Dielectric phase transition into a current state

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Dielectric pairing in a two-band model with band extrema that coincide in momentum space is investigated. It is shown that if the order parameter is imaginary and dipole interband transitions are allowed then the state of the system is characterized by a homogeneous current.

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It is known that in the case of electron-hole pairing, depending on the phase of the order parameter and on its spin structure, anomalous mean values of four types are possible.[1] The purpose of the present paper is to establish the connection of these anomalous mean values with the physically observable quantities that are produced in the phase transition, as a function of the symmetry of the paired bands.

It is known that when a system goes over into the state of the excitonic insulator, there appear anomalous mean values of the type:

$$\langle a_1^+ a_2 \rangle = \langle a_2^+ a_1 \rangle^* = \Delta , \quad (1)$$

where a_1 and a_2 are the electron-annihilation operators in bands 1 and 2, respectively. If now there exists an operator $\hat{A}$ whose interband matrix elements $A_{12}=A^*_{21}$ are different from zero for transitions between bands 1 and 2, then the formation of anomalous mean values (1) in the system is accompanied by the appearance in the system of the mean value

$$< A > = A_{12}\Delta + A_{21}\Delta^* . \qquad (2)$$

Assume for simplicity that in the unaltered phase the wave functions ϕ_1 and ϕ_2 of the electrons at the extrema of both bands can be chosen to be real. In this case, as shown in,[2] the self-consistency equations for the determination of Δ turn out to be compatible only for either real or pure imaginary Δ.

We consider now (for the time being, without allowance for the spin variable) the possibility of a change occuring in the local density $n(\mathbf{r})$ of the electrons and of the appearance of local currents $\mathbf{j}(\mathbf{r})$ in the system during the phase transition. The corresponding operators are of the form

$$\hat{n}(\mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}), \qquad \hat{\mathbf{j}}(\mathbf{r}) = \frac{e}{m}\frac{\hbar}{i}\delta(\mathbf{r}' - \mathbf{r})\,\mathrm{grad}\,; \qquad (3)$$

and their interband matrix elements are:

$$n_{12}(\mathbf{r}) = \phi_1(\mathbf{r})\phi_2(\mathbf{r}),$$

$$\mathbf{j}_{12}(\mathbf{r}) = \frac{e}{m}\frac{\hbar}{i}\phi_1(\mathbf{r})\,\mathrm{grad}\,\phi_2(\mathbf{r}). \qquad (4)$$

It is easy to verify with the aid of (2) that if the parameter Δ is real, then a change takes place of the local density $\langle n(\mathbf{r})\rangle = 2\Delta n_{12}(\mathbf{r})$ of the electrons in the system, and there are no local currents, since the matrix elment $\mathbf{j}_{12}(\mathbf{r})$ is imaginary. Conversely, if the parameter Δ is pure imaginary, then a nonzero mean current density $\langle \mathbf{j}(\mathbf{r})\rangle = 2j_{12}(\mathbf{r})\Delta$ is produced, and the change of the local charge density is identically equal to zero. Of course, in the latter case, owing to the absence of charge accumulation, $\langle \mathbf{j}(\mathbf{r})\rangle$ is solenoidal: $\mathrm{div}\langle \mathbf{j}(\mathbf{r})\rangle = 0$.

It can thus be concluded that when no account is taken of the spin degree of freedom and the order parameter is real, the system goes over into a state with a charge-density wave (ChDW) $\langle n(\mathbf{r})\rangle$, and if the order parameter is imaginary the system goes over into a state with a current density wave (CuDW) $\langle \mathbf{j}(\mathbf{r})\rangle$. If we now take into account the spin and the ensuing different choice of the sign of Δ for opposite spin directions $\Delta_\uparrow = \pm\Delta_\downarrow$, then we can see the following:

1) At $\Delta = \mathrm{Re}\Delta$, $\Delta_\uparrow = \Delta_\downarrow$ there is produced a local charge-density wave $\langle n(\mathbf{r})\rangle = 2(\Delta_\uparrow + \Delta_\downarrow)n_{12}(\mathbf{r})$, (ChDW);

2) At $\Delta = \mathrm{Re}\Delta$, $\Delta_\uparrow = -\Delta_\downarrow$ there is produced a spin density wave $\langle S(\mathbf{r})\rangle = 2(\Delta_\uparrow - \Delta_\downarrow)n_{12}(\mathbf{r})$, (SDW);

3) At $|\Delta| = \mathrm{Im}\Delta$, $\Delta_\uparrow = \Delta_\downarrow$ there is produced an orbital-current density wave $\langle \mathbf{j}(\mathbf{r})\rangle = 2(\Delta_\uparrow + \Delta_\downarrow)\mathbf{j}_{12}(\mathbf{r})$, (CuDW);

4) At $|\Delta| = \mathrm{Im}\Delta$, $\Delta_\uparrow = -\Delta_\downarrow$ there is produced a spin flux-density wave $\langle \mathbf{S}(\mathbf{r})\mathbf{j}(\mathbf{r})\rangle = 2(\Delta_\uparrow - \Delta_\downarrow)\mathbf{j}_{12}(\mathbf{r})$, (SFDW).

In the preceding part of the article we did not specify the symmetry and the relative positions of the bands in momentum space. We shall now show that special attention must be paid to the case when the extrema of bands between which dipole transitions are allowed coincide in momentum space. We designate the matrix element of the corresponding dipole transition by $\mathbf{d}=\langle\phi_1|\mathbf{r}|\phi_2\rangle$. It can easily be connected with the matrix elements of the interband current density:

$$\mathbf{j} = \langle \phi_1 | \hat{\mathbf{j}}(\mathbf{r}) | \phi_2 \rangle = ie\frac{\epsilon_g}{\hbar}\mathbf{d} \cdot \tag{5}$$

Here ϵ_g is the width of the forbidden band in the unaltered phase.

Using (2) and (5) we can now obtain the following curious result. If the parameter Δ is pure imaginary, then the ground state of the system with broken symmetry is characterized by an undamped macroscopic homogeneous current with density $\langle\mathbf{j}\rangle=2\Delta\mathbf{j}$, proportional to Δ. A different choice of the phase of Δ (real Δ) leads to the appearance in the system of a spontaneous electric moment, i.e., to ferroelectricity.

To realize the current solution it is necessary that it correspond to a maximum coupling constant. It was shown in[2] that in the isotropic-semimetal model the effective coupling constant for the solution with imaginary Δ is equal to:

$$g_{im} = g_1 - \tilde{g}_2; \tag{6}$$

whereas the constants corresponding to solutions with ChDW and SDW are respectively:

$$g_s = g_1 + \tilde{g}_2 + 4(g_{ph}^2 - g_2),$$
$$g_t = g_1 + \tilde{g}_2 \; . \tag{7}$$

Here g_1 is the constant of the density–density type of interaction, g_2 is the bare interaction connected with the transition of a pair from one band to another (of the type $g_2a^+_1a^+_1a_2a_2$), $\tilde{g}_2$ is the same interaction but renormalized by screening, and g_{ph} is the electron-phonon interband interaction. It is seen from (6) and (7) that a situation with a current is realized if electron-electron attraction exists in the interband channel, i.e., when

$$\tilde{g}_2 < 0 \quad \text{and} \quad \tilde{g}_2 < 2(g_2 - g_{ph}^2). \tag{8}$$

It must also be noted that in contrast to the case of real Δ, when scattering by charged impurities suppresses the pairing effect, when Δ is imaginary the intraband scattering effects are partially cancelled out by scattering connected with the transition of the electron between bands. The latter is due to the reversal of the sign of the product of the two anomalous Green's function at imaginary Δ.

Owing to the requirement div$\langle\mathbf{j}\rangle=0$, a homogeneous current state might be realized in a closed-ring geometry. In the case of a sample of arbitrary shape, one should expect the sample to be broken up into a system of macroscopic domains.

There exists a clear-cut analogy between the thermodynamic-equilibrium current state considered above, and the situation that arises in a straight-band semiconductor with allowed interband dipole transitions, in which a Bose condensate of real non-equilibrium excitons is obtained by pumping. Thus, at real Δ this condensate is coupled via electric-dipole transitions with the condensate of photons in the $E1$ state (in accordance with the terminology of[3]), but if Δ is imaginary it is coupled via magnetic-dipole transitions with the condensate of photons in the $M1$ state.

In conclusion, we wish to note one more curious property that appears in an equilibrium system with straight bands in the case of dielectric pairing in a state with imaginary Δ. If only transitions with a change of the total angular momentum **J** are allowed in the system (as in HgTe), then the ordering is accompanied in this case by the appearance of ferromagnetic properties. Obvious, a most important role is assumed here by spin-orbit interaction. This interaction, incidentally, should produce differences between the effective interaction constants for transitions into the states with CuDW and SFDW.

Thus, in the two-band model, in contrast to the single-band model with flat sections of the Fermi surface, the additional degree of freedom due to the presence of two bands of different symmetry causes the choice of the phase of the order parameter to lead to new physical effects (current in the ground state or photomagnetism). In the one-band model, the phase of Δ plays a trivial role, and it determines only the position of the antinodes and the nodes of the charge or spin density waves.

The conclusion that a homogeneous spontaneous current exists in a system with broken symmetry is in contradiction with Bloch's theorem. However, Bloch's theorem was proved for neutral particles. Actually the spontaneous currents produce a magnetic field, which in turn alters the currents. This leads to inhomogeneous solutions, for which the conditions of the theorem are not satisfied.[4]

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