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Can excitons produce superdiamagnetic currents ?

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Résumé. — Nous montrons que la condensation de Bose des excitons ne peut pas produire de courants diamagnétiques. Ceux-ci sont nuls dans une approximation de champ moyen cohérente, qui inclut à la fois les termes normaux et anormaux.

Abstract. — It is shown that Bose condensation of excitons cannot produce superdiamagnetic currents. The latter vanish within a consistent mean field approximation when both normal and anomalous pairings are retained.

It has been claimed recently that Bose condensation of optically active excitons could give rise to electric currents — yielding a superdiamagnetism reminiscent of superconductivity [1], [3]. Such a conclusion is puzzling, since it amounts to producing a *charged* current *via* the condensation of *neutral* entities (the excitons). In the present note, we argue that such diamagnetic currents do not exist : they appear only as a consequence of inconsistent approximations.

Let μ be the net electric dipole moment of the electron system

$$\mu = \sum_i \mathbf{X}_i.$$

An unambiguous definition of the current operator is $\mathbf{J} = \dot{\mu}$. Usually, μ will contain a free carriers unbounded part together with an atomic polarization term. More specifically, we use a basis of *orthogonal* Wannier functions $\varphi_n(\mathbf{r} - \mathbf{R}_i)$ (n is the band index, $\mathbf{R}_i$ the lattice site). Then

$$\begin{aligned} \mu &= \mu_{in}^{jn'} a_{in}^* a_{jn'} \\ \mu_{in}^{jn'} &= \int \varphi_n^*(\mathbf{r} - \mathbf{R}_i) \mathbf{r} \varphi_n(\mathbf{r} - \mathbf{R}_j) d\tau. \end{aligned}$$

Because the φ_n are orthogonal,

$$\mu_{in}^{jn'} = \mathbf{R}_i \delta_{ij} \delta_{nn'} + \bar{\mu}_{in}^{jn'}. \quad (1)$$

The first term μ_f in (1) is the band diagonal usual

position operator, while $\bar{\mu}$ is the bounded atomic polarization term.

For instance, let us consider a highly simplified model : a two band system of spinless electrons, in which each site is a symmetry centre. Let one band have s-symmetry (creation operator a_i^*), the other one being p_z-type (creation operator b_i^*) ⁽¹⁾. To the extent that the overlap between neighbouring site is small, the dominant contribution to μ may be written

$$\mu = \sum_i \{ \mathbf{R}_i (a_i^* a_i + b_i^* b_i) + \mathbf{d} (a_i^* b_i + b_i^* a_i) \} \quad (2)$$

($\mathbf{d}$ is the usual interband dipole matrix element, parallel to Oz). The free carrier and atomic contributions, μ_f and $\bar{\mu}$, are clearly separated.

We now return to the general case. The Hamiltonian is written as

$$H = \sum_{i,j,n} T_{in}^{jn} a_{in}^* a_{jn} + U. \quad (3)$$

The first term of (3) embodies kinetic energy and the one body lattice potential ; U is the particle interaction. Since U depends only on positions, it *must commute with* μ . Thus only the first term in (3) contributes to the current $\dot{\mu}$ (actually, only the kinetic energy). Making use of (1), we see that the current may be split into two parts

$$\mathbf{J} = \frac{i}{\hbar} [H, \mu] = \mathbf{J}_f + \bar{\mathbf{J}}$$

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⁽¹⁾ We consider a single p-subband, which implies either uniaxial symmetry, or excitons all polarized in a single direction, here the z-axis.

J_f is the usual *intraband conduction current* :

$$J_f = \frac{i}{\hbar} \sum_{i,j,n} T_{in}^{jn} (\mathbf{R}_j - \mathbf{R}_i) a_{in}^* a_{jn}.$$

It is the quantity one deals with in transport phenomena. $\bar{J}$, instead, arises from the atomic polarization $\bar{\mu}$; it involves interband processes, supposedly responsible for superdiamagnetism.

We now argue that any quantity which is the time derivative of a *bounded* operator has a zero expectation value in any *eigenstate* $|\psi\rangle$ of the Hamiltonian. Consequently

$$\langle \psi | \bar{J} | \psi \rangle = \frac{i}{\hbar} \langle \psi | [H, \bar{\mu}] | \psi \rangle \equiv 0. \quad (4)$$

There cannot exist a *steady* superdiamagnetic current (note that such a conclusion would not apply to the ordinary current J_f , since μ_f is not a bounded operator : one must worry about boundary conditions). If an approximate calculation yields a finite value of $\bar{J}$, it means that either $\bar{J}$ is inaccurately defined, or that the approximations violate the condition $[U, \bar{\mu}] = 0$, or both. In any case, a finite $\langle \bar{J} \rangle$ should be an artefact.

In a recent letter, Batyev [4] considered the same problem. He noted that the current operator used by Volkov *et al.* was inaccurate, as it violates the continuity equation (equivalent to our $J = \dot{\mu}$). Within a BCS type effective Hamiltonian, he restored charge conservation by modifying the current operator, introducing as an extra term the commutator of position with the BCS potential. He then showed that if the continuity equation is obeyed, then $\langle J \rangle$ vanishes, a conclusion which is essentially equivalent to our general argument (4). While we agree with the result, we claim that such a procedure is incorrect. Since the position commutes with U , the mean field BCS potential should not, on the average, affect the current operator (which is defined from first principles). The violation of charge conservation must be cured not by an *ad hoc* redefinition of J , but by a *consistent* mean field approximation.

In order to see explicitly how the cancellation occurs, we return to our spinless two band model. We assume a local interaction :

$$U = g \sum_i a_i^* b_i^* b_i a_i.$$

The bands are assumed to be symmetric with respect to some energy ξ , so that

$$H = \xi \sum_i (a_i^* a_i + b_i^* b_i) + \sum_{i,j} T_{ij} (a_i^* a_j - b_i^* b_j) + U.$$

The constant ξ is irrelevant : it may be absorbed in a redefinition of the energy origin. It is readily verified

that $[U, a_i^* b_i] = 0$: U does commute with $\bar{\mu}$, as it should. The two contributions to the current are

$$\begin{aligned} J_f &= \frac{i}{\hbar} \sum_{ij} T_{ij} (\mathbf{R}_j - \mathbf{R}_i) (a_i^* a_j - b_i^* b_j) \\ \bar{J} &= \frac{i}{\hbar} 2 \mathbf{d} \sum_{ij} T_{ij} (a_i^* b_j - b_i^* a_j) \end{aligned} \quad (5)$$

They are best expressed in terms of the Fourier transformed Bloch waves

$$\begin{aligned} J_f &= \frac{1}{\hbar} \sum_{\mathbf{k}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} [a_{\mathbf{k}}^* a_{\mathbf{k}} - b_{\mathbf{k}}^* b_{\mathbf{k}}] \\ \bar{J} &= \frac{id}{\hbar} \sum_{\mathbf{k}} 2 \varepsilon_{\mathbf{k}} [a_{\mathbf{k}}^* b_{\mathbf{k}} - b_{\mathbf{k}}^* a_{\mathbf{k}}] \end{aligned} \quad (6)$$

where $\varepsilon_{\mathbf{k}}$ is the Bloch state energy

$$\varepsilon_{\mathbf{k}} = \frac{1}{N} \sum_{i,j} T_{ij} \exp[i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)]$$

Note that $\bar{J}$ involves the *full* energy $\varepsilon_{\mathbf{k}}$. Replacing the latter by the local atomic quantity T_{ii} would violate the relationship $\bar{J} = \dot{\bar{\mu}}$, thereby introducing a spurious current.

In order to proceed, we treat U within a molecular field approximation. We may assume an equal number of electrons and holes. In order to preserve electron hole symmetry, we write U as

$$U = -g \sum_i a_i^* a_i b_i b_i^* + g \sum_i a_i^* a_i. \quad (7)$$

The last term of (7) may be incorporated into the one body Hamiltonian : we assume that has been done and we discard it. We moreover set $\xi = 0$ via an appropriate choice of the origin. The resulting mean field hamiltonian displays full electron hole symmetry :

$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - V) (a_{\mathbf{k}}^* a_{\mathbf{k}} - b_{\mathbf{k}}^* b_{\mathbf{k}}) + \Delta \sum_{\mathbf{k}} b_{\mathbf{k}}^* a_{\mathbf{k}} + \Delta^* \sum_{\mathbf{k}} a_{\mathbf{k}}^* b_{\mathbf{k}}. \quad (8)$$

In (8), V and Δ are the self consistent potentials

$$\begin{aligned} V &= -g \{ \langle a_i^* a_i \rangle - \langle b_i^* b_i \rangle \} \\ &= -\frac{g}{N} \sum_{\mathbf{k}} \{ \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle - \langle b_{\mathbf{k}}^* b_{\mathbf{k}} \rangle \} \\ \Delta &= -g \langle a_i^* b_i \rangle = -\frac{g}{N} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^* b_{\mathbf{k}} \rangle. \end{aligned} \quad (9)$$

Bose condensation of excitons is signalled by the *anomalous* pairing Δ . The hamiltonian H_{eff} is diagonalized by the familiar Bogoliubov transformation.

The resulting self consistency equations read

$$\begin{aligned}\Delta &= -\frac{g}{N} \sum_{\mathbf{k}} U_{\mathbf{k}} V_{\mathbf{k}} = \frac{g}{N} \sum_{\mathbf{k}} \frac{\Delta}{E_{\mathbf{k}}} \\ V &= -\frac{g}{N} \sum_{\mathbf{k}} (U_{\mathbf{k}}^2 - V_{\mathbf{k}}^2) = -\frac{g}{N} \sum_{\mathbf{k}} \frac{(\varepsilon_{\mathbf{k}} - V)}{E_{\mathbf{k}}}\end{aligned}\quad (10)$$

$E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - V)^2 + |\Delta|^2}$ is here the quasiparticle energy. We note that (10) leaves the phase of Δ arbitrary : this is a result of the *gauge invariance* of (7) : the interaction is unchanged if one shifts the *relative* phase of a_i and b_i by an arbitrary amount. Such an invariance would not persist if one were to include non local interactions (terms such as $a^* a^* b b$ are then quite possible).

From (6), we see that

$$\langle \bar{\mathbf{J}} \rangle = \frac{2 i d}{\hbar} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}} (\Delta - \Delta^*). \quad (11)$$

If it existed, $\langle \bar{\mathbf{J}} \rangle$ would depend on the choice of the gauge, a surprising result. In ref. [1], the authors consider the atomic quantity in which $\varepsilon_{\mathbf{k}}$ is replaced by T_{ii} in (11). We saw that such a term only represents part of the story. Restoring $\varepsilon_{\mathbf{k}}$ in (11), we might follow the usual practice of ignoring V , on the grounds that it just renormalizes $\varepsilon_{\mathbf{k}}$: then there is no clear reason why (11) should vanish. The paradox disappears if we consider the self consistency equations *together*. Then, by subtraction, we see that V adjusts in such a way that

$$\sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \equiv 0.$$

Thus, the diamagnetic current J vanishes identically, irrespective of the gauge, as it should.

We see that a proper solution requires a *consistent* calculation of *both* the anomalous and normal potentials, Δ and V . The origin of that fact is clear. When we replace U by its linearized form (8), the commutator $[U, a_i^* b_i]$ is no longer zero :

$$[U, a_i^* b_i] = \frac{\Delta}{N} \sum_{\mathbf{k}} [b_{\mathbf{k}}^* b_{\mathbf{k}} - a_{\mathbf{k}}^* a_{\mathbf{k}}] - \frac{2 V}{N} \sum_{\mathbf{k}} a_{\mathbf{k}}^* b_{\mathbf{k}}. \quad (12)$$

Still, if we retain *both* pairings, and use (9), we see that (12) vanishes *on the average* : mean field linearization preserves the conservation law $[U, \bar{\mu}] = 0$ as far as physical expectations are concerned. If however we discard the last term of (12), our conservation law is definitely ruined. The current $\bar{\mathbf{J}}$ given by (6) is no longer the commutator of $\bar{\mu}$ with H , and a spurious finite result ensues.

The above model could be generalized to more complicated situations, for instance non local interactions U . In such a case, however, the commutation rule $[U, \mu] \equiv 0$ is no longer automatic. It results on constraints on the various coupling matrix elements : these constraints will be vital in guaranteeing $\bar{\mathbf{J}} = 0$. Over again, we expect that steady diamagnetic currents will cancel as a result of subtle compensations between selfconsistency equations for the numerous pairings $\langle a_{in}^* a_{jm} \rangle$. Any approximation that distroys these compensations would introduce a spurious commutator $[U, \mu]$, responsible for the expectation value $\langle \bar{\mathbf{J}} \rangle$. Thus, considerable care must be exerted in order to preserve the correct definition $\bar{\mathbf{J}} = \bar{\mu}$. An innocent looking mean field linearization may prove very misleading.

We did not consider the extension to spin 1/2 particles. We do not expect major corrections to the above simple arguments.

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