Magnetic energy of a quantum current

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PACS. 03.65.-w – Quantum mechanics.
PACS. 74.20.-z – Theories and models of superconducting state.
PACS. 11.10.-z – Field theory.

Abstract. – It is shown that the magnetic energy of a quantum current, contrary to the classical case, is essentially negative. Since this result allows to escape a famous theorem by Bloch, it can be expected that, under appropriate conditions, the ground state of a quantum conductor may be characterized by a spontaneous current. A similar idea was suggested, many years ago, by Heisenberg and by Born and Cheng as a possible mechanism for superconductivity.

Introduction. – It is well-known, from the study of the infra-red divergence problem in relativistic QED, that a charged particle cannot be separated from its classical field [1] [2]. It is known also that the motion of a classical particle cannot be described correctly, if the interaction with the self-generated field is not taken into account properly [3].

In this paper we analyse the effects induced by the self-generated classical (i.e. coherent) field on a stationary current flowing in a macroscopic quantum conductor. In particular we will estimate the contribution to the total energy of the system due to the classical magnetic field and to its interaction with the current. The analysis will concern explicitly two geometrically different models. In both cases we will obtain the remarkable result that the magnetic energy associated to the current is essentially negative. A completely different result would be obtained for a current due to a system of classical charged particles. Such a difference descends from the fact that, in classical mechanics, the kinetic energy of a particle is expressed, in a natural way, in terms of the velocity. We remark that the velocity is essentially a classical concept. In quantum mechanics the velocity of an electron corresponds to the following operator

\[ \mathbf{v} = m^{-1}[-i\hbar \nabla + e\mathbf{A}_c(t, r)], \]

where \( \mathbf{A}_c \) is the classical vector potential. Owing to the presence of \( \mathbf{A}_c \), which depends on the other particles of the system as well as on the external environment, the velocity \( \mathbf{v} \), given by eq.(1), is essentially a collective operator. On the other hand, the canonical momentum is connected directly to the particle wave-length, which in turn is involved by a boundary

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condition like periodicity. For these reasons it looks more proper, in our opinion, to analyse a quantum many-body system in terms of the canonical momenta and not in terms of the velocities of the particles.

As previously mentioned, in this paper we will obtain the result that the magnetic self-interaction energy of a quantum current is essentially negative. This result may have unexpected consequences concerning e.g. the ground state of a system of electrons subject to periodic boundary conditions. In fact, as it will be discussed in the sequel, it is conceivable that, under appropriate conditions, a physical situation corresponding to a spontaneous current may be favoured with respect to a current-less situation. We recall that attempts to explain superconductivity in terms of spontaneous currents have been made long ago by Heisenberg [4] and by Born and Cheng [5]. However such theories have been ruled out by a theorem by Bloch [6], owing to the lack, in our opinion, of a proper analysis of the magnetic self-interaction.

The Schrödinger equation for a quantum system interacting with its classical field is given by

\[ i\hbar \partial_t |\psi\rangle = H[A_c] |\psi\rangle, \]  

where

\[ H[A_c] = H_M - \int dr \ A_c \cdot (j_p + \frac{1}{2} j_A). \]  

We have assumed the Coulomb gauge. In eq.(3) \( H_M \) represents the Hamiltonian for the matter, including the Coulomb interaction among charged particles. In the interaction term the current-density operator \( j \) has been split into two contributions. The first one, which will be called canonical current, consists of

\[ j_p(r) = -i\hbar \sum_a (q_a/2m_a) [\delta(r - r_a) \nabla_a + \nabla_a \delta(r - r_a)]. \]  

The second contribution, involving the potential \( A_c \), consists of

\[ j_A(r) = -\sum_a (q_a^2/m_a) n_a(r) A_c(r), \]  

where \( n_a(r) = \delta(r - r_a) \) represents the density operator for the \( a \)-th particle. A third contribution due to the spin magnetization-density has been neglected, for the sake of simplicity.

The classical potential \( A_c \) is solution to the Maxwell equation

\[ \nabla \times B_c - c^{-2} \partial_t E_{\perp c} = c_0^{-1} c^{-2} \langle \psi | (j_p + j_A) |\psi\rangle_{\perp}, \]  

with the transverse electric field given by

\[ E_{\perp c} = -\partial_t A_c. \]  

Both eq.(6) and eq.(7) can be obtained, in the framework of QED, by use of the coherent-state formalism [7].

In this paper we limit ourselves to consider the interaction of the system with the classical field, neglecting any residual interaction with the quantum field (uncoherent photon emission and reabsorption). In this approximation, a simple expression for the conserved total energy of the whole system (matter plus classical field) can be given, in the form:

\[ \mathcal{E} = \langle \psi | H[A_c] |\psi\rangle + \left( e_0/2 \right) \int dr (|E_{\perp c}|^2 + c^2 |B_c|^2). \]
It can be verified easily that $\mathcal{E}$ is conserved. In fact, by differentiating both sides of eq. (8) with respect to time, we obtain, in the absence of emission of radiation,

$$\frac{d\mathcal{E}}{dt} = -\frac{i}{\hbar} \langle \psi | [H[A_c], H[A_c]] | \psi \rangle + \int dr \frac{\partial A_c}{\partial t} \cdot \{-\langle \psi | (j_p + j_A) | \psi \rangle \}$$

where eq.s (2) and (6) have been used.

The second term in the r.h.s. of eq.(8) represents the (positive) energy of the classical field. By a simple calculation, this term can be cast in the form

$$\frac{\epsilon_0}{2} \int dr \left( |E_{\perp c}|^2 + c^2 |B_c|^2 \right) = \frac{1}{2} \int dr A_c \cdot \langle \psi | (j_p + j_A) | \psi \rangle + \epsilon_0 \int dr |E_{\perp c}|^2$$

and

$$- \frac{\epsilon_0}{4} \frac{d^2}{dt^2} \int dr |A_c|^2 + \frac{1}{2} \epsilon_0 c^2 \int ds \cdot (A_c \times B_c),$$

where eq.s (6) and (7) have been used. In the absence of a significant emission of coherent radiation the last term can be neglected, for a finite system. By use of this result we obtain from eq.(8)

$$\mathcal{E} = \langle H_M \rangle - \frac{1}{2} \int dr A_c \cdot \langle j_p \rangle + \epsilon_0 \int dr |E_{\perp c}|^2 - \frac{\epsilon_0}{4} \frac{d^2}{dt^2} \int dr |A_c|^2. \quad (11)$$

We notice the absence of any contribution due to $j_A$. We notice also the factor of 1/2, as well as the minus sign, in the second term in the r.h.s. of eq.(11). In stationary conditions, eq.(11) reads

$$\mathcal{E} = \mathcal{E}_M + \mathcal{E}_F = \langle H_M \rangle - \frac{1}{2} \int dr A_c \cdot \langle j_p \rangle, \quad (12)$$

where the Coulomb gauge is understood. The analysis of the physical content of eq.(12), in particular of the minus sign in the r.h.s., can be simplified if the potential $A_c$ is expressed in terms of the canonical current $j_p$ and not in terms of the total current appearing in the r.h.s. of the Maxwell equation (6). This result will be obtained explicitly for two models.

**First model.** – The first model consists of a hollow cylinder with a current flowing around it. Let $L$ be the height, $R$ the inner radius, $a$ the thickness and let us assume, in order to simplify the calculations, $a \ll R \ll L$. Let us assume an uniform canonical current, flowing around the cylinder, given by

$$\langle j_p \rangle = -en(hp/m) = -en(h\mu/mR), \quad (13)$$

where $n$ is the (constant) electron density. We observe that $\mu$ is related to the total orbital angular momentum $\hbar M$ of the electrons by the relation $\mu = MN^{-1}$, where $N = 2\pi Ra Ln$ represents the total number of electrons involved in the process.

From eq.(6) we obtain the following expression for the magnetic flux $\Phi_B$

$$\Phi_B \simeq -he^{-1} \mu/2 = -he^{-1} \mu[1 + (2/\gamma^2 aR)]^{-1} \simeq -he^{-1} \mu, \quad (14)$$

where $\gamma$ is given by
\[ \gamma = \sqrt{\frac{e^2 n}{\epsilon_0 mc^2}}. \]  

(15)

For copper e.g. \( \gamma^{-1} \approx 1.8 \times 10^{-8} \) m (in the theory of superconductivity \( \gamma^{-1} \) is known as penetration depth \([\text{3}]\)). The last expression in eq.(14), corresponding to the case in which \( \gamma^2 aR \gg 1 \), is independent of geometrical details. The following relation

\[ \langle j_A \rangle \propto -\left(\frac{e^2 n}{2\pi R m}\right) \Phi_B \]  

(16)

has been used in the derivation of eq.(14). Eq.(14) gives an expression for the flux \( \Phi_B \) in terms of \( \mu \), i.e. in terms of the total angular momentum \( M = \mu N \).

For this model the magnetic energy \( E_F \), defined in eq.(12), is negative:

\[ E_F \simeq -\left(\frac{1}{2}\right) \langle j_p \rangle \Phi_B aL = -N\hbar^2 \mu^2 \left(1 + \frac{2}{\gamma^2 aR}\right)^{-1} \simeq -N\hbar^2 p^2 \]  

(17)

Second model. – Now let us consider a second model, consisting of a long, thin cylindrical conductor, with a current flowing along it. Let \( L \) be the length and \( \rho_0 \) the radius, with \( \rho_0 \ll L \).

We assume an uniform stationary canonical current, flowing inside the conductor, given by

\[ \langle j_p \rangle = -em^{-1}n\hbar p, \]  

(18)

where \( \hbar = N^{-1}hP \) is the canonical momentum per electron (in this case the total number of electrons is given by \( N = \pi \rho_0^2 Ln \)).

For a very long conductor we may assume that \( A_c \) is approximately oriented in the direction of the current (z-direction) and that it depends, approximately, on the distance \( \rho \) from the axis of the cylinder only. Putting \( x = \gamma \rho \), we obtain from eq.(6)

\[ \nabla^2 A_c - \theta(x_0 - x)A_c = \theta(x_0 - x)\hbar^{-1}p. \]  

(19)

The solution to eq.(19) has the form

\[ A_c = -\hbar \theta^{-1}p + \theta(x_0 - x)A_{int} \]  

(20)

where \( A_{int} \) is solution to

\[ \frac{d^2 A_{int}}{dx^2} + \frac{1}{x} \frac{dA_{int}}{dx} - A_{int} = 0 \]  

(21)

and \( A_{ext} \) is solution to

\[ \frac{d^2 A_{ext}}{dx^2} + \frac{1}{x} \frac{dA_{ext}}{dx} = 0 \]  

(22)

We assume that, for \( \rho_0 \ll \rho \ll L \), the solution of eq.(22) must coincide with the expression for the potential generated by a current \( i_T \) flowing through a one-dimensional wire

\[ A_w(\rho) \simeq 2 \frac{i_T}{4\pi \epsilon_0 c^2} \int_0^{L/2} dz (\rho^2 + z^2)^{-1/2} \]  

(23)

\[ = \frac{i_T}{2\pi \epsilon_0 c^2} \ln \left| \frac{L}{2\rho} + (1 + \frac{L^2}{4\rho^2})^{1/2} \right| \simeq \frac{i_T}{2\pi \epsilon_0 c^2} \ln \frac{L}{\rho}. \]

Taking into account the regularity of \( A_c \) for \( x = 0 \), as well as the continuity of both \( A_c \) and its gradient across the surface \( x = x_0 \), we obtain
Fig. 1 – Plot of $e_F$ versus $x_0$, for a conducting wire. The function $e_F$ represents the ratio between the total current $i_T$ and the canonical one $i_p$. The reduced radius $x_0 = \gamma \rho_0$ represents the radius of the wire in units with $\gamma^{-1} = 1$, where $\gamma^{-1}$ is the penetration depth. For copper e.g. $x_0 = 1$ corresponds to a radius $\rho_0 \approx 1.8 \times 10^{-8}$ m. Corrections due to surface effects can be expected. The plot is given for $L/\rho_0 = 10^4$, where $L$ is the length and $\rho_0$ the radius of the conducting wire.

$$A_{int} = -\left[i_T/2\pi\epsilon_0 c^2 x_0 I_1(x_0)\right] I_0(x),$$

(24)

where the $I$’s are modified Bessel functions (imaginary-argument Bessel functions) [9]. We obtain also

$$A_{ext} = -\frac{i_T}{2\pi\epsilon_0 c^2} \left[\ln \frac{x}{x_0} + \frac{I_0(x_0)}{x_0 I_1(x_0)}\right].$$

(25)

By a comparison of eq.(20), for $x > x_0$, with eq.(23) we obtain

$$i_T = e_F(x_0) i_p,$$

(26)

with $i_p = \pi \rho_0^2 \langle j_p \rangle$ and $e_F$ given by

$$e_F = 2[x_0^2 \ln(X_L/x_0) + x_0 I_0(x_0)/I_1(x_0)]^{-1},$$

(27)

where we have put $X_L = \gamma L$. Physically eq.(26) is a consequence of the skin-effect. A plot for $e_F$ versus $x_0$ is given in Fig.1, for $X_L/x_0 = 10^4$.

According to eq.(12) the magnetic energy $E_F$ is given by

$$E_F \simeq -\frac{(N\hbar^2 p^2/2m)[1 - e_F(x_0)]}{1 - e_F(x_0)} \simeq -(N\hbar^2 p^2/2m).$$

(28)

The last expression in eq.(28) represents the asymptotic limit for $x_0 \gg 1$ (bulk limit). It is independent of geometric details and coincides with the r.h.s. of eq.(17) obtained for the previous model. Such a coincidence ascribes a sort of universality to this result. In the derivation of eq.(28) the following identity

$$\int_0^{x_0} dx x I_0(x) = x_0 I_1(x_0)$$

has been used.
Conclusions. – Let $\mathcal{E}_M$ be the ground-state energy for a system of electrons, in the absence of current. Let $\Delta \mathcal{E}_M$ be the variation for $\mathcal{E}_M$, corresponding to a translation in momentum space, assuming that such a translation is allowed by the electron state. According to eq.(12), the corresponding variation for the total energy of the system is given by

$$\Delta \mathcal{E} = \mathcal{E}_F + \Delta \mathcal{E}_M.$$  

(30)

Since the magnetic energy $\mathcal{E}_F$ is negative, a physical situation, in which $\Delta \mathcal{E}$ is negative, is possible. In such a case the true ground state of the system would be characterized by a spontaneous current, as supposed in Refs. [4] and [5].

It can be demonstrated that, as a consequence of eq.(28), the ground state of a system of electrons in a periodic potential, with periodic boundary conditions, is at least degenerate, up to finite-size effects. In fact, let $|\psi_0\rangle$ be the ground state of $H_M$ and let $\mathcal{E}_M$ be the corresponding eigenvalue. In the state $|\psi_0\rangle$ the total canonical momentum, as well as the total current, vanish. Let $|\psi'\rangle$ be the state obtained from $|\psi_0\rangle$ through a rigid translation in momentum space

$$|\psi'\rangle = \exp[i\bar{\hbar}^{-1} \mathbf{p} \cdot \sum_j \mathbf{r}_j] |\psi_0\rangle.$$  

(31)

We obtain

$$\langle \psi'|H_M|\psi'\rangle = \mathcal{E}_M + N(h^2 \mathbf{p}^2 / 2m),$$  

(32)

and, according to eq.(28), $\Delta \mathcal{E} \approx 0$. However this result, since it holds up to finite-size effects only, is not sufficient to allow a spontaneous current.

The possibility for $\Delta \mathcal{E} < 0$ is investigated, for the sake of simplicity, in the case of a system of Bloch electrons in a conducting band. However a similar analysis could be applied, in principle, to more complicated electron states. In this simple case we have

$$\mathcal{E}_M = \frac{V}{8\pi^3} \int d\mathbf{k} n(k) \varepsilon(k)$$  

(33)

and [8]

$$\mathbf{p} = \frac{V}{8\pi^3 N\hbar} \int d\mathbf{k} n(k) \langle \psi_k | (-i\hbar \nabla) | \psi_k \rangle = \frac{mV}{8\pi^3 N\hbar^2} \int d\mathbf{k} n(k) \nabla_k \varepsilon(k).$$  

(34)

Neglecting the magnetic energy of eq.(28), in the ground state one would obtain, for $n(k)$, the zero-temperature Fermi-Dirac distribution function

$$n_F(k) \equiv n_F(\varepsilon(k)) = 2\theta(\varepsilon_F - \varepsilon(k))$$  

(35)

and correspondingly $\mathbf{p} = 0$ and vanishing current. However, owing to the negative value of $\mathcal{E}_F$, it may happen that the solution given in eq.(35) is unstable, when the magnetic interaction is switched on. In fact let us consider the following distribution function

$$n(k) = n_F(k - e_z q),$$  

(36)

obtained from $n_F$ through a shift of the argument. We observe that the transformation of the distribution function given in eq.(36) represents a sort of energy-weighted translation in momentum space, not a rigid one as given in eq.(31). In this case we have
\[ p = -\frac{mVq}{8\pi^3N\hbar^2} \int d\mathbf{k} \frac{dn_F}{d\varepsilon} \left( \frac{\partial \varepsilon}{\partial k_z} \right)^2 = \frac{mVq}{4\pi^3N\hbar^2} \int d\mathbf{k} \delta(\varepsilon - \varepsilon_F) \left( \frac{\partial \varepsilon}{\partial k_z} \right)^2 \]  

(37)

and

\[ \Delta \mathcal{E}_M = -\frac{Vq^2}{16\pi^3} \int d\mathbf{k} \frac{dn_F}{d\varepsilon} \left( \frac{\partial \varepsilon}{\partial k_z} \right)^2 = \frac{N\hbar^2}{2m}pq, \]

(38)

where the parity of \( \varepsilon(k) \) has been used. Now eq.(30) reads

\[ \Delta \mathcal{E} \simeq (N\hbar^2/2m) p(q - p) \]

(39)

and the condition for \( \Delta \mathcal{E} < 0 \) consists of \( p > q \), i.e.

\[ \left( \frac{V}{4\pi^3N} \right) \int d\mathbf{k} \delta(\varepsilon - \varepsilon_F) \left( \frac{\partial \varepsilon}{\partial k_z} \right)^2 > \left( \hbar^2/m \right), \]

(40)

where \( m \) is the physical mass of the electron.

In the simple case of a spherically symmetric \( \varepsilon \) we obtain from eq.(40)

\[ k_F^{-1}|d\varepsilon/dk|_{k=k_F} > \left( \hbar^2/m \right), \]

(41)

where the expression \( k_F^2 = 3\pi^2NV^{-1} \) has been used for the Fermi momentum \( k_F \). This is the condition for a superconductivity à la Heisenberg [4]. Finite-size effects could destroy the superconductivity e.g. in the case of a very small ring, according to eq.(17), or of a very thin wire, according to eq.(28).

For a free-electron gas in the bulk limit, the l.h.s. and the r.h.s. of eq.(41) coincide. This result indicates that, for such a system, the ground state is degenerate, up to finite-size effects, provided that the magnetic self-interaction energy is taken into account properly.

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