

On the possibility of a current state of an excitonic dielectric

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We show that in the case of an excitonic dielectric model it is necessary to redetermine an expression for the current, otherwise a contradiction occurs. We conclude that a current state of an excitonic dielectric can not occur.

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Volkov and Kopaev¹ showed that (in an excitonic dielectric) under certain conditions a state involving a non-dissipative current is possible.

In this article we show that this effect disappears in subsequent examination of this question using a simple model.

In fact, the authors' reasoning reduces to the following. The eigenstates of an electron in the excitonic dielectric have the following form:

$$\psi_k = u_k \psi_{1k} + v_k \psi_{2k}, \quad (1)$$

where ψ_{1k} and ψ_{2k} are the electron eigenfunctions with quasi-momentum k in the original, undisturbed bands (conduction and valence). It is assumed that $\psi_{1,2}$ satisfy the Shroedinger equation with the periodic potential:

$$H_0 \psi_{nk} = \xi_{nk} \psi_{nk}, \quad H_0 = \frac{-1}{2m} \nabla^2 + U(r). \quad (2)$$

When the well-known formula is used to calculate the current

$$j_0 = \frac{1}{2m} (\psi^* \hat{p} \psi + \text{c.c.}) \quad (3)$$

($\hat{p} \equiv -i\nabla$) the interference of ψ_1 and ψ_2 in the state with wave function [Eq.(1)] gives rise to, among others, a contribution which shall solely interest us; its magnitude is

$$j_{12} = \frac{1}{2m} \{ (u^* v \psi_1^* \hat{p} \psi_2 + u v \psi_2^* \hat{p} \psi_1) + \text{c.c.} \} \quad (4)$$

(here and further the index k is omitted). The non-dissipative current¹ constitutes the current j_{12} averaged over coordinates.

This leads to a contradiction: the continuity equation does not hold for the state in Eq. (1) if Eq. (3) is picked to represent the current. This may be ascertained as follows. The parameter $\text{div } j_{12}$ may be calculated taking into account the fact that the function

$$\phi = u \psi_1 e^{-i\xi_1 t} + v \psi_2 e^{-i\xi_2 t}$$

constitutes a solution of the time-dependent Schrödinger equation with the Hamiltonian H_0 ; we shall write the continuity equation for this state [naturally, including the current in Eq. (3)] and set to zero the coefficients of $\exp\{\pm i(\xi_1 - \xi_2)t\}$. Combining the resultant expressions we get

$$\operatorname{div} \mathbf{j}_{12} + i(\xi_1 - \xi_2) [\mathbf{u}^* \mathbf{v} \psi_1^* \psi_2 - \text{c.c.}] = 0. \quad (5)$$

It may be readily established that the second term in Eq. (5) is, generally speaking, nontrivial. We should emphasize that Eq. (5) constitutes a simple property of the solutions of the Schrödinger equation.

In the case of the steady state [Eq. (1)], $\partial |\psi|^2 / \partial t = 0$, while $\operatorname{div} \mathbf{j} \neq 0$ [see Eq. (5)] so that there is an obvious contradiction, the continuity equation is not satisfied.

In order to understand what is happening, we shall consider the simplest model of the excitonic dielectric with an effective Hamiltonian (for singlet coupling):

$$H = \sum_{k; n=1,2} \xi_{nk} a_{nk}^+ a_{nk} + \sum_k \{ \Delta a_{1k}^+ a_{2k} + \Delta^* a_{2k}^+ a_{1k} \}, \quad (6)$$

where the operators a_{1k} and a_{2k} pertain to conduction and valence bands, respectively, Δ is the order parameter, and the energy in the isotropic case is

$$\xi_{1k} = \frac{k^2 - k_0^2}{2m_1}, \quad \xi_{2k} = -\frac{k^2 - k_0^2}{2m_2}.$$

Evidently, a mode of this type [if we take into account an insignificant constant term dropped from Eq. (6)] is equivalent, after self-consistent determination of Δ , to the BCS model; in any case, it correctly describes the equilibrium properties of the ordered phase. This type of Hamiltonian may be treated as conventional, i.e., we may consider Δ a fixed quantity and not be concerned with its origin and means of determination (in particular, it is unimportant whether the phase is fixed or not). As long as we are dealing with equilibrium properties, there are no doubts concerning the correctness of the obtained results.

The single-electron eigenfunctions of the Hamiltonian [Eq. (6)] are functions of the type of Eq. (1), for which u and v may be expressed as follows:

$$|u|^2 = \frac{1}{2} \left(1 \pm \frac{\xi}{\sqrt{\xi^2 + |\Delta|^2}} \right); \quad |v|^2 = \frac{1}{2} \left(1 \mp \frac{\xi}{\sqrt{\xi^2 + |\Delta|^2}} \right); \quad (7)$$

$$u|v| = \pm \frac{|\Delta|}{2\sqrt{\xi^2 + |\Delta|^2}}; \quad v = |v| e^{-i\phi}, \quad \phi = \arg \Delta, \quad \xi \equiv \frac{1}{2}(\xi_1 - \xi_2).$$

Here, the upper (lower) sign pertains to the upper (lower) reconstructed band and the corresponding energies are $E = [(\xi_1 + \xi_2)/2] \pm (\xi^2 + |\Delta|^2)^{1/2}$.

In order to obtain the continuity equations we shall write the single-electron wave equation that corresponds to the Hamiltonian [Eq. (6)]:

$$i \frac{\partial \psi}{\partial t} = H_0 \psi + \hat{K} \psi, \quad (8)$$

where upon determining $\hat{K}\psi(r) = \int d\mathbf{r}' K(r, r')\psi(r')$,

$$K(r, r') = \Delta \sum_k \psi_{1k}(r) \psi_{2k}^*(r') + \Delta^* \sum_k \psi_{2k}(r) \psi_{1k}^*(r'). \quad (9)$$

With the aid of Eq. (8) we get the following equation of continuity:

$$\frac{\partial |\psi|^2}{\partial t} + \text{div } \mathbf{j}_0 + i(\psi^* \hat{K} \psi - \psi \hat{K}^* \psi^*) = 0. \quad (10)$$

For the steady state [Eq. (1)], Eq. (7) yields Eq. (5) and the contradiction is eliminated.

Thus, as soon as we assume that the state of an electron in the excitonic dielectric is described by a wave function [Eq. (1)] (which is the result of a mean field approximation), we arrive at the wave equation [Eq. (8)] and the continuity equation [Eq. (10)], i.e., an expression for the current that is different from Eq. (3). Specifically, the current density

$$\mathbf{j} = \mathbf{j}_0 + \mathbf{j}_1, \quad \text{div } \mathbf{j}_1 = i(\psi^* \hat{K} \psi - \psi \hat{K}^* \psi^*), \quad (11)$$

where \mathbf{j}_0 is given by Eq. (3). With regard to an equation for \mathbf{j}_1 , it may be analyzed similarly to the corresponding equation of electrostatics. The derivation of an expression for an averaged parameter $\langle \mathbf{j}_1 \rangle$ is relatively simple. For the states given by Eqs. (1) and (7), the mean "charge" in Eq. (11) is trivial and the mean "dipole moment" of a unit volume ("polarization") $\mathcal{P} \neq 0$ (if the corresponding condition is satisfied as proposed in Ref. 1). The "electric field" $\langle \mathbf{j}_1 \rangle = -4\pi\mathcal{P}$; moreover, we get the following for the state in Eqs. (1) and (7):

$$\langle \mathbf{j}_1 \rangle = \frac{i}{V} (|u|^2 - |v|^2) \{ \Delta \int d\mathbf{r} \psi_2^* \mathbf{r} \psi_1 - \text{c.c.} \} \quad (12)$$

(V is volume). A comparison with the averaged value $\langle \mathbf{j}_{12} \rangle$ shows that $\langle \mathbf{j}_1 \rangle + \langle \mathbf{j}_2 \rangle = 0$ [in this case we must use the known relationship between the matrix elements of momentum and the coordinate $(\hat{\mathbf{p}}_{12}/m) = i(\xi_1 - \xi_2)\mathbf{r}_{12}$].

An alternate approach involves looking at velocity instead of current. The velocity operator is:

$$\hat{\mathbf{v}} = i(H\mathbf{r} - \mathbf{r}H) = \frac{\hat{\mathbf{p}}}{m} + i(\hat{K}\mathbf{r} - \mathbf{r}\hat{K}). \quad (13)$$

The calculation of the mean value $\langle \hat{\mathbf{v}} \rangle$ in the state described by Eqs. (1) and (7) again leads to realization that the interference part of $\langle \hat{\mathbf{p}}/m \rangle$ and the mean of the second term in Eq. (13) mutually eliminate each other.

Thus, the interference part of the current reduces on the average to zero and the expression for $\langle \hat{\mathbf{v}} \rangle$ is simply

$$\langle \dot{\mathbf{r}} \rangle = \frac{\mathbf{k}}{m_1} |u|^2 - \frac{\mathbf{k}}{m_2} |v|^2,$$

which coincides, as can be readily shown, with $\partial E / \partial \mathbf{k}$, which was to be expected.

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¹B.A. Volkov and Yu.V. Kopaev, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 10 (1978) [JETP Lett. **27**, 7 (1978)].