\gamma_g$). The triangular diagrams can be expanded in odd powers of $i\bar{\omega}$, so that in the limit of small q the contribution from the diagrams (b) and (c) is positive:

$$\Gamma_o^{(4)}(q, \tau) = -\gamma_g [1 - ab\bar{\omega}^2 / (m + q^2 R^2)]. \quad (14)$$

Here a is a numerical coefficient that turns out to be equal to

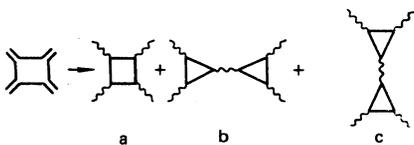


FIG. 2. Averaging of the simplest eight-vertex part in the self-consistent field approximation.

18 in perturbation theory. In the dielectric phase we have $\bar{\omega} = 0$ and $m = 0$ at $\omega = 0$, so that the vertex part (14) changes sign when we go from the metallic into the dielectric phase. Thus, in the metallic phase we find with the aid of (2) that as $q^2 \rightarrow 0$ and $\omega \rightarrow 0$

$$\Gamma_o^{(4)}(0, \tau) = \gamma_g(a/2 - 1). \quad (15)$$

The vertex part for high frequencies, i.e., for $|\tau|^{3/2} \ll |\omega| \ll b^{-1/2}$, has the same sign as the vertex part in the metallic phase. In this case we can set $\tau = 0$ in (2) and (14), so that as $q^2 \rightarrow 0$, $\tau \rightarrow 0$

$$\Gamma_o^{(4)}(0, 0) = \gamma_g = \gamma_g(a/3 - 1). \quad (16)$$

We can generally assert on the basis of (14) that there exists in the gapless region a value $q = q_0(m)$ at which the vertex part reverses sign. We shall assume that the coefficients a is so large that in the metallic and high-frequency regions

$$q_0^2(m) \gg m. \quad (17)$$

The critical exponents that will be computed in the following section do not depend on the coefficient a , so that we make no attempt to compute its exact value in the region of strong correlations.

3. EQUATION FOR THE FLUCTUATIONS; THE CRITICAL EXPONENTS IN THE METALLIC PHASE

Let us assume that there exists in the region of strong correlations in the metallic phase a self-energy part $i\bar{\omega}$ that does not vanish in the limit as $i\omega \rightarrow 0$. Besides the simplest diagram representing the scattering of an electron on an impurity, all the diagrams that cannot be reduced by cutting along a single line, but can be reduced by cutting along two lines with opposite or identical directions and zero momentum transfer or zero total momentum must be referred to the self-energy part.

With this definition, the equation for the self-energy part has the same form as (2), but with coefficients that depend on the self-energy part m for the critical vibrations. We should then replace b by the irreducible four-vertex part Γ_1 for the critical vibrations corresponding to small momentum transfers $q^2 \ll m$; the parameter τ should be multiplied by $\mathcal{T}_a(m)$, the two-vertex part with oppositely directed lines, computed in the same limit:

$$\bar{\omega} \tau \mathcal{T}_a(m) + \bar{\omega}^3 \Gamma_1(m) = \omega. \quad (18)$$

The equation for m is none other than the Dyson equation for the correlation function, which equation has, after expansion in powers of $\bar{\omega}$, the same form as Eq. (13), but with b and τ replaced respectively by $\Gamma_1(m)$ and $\tau \mathcal{T}_a(m)$:

$$m = \tau \mathcal{T}_a(m) + 3\bar{\omega}^2 \Gamma_1(m). \quad (19)$$

In the theory of phase transitions¹¹ the functions Γ and \mathcal{T} are computed first in the disordered phase in the region of momenta $q^2 \gg m$ and are then used, with logarithmic accuracy, for the same values of m in the ordered phase. As shown in the preceding section, such a computation is impossible in the low-frequency region of the dielectric phase. But if we

assume that the condition (17) is fulfilled, so that there exists a region of momenta $m \ll q^2 \ll q_0^2$ where the corrections to the vertex have the "right" sign, then the coefficients Γ_1 and \mathcal{F}_a can be determined in a space with $d = 4 - \varepsilon$ (where $\varepsilon \ll 1$) dimensions.

We can easily write down the equations for the vertex part containing four pairs of electronic end points if we first use perturbation theory. It then turns out that the sought vertex part Γ_1 can be expressed in terms of the products of the other vertices Γ_k ($1 < k < 4$), which differ from Γ_1 in that the electron lines that are to be averaged have a different direction. A more exact definition of the vertices Γ_k is given in Appendix A. The coefficients entering into the corresponding parquet equations do not depend on the dimensionality d , and are computed in Appendix B for $d = 4$. If, on the other hand, $d = 4 - \varepsilon$, we shall seek the solution in the form of a product of the rapidly varying quantities $A_d q^\varepsilon$ and a slowly varying function g_k that depends on the logarithmic variable $t = -\ln q$.

In the new variables we obtain

$$\begin{aligned} \dot{g}_1 &= \varepsilon g_1 - (2g_2 + g_3)^2, \\ \dot{g}_2 &= \varepsilon g_2 - (g_1 g_3 + 2g_2 g_3 + 2g_2 g_4 + g_3^2 + 2g_2^2 + g_3 g_4), \\ \dot{g}_3 &= \varepsilon g_3 - (4g_2 g_3 + 4g_2^2 + g_1 g_3), \quad \dot{g}_4 = \varepsilon g_4 - (5g_4^2 + 4g_2 g_3). \end{aligned} \quad (20)$$

The constant A_d has been chosen such that the right-hand side of the system (20) has a universal form with coefficients that coincide with the number of topologically nonequivalent diagrams of second-order perturbation theory.

Similarly, let us write down the equations for the two-vertex singular diagrams \mathcal{F}_a containing one angle ($\alpha = a, b$). If we set $\mathcal{F}_a = A_d q^\varepsilon \gamma_a$, we can write down the equations for γ_a by using the universal coefficients obtained for $d = 4$ in Appendix B:

$$\dot{\gamma}_a = \varepsilon \gamma_a - (2g_2 + g_3) \gamma_b, \quad \dot{\gamma}_b = \varepsilon \gamma_b - 2g_4 \gamma_b - g_3 \gamma_a. \quad (21)$$

In the metallic phase

$$\mathcal{F}_a(m) \propto q^\varepsilon \gamma_a(t), \quad \Gamma_1(m) \propto q^\varepsilon g_1(t),$$

where we should replace q and t by $m^{1/2}$ and $-(\ln m)/2$ ($m \ll 1$, so that $t \gg 1$).

The equations have a completely symmetric solution, with $g_k = g(t)$ and $\gamma_a = \gamma(t)$:

$$\dot{g} = \varepsilon g - 9g^2, \quad \dot{\gamma} = \varepsilon \gamma - 3\gamma g. \quad (22)$$

From this we find the solutions corresponding to the singular point $g = \varepsilon/9$ in the limit $t \gg 1$:

$$\Gamma(m) \propto m^{\varepsilon/2}, \quad \mathcal{F}(m) \propto m^{\varepsilon/6}. \quad (23)$$

Substituting these solutions into (2) and (13), we find that in the low-frequency region

$$\begin{aligned} \bar{\omega} &\propto |\tau|^\beta, \quad \partial \bar{\omega} / \partial \omega \propto |\tau|^{-1}, \\ \beta &= 1/2 - \varepsilon/6, \quad \gamma = 1 + \varepsilon/6. \end{aligned} \quad (24)$$

In the high-frequency region

$$\omega \gg |\tau|^{\beta+1} \quad (25)$$

we can set $\tau = 0$ in Eqs. (2) and (13). Then

$$|\bar{\omega}| \propto |\omega|^{1/\delta}, \quad \delta = 3 + \varepsilon. \quad (26)$$

The relations (24) can be used to determine more precisely the character of the transition into the dielectric state. The singular part of the energy at absolute zero is given by the general relation (7). Therefore,

$$\Delta E \propto |\tau|^{e'}, \quad e' = 1 + \gamma + 3\beta = 7/2 - \varepsilon/3. \quad (27)$$

The obtained critical exponents do not correspond to an absolutely stable solution if the symmetry $g_k = g(t)$ is not exact. An arbitrarily small deviation, caused for example by an external magnetic field, leads to the rapid growth of the fluctuations. The detailed investigation, carried out in Appendix C, of the system (20) leads to the conclusion that the only point of absolute stability is the following point:

$$g_1 = g_2 = -g_3 = g_4 = \varepsilon. \quad (28)$$

For $t \gg 1$ we find in the vicinity of this point that

$$\gamma_a = \gamma_b = \text{const}. \quad (29)$$

From this we find the values of the critical exponents of interest to us:

$$\beta = 1/2, \quad \gamma = 1 + \varepsilon/2, \quad \delta = 3 + \varepsilon. \quad (30)$$

Using the general relation (7), we find that, in contrast to the symmetric case (27), the singularity in the anomalous part of the energy in this case is weaker than the one predicted by the self-consistent-field theory:

$$e' = 7/2 + \varepsilon/2. \quad (31)$$

Let us determine the critical exponent for the correlation length from the condition $R_c \propto m^{-1/2}$. In the low-frequency region $|\omega| \ll |\tau|^{\gamma+\beta}$

$$R_c \propto |\tau|^{-\nu}, \quad \nu = \gamma/2. \quad (32)$$

In the high-frequency region (25)

$$R_c \propto |\tau|^{-\mu}, \quad \mu = 1/3 + \varepsilon/18. \quad (33)$$

It is clear that the results (25) and (33), which are valid for high frequencies, can be used in the dielectric phase as well. In this region the states are delocalized, and the high-frequency dynamics is valid when the real part of the energy of the elementary excitations is of the order of the imaginary part. To verify this, we need only continue all the relations analytically:

$$i\omega \rightarrow \omega, \quad i\bar{\omega} \rightarrow \Sigma_R + i\delta.$$

Then for high frequencies

$$\Sigma_R(\omega) \propto |\omega|^{1/\delta} \text{sgn } \omega \exp \left\{ \frac{i\pi}{3} \text{sgn } \omega \left(1 + \frac{\varepsilon}{6} \right) \right\}. \quad (34)$$

For low frequencies in a metallic medium

$$\Sigma_R(\omega) \propto i |\tau|^\beta. \quad (35)$$

Thus, for all frequencies the imaginary part of the energy of

the excitations turns out to be higher than the real part, and the damping increases with decreasing dimensionality.

4. CRITICAL EXPONENTS IN SYSTEMS NONDEGENERATE IN SPIN

As in the localization theory,⁹ an external magnetic field and paramagnetic impurities weaken the correlation effects in the channel with low total momentum, as a result of which the integrals containing electron lines having the same direction become truncated. The corrections Γ_1 and \mathcal{S}_a to the vertex part then vanish, so that in the approximation linear in ε the critical exponents has the same form as in the self-consistent field theory.

Under conditions of weakly-broken symmetry the critical exponents are determined by the behavior of the system in the vicinity of the stable center (28). The character of the phase transition can then be determined from (31), and in the approximation linear in ε the critical exponent β is equal as before to $\frac{1}{2}$.

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A similar situation obtains in the nonideal Hubbard model. As has already been noted, in this case there are two types of critical vibrations—for the low total momentum and for the small momentum transfer—in each of which the two-particles states with identical spin components are mixed. In consequence, we may obtain the same results obtained for the excitonic dielectric.

Of special interest is a superconductor with paramagnetic impurities, in which the states with oppositely directed momenta and spins are mixed. We can easily write down the equations for the vertex part if we take into account the fact that, after averaging, the diagrams that differed earlier only in the directions of the electron lines are now topologically equivalent. Then, instead of (22), we obtain

$$\dot{g} = \varepsilon g - 5g^2, \quad \dot{\gamma} = \varepsilon \gamma - 2\gamma g. \quad (36)$$

From this we find the critical exponents in the low-frequency limit, (31):

$$\beta = \frac{1}{2} - 3\varepsilon/20, \quad \gamma = 1 + \varepsilon/5, \quad \varepsilon' = \frac{7}{2} - \varepsilon/4. \quad (37)$$

The high-frequency limit is determined as before by the exponents in (33) and (26).

5. THE DIELECTRIC PHASE

To find the "tail" of the density of states, let us construct the functional whose variation gives Eq. (1) together with gradient terms. We can find the normalization constant for the free-energy functional without difficulty if we compute the energy of the system in the single-loop approximation.¹²

Taking into account the possibility of slow fluctuations in the quantity $\bar{\omega}$, we obtain the following functional density

$$\mathcal{F}(\mathbf{r}) = \left[\frac{\bar{\omega}^2 \tau}{2} - \omega \bar{\omega} + \frac{b \bar{\omega}^4}{4} + \frac{R^2 (\nabla \bar{\omega})^2}{2} \right] \lambda. \quad (38)$$

In an excitonic dielectric λ is the product of density of states at the Fermi level in the absence of interactions and the doubled characteristic time of the relaxation on the impurities; the remaining symbols have the same meaning as in the first section. The variation of the functional (38) leads us to an equation of the Ginzburg-Landau type:

$$\bar{\omega} \tau + b \bar{\omega}^3 - R^2 \Delta \bar{\omega} = 0. \quad (39)$$

The solution of this equation in the dielectric phase, i.e., for $\tau > 0$, and at the band center $\omega = 0$ is purely imaginary, and can be found by numerical integration:

$$i \bar{\omega} = (\tau/b)^{1/2} f(r \tau^{1/2}/b). \quad (40)$$

Substituting it into the original functional, and performing the integration over the entire volume, we obtain an expression for the exponential "tail" of the density of states ρ :

$$\ln \left(\frac{\rho}{\rho_0} \right) = - \frac{R^d \lambda \tau^{2-d/2}}{b} \kappa_d, \quad (41)$$

where κ_d is a numerical coefficient: $\kappa_2 = 2.9$; $\kappa_3 = 13.2$. Let r_0 and l be the mean distance between the electrons and the mean free path in the metallic phase; then

$$R^d \lambda / b \propto (l/r_0)^{d-1}. \quad (42)$$

In an excitonic dielectric, in the nonideal Hubbard model (at $T = 0$), and in superconductors, where $l \gg r_0$, the density-of-states "tail" does not extend far ($d > 1$), only to

$$\tau \propto (r_0/l)^{2(d-1)/(4-d)} \quad (43)$$

In the ideal Hubbard model (at $T \gg T_N$) and in a binary solid solution we have $l \sim r_0$, so that the "tail" makes a significant contribution to all the observable effects, even at $\tau \sim 1$.

CONCLUSION

The critical exponents characterizing the metallic phase are well known in the region of applicability of the self-consistent field theory:

$$\beta = \frac{1}{2}, \quad \gamma = 1, \quad \delta = 3, \quad \mu = \frac{1}{3}, \quad \nu = \frac{1}{2}, \quad \varepsilon' = \frac{7}{2}. \quad (44)$$

The assumption that the four-vertex irreducible part has a repulsive sign can, as follows from the expansion (38), be justified by using the Stratonovich-Hubbard model.^{13,14} All the possible limiting cases can be obtained by computing the single critical exponent m/n , where m and n are the numbers of the topologically nonequivalent diagrams determining the two-vertex and four-vertex correlators for the critical vibrations. Then

$$\beta = \frac{1}{2} - \frac{\varepsilon}{4} \left(1 - \frac{m}{n} \right), \quad \gamma = 1 + \frac{\varepsilon m}{2n},$$

$$\delta = 3 + \varepsilon, \quad \mu = \frac{1}{3} + \varepsilon/18,$$

and the remaining exponents can be expressed in terms of β and γ . For the symmetric case $m/n = 1/3$, for the slightly nonsymmetric case $m/n = 1$, and for a superconductor with

paramagnetic impurities $m/n = \frac{2}{3}$. In the present investigation we did not consider the case of strong spin-orbit interaction and strong magnetic interactions, when $m = n = 0$.

We find the usual exponential density-of-states "tails" far from the transition point in the dielectric phase. All the kinetic coefficients exhibit strong dispersion in this region, but vanish in the static limit. In the metallic phase the static kinetic coefficients are small and vanish at the transition point. The computation of these coefficients, as well as the study of the M transition as $d \rightarrow 2$, is beyond the scope of the present paper.

APPENDIX A

Let us classify the irreducible blocks having the same number of incoming and outgoing electron lines. In first order, the irreducible vertex part is a quadrangle from each corner of which emanates a pair of electron lines having either identical or mutually opposite directions (see Fig. 3). Let us place in the first class all those diagrams that have as incoming lines only those pairs of lines which, after averaging, form ladders of oppositely directed electron lines. The simplest diagram of the first class is shown in Fig. 3a. Let us number all the pairs of electron lines and introduce a replica index that is preserved along an electron line. Let us denote the irreducible eight-vertex part of the first class by $\Gamma_{1\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4}$, so that the superscripts number the incoming lines, while the subscripts number the outgoing lines. An irreducible vertex should not have continuous lines entering and leaving one and the same corner, and this corresponds to the presence of the factor $\delta_{\alpha_i\beta_k}$. A similar argument pertains to the factors $\delta_{\alpha_i\beta_p} \delta_{\alpha_j\beta_k}$, which correspond to a disconnected pair of lines coming through corners with numbers k and p . Discarding such terms, we obtain the general form of the irreducible vertex:

$$\Gamma_{1\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4} = \Gamma_1 \left\{ (\delta_{\alpha_1\beta_1} \delta_{\alpha_2\beta_2} \delta_{\alpha_3\beta_3} \delta_{\alpha_4\beta_4} + \delta_{\alpha_1\beta_2} \delta_{\alpha_2\beta_1} \delta_{\alpha_3\beta_4} \delta_{\alpha_4\beta_3}) + \text{two cyclic} \right\} / \text{permutations of the subscripts } \beta_k \quad (\text{A.1})$$

The diagrams of the fourth class have as their incoming lines pairs of lines that form ladders of lines with the same direction (see Fig. 3d). If we number each pair of lines, it immediately becomes clear that a vertex part of the fourth class should be symmetric with respect to the interchange of any pair of indices with the same number:

$$\Gamma_{4\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4} = \Gamma_4 \{ [\delta_{\alpha_1\beta_1} \delta_{\alpha_2\beta_2} (\delta_{\alpha_3\beta_3} \delta_{\alpha_4\beta_4} + \delta_{\alpha_3\beta_4} \delta_{\alpha_4\beta_3}) + (\alpha_3 \neq \alpha_4)] + (\beta_3 \neq \beta_4) \} + (\beta_1 \neq \beta_2). \quad (\text{A.2})$$

The vertex parts of the intermediate type in their turn split

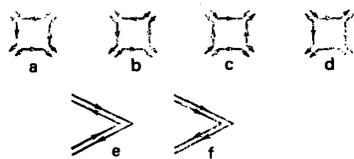


FIG. 3. Different types of four-vertex (a-d) and two-vertex (e, f) diagrams for the critical vibrations before averaging over the impurities.

up into two classes. In diagrams of the Γ_2 type, the angular vertex with lines of the same direction are necessarily joined by one electron line (see Fig. 3b). In diagrams of the Γ_3 type, on the other hand, the angular vertices with lines of the same direction are joined to angular vertices where pairs of lines of opposite directions meet (as shown in Fig. 3c). In analytic form

$$\Gamma_{2\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4} = \Gamma_2 \{ \delta_{\alpha_1\beta_1} [(\delta_{\alpha_2\beta_2} \delta_{\alpha_3\beta_3} \delta_{\alpha_4\beta_4} + \alpha_3 \neq \alpha_4)] + (\beta_1 \neq \beta_2) \} + \{ 1 \neq 2 \}. \quad (\text{A.3})$$

A diagram of the $\Gamma_{3\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4}$ type has only four terms, since the interchange of the first and second pairs of lines is equivalent to the simultaneous interchanges $\alpha_3 \rightleftharpoons \alpha_4$ and $\beta_3 \rightleftharpoons \beta_4$:

$$\Gamma_{3\beta_1\beta_2\beta_3\beta_4}^{\alpha_1\alpha_2\alpha_3\alpha_4} = \Gamma_3 [\delta_{\alpha_1\beta_1} \delta_{\alpha_2\beta_2} \delta_{\alpha_3\beta_3} \delta_{\alpha_4\beta_4} + (\alpha_3 \neq \alpha_4)] + [\beta_3 \neq \beta_4]. \quad (\text{A.4})$$

The angular-vertex part \mathcal{F}_a has on each side two electron lines with opposite directions. It is easy to see that the irreducible vertex part should have the following form (see Fig. 3e):

$$\mathcal{F}_{a\beta_1\beta_2}^{\alpha_1\alpha_2} = \delta_{\alpha_1\beta_1} \delta_{\alpha_2\beta_2} \mathcal{F}_a. \quad (\text{A.5})$$

The angular-vertex part \mathcal{F}_b has on the side a pair of incoming, and on the other side a pair of outgoing, lines, as shown in Fig. 3f. From symmetry consideration we can immediately write

$$\mathcal{F}_{b\beta_1\beta_2}^{\alpha_1\alpha_2} = (\delta_{\alpha_1\beta_1} \delta_{\alpha_2\beta_2} + \delta_{\alpha_1\beta_2} \delta_{\alpha_2\beta_1}) \mathcal{F}_b. \quad (\text{A.6})$$

APPENDIX B

To find the second-order perturbation theory corrections, it is sufficient to compute all the possible pair products of the vertices listed in Appendix A. In doing this, we must

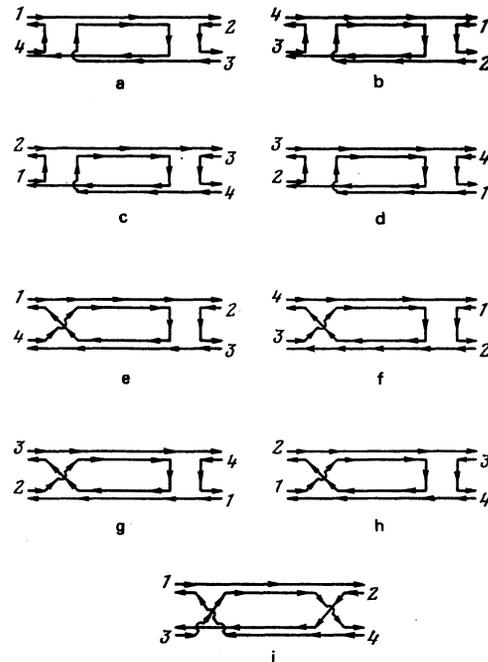


FIG. 4. Different kinds of nonequivalent diagrams of the type Γ_2^2 (a-d), $\Gamma_2\Gamma_3$ (e-h), and Γ_3^2 (i) giving second-order corrections to vertices of the first class.

bear in mind that, in our case of scattering by static impurities, the electron Green function is diagonal in both the frequency and the replica index, on which it does not depend at all.

1. Computation of the corrections to the Γ_1 vertex

The direct computation of a correction of the Γ_1^2 type shows that there arise either closed loops or disconnected diagrams, following the summation over the replica indices. A nonzero correction appears after the multiplication of the vertex Γ_2 by itself, as a result of which we obtain four topologically nonequivalent diagrams (see Figs. 4a–4d). After averaging, the pairs of long parallel lines become anomalous correlation functions corresponding to critical vibrations.

We can similarly depict the four diagrams that are obtained after averaging the products $\Gamma_2\Gamma_3$ and $\Gamma_3\Gamma_2$ and one other diagram corresponding to the averaging of Γ_3^2 (see Figs. 4e–4i). As a result we obtain in the $d = 4$ case an equation for the $t = -\ln q$ derivative of Γ_1 :

$$\dot{\Gamma}_1 = -A_4(2\Gamma_2 + \Gamma_3)^2, \quad (\text{B.1})$$

where A_4 is a positive coefficient that is unimportant for what follows

2. Computation of the corrections to the Γ_2 vertex

It is not difficult to understand that, to find the diagrams corresponding to the sought corrections, it is sufficient to change the direction of the lines labeled by one and the same number in all the figures depicting the corrections to the Γ_1 vertex. If, for example, we change the direction of the lines labeled by the number 3, then the diagrams (a)–(d) will respectively represent

$$\overline{\Gamma_2^2}; \overline{\Gamma_2\Gamma_4}; \overline{\Gamma_3^2}; \overline{\Gamma_2\Gamma_4}$$

(the bar denotes logarithmic integration). Similarly, the diagrams (e)–(i) will represent

$$\overline{\Gamma_2\Gamma_3}; \overline{\Gamma_1\Gamma_3}; \overline{\Gamma_3\Gamma_2}; \overline{\Gamma_3\Gamma_4}; \overline{\Gamma_2^2}.$$

As a result we can derive a second equation:

$$\dot{\Gamma}_2 = -A_4(\Gamma_1\Gamma_3 + 2\Gamma_2\Gamma_3 + 2\Gamma_2\Gamma_4 + \Gamma_3^2 + 2\Gamma_2^2 + \Gamma_3\Gamma_4). \quad (\text{B.2})$$

3. Equations for Γ_3 and Γ_4

It is clear that the corrections to Γ_3 and Γ_4 can be obtained by changing the directions of the two lines in the equations for Γ_1 . It is easy to see that the change in direction of two lines with adjacent numbers gives a correction to Γ_3 . But if we change the directions of lines having the same parity, we obtain a correction to Γ_4 . As a result, we obtain the following equations:

$$\dot{\Gamma}_3 = -A_4[4\Gamma_2\Gamma_3 + 4\Gamma_2^2 + \Gamma_1\Gamma_3], \quad \dot{\Gamma}_4 = -A_4[5\Gamma_4^2 + 4\Gamma_2\Gamma_3]. \quad (\text{B.3})$$

4. Equations for the angular vertices

Let us first write down the corrections to the angular vertex \mathcal{T}_a in first-order perturbation theory (see Fig. 5). After averaging, the diagrams (a)–(c) become integrals of the

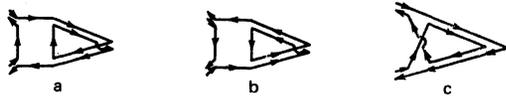


FIG. 5. The first three corrections to an angular vertex of the \mathcal{T}_a type.

logarithmic type: $\overline{\Gamma_2\mathcal{T}_b}$, $\overline{\Gamma_2\mathcal{T}_b}$, and $\overline{\Gamma_3\mathcal{T}_b}$. From this we obtain an equation for \mathcal{T}_a :

$$\dot{\mathcal{T}}_a = -A_4(2\Gamma_2 + \Gamma_3)\mathcal{T}_b. \quad (\text{B.4})$$

We can write down a similar equation for the angular vertex \mathcal{T}_b , which differs from \mathcal{T}_a in that one of the continuous electron lines has been reversed:

$$\dot{\mathcal{T}}_b = -A_4(2\Gamma_4\mathcal{T}_b + \Gamma_3\mathcal{T}_a). \quad (\text{B.5})$$

APPENDIX C

Let us investigate the stability of the system (17). To begin with, let us note that, as in the theory of phase transitions, the Gaussian critical point $g_k = 0$ is stable at $d > 4(\epsilon < 0)$. But if $\epsilon > 0$, a fixed critical point cannot be one that coincides with the Gaussian point. An elementary investigation shows that the system (17) possesses (besides the Gaussian critical point) six real singular points:

$$\begin{aligned} A_1 &= \frac{\epsilon}{9}(1, 1, 1, 1), \quad A_2 = \epsilon(1, 1, -1, 1), \\ A_{3,4} &= \epsilon\left(0, \frac{1}{2}, -1, \frac{1 \pm \sqrt{41}}{10}\right), \\ A_5 &= \epsilon(0.0945; 0.1084; 0.0945; 0.13746), \\ A_6 &= \epsilon(0.3371; -0.4594; 0.3371; 0.4659). \end{aligned} \quad (\text{C.1})$$

The symmetric point A_1 has only one negative eigenvalue $\lambda_1^{(0)} = -\epsilon$, which corresponds to the symmetric particular solution $\delta g_k = g(0)e^{-\epsilon t}$. All the remaining eigenvalues pertaining to the point are positive:

$$\lambda_1^{(1)} = \epsilon/9, \quad \lambda_1^{(2)} = 10\epsilon/9, \quad \lambda_1^{(3)} = 11\epsilon/9. \quad (\text{C.2})$$

A similar situation in which at least one of the eigenvalues is positive is found to exist on moving around each of the singular points except A_2 . For this point

$$\begin{aligned} \lambda_2^{(0)} &= \epsilon \frac{\sqrt{73}-9}{2} \approx -0.228\epsilon, \quad \lambda_2^{(1)} = -\epsilon, \\ \lambda_2^{(2)} &= -5\epsilon, \quad \lambda_2^{(3)} = -\frac{9+\sqrt{73}}{2}\epsilon \approx -8.772\epsilon. \end{aligned} \quad (\text{C.3})$$

In the region of small $|\tau|$, the critical behavior is determined by the evolution of the system with the smallest—in absolute value—eigenvalue $\lambda_2^{(0)}$ if, of course, the initial conditions will allow the system to reach the vicinity of the point A_2 .

In Sec. 2 we showed that, for the standpoint of perturbation theory, the vicinity of the symmetric point A_1 is accessible in the metallic phase, while the region of absolute instability, i.e., the region where all $g_k(0) < 0$, corresponds to the dielectric phase. It only remains to find out whether the points A_1 and A_2 are not separated by some integral surface.

The answer to this question can be given only by a numerical integration.

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