

The nonrelativistic Quantum-Mechanical Hamiltonian with diamagnetic current-current interaction.

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Abstract

We extend the standard solid-state quantum mechanical Hamiltonian containing only Coulomb interactions between the charged particles by inclusion of the (transverse) current-current diamagnetic interaction starting from the non-relativistic QED restricted to the states without photons and neglecting the retardation in the photon propagator. This derivation is supplemented with a derivation of an analogous result along the non-rigorous old classical Darwin-Landau-Lifshitz argumentation within the physical Coulomb gauge.

1 Introduction

The standard Hamiltonian of solid-state theory considers a system of electrons and ions interacting only through Coulomb forces. Magnetic interaction between the moving charges is not included. Only the spin-spin and spin-orbit magnetic interactions may be considered. The former is needed for the explanation of ferromagnetism, whereas the latter for the valence-band-splitting in semiconductors is important. However, the non-relativistic magnetic interactions between the moving charges of order $1/c^2$ responsible for diamagnetism are ignored.

Already 100 years ago Darwin [1] has argued in the frame of the classical electrodynamics of point-like particles, that up to order $1/c^2$ one might separate the motion of the particles from that of the electromagnetic field. From this separation emerges a magnetic current-current interaction. Since the classical electrodynamics of point-like charged particles is a vicious theory having neither Lagrangian, nor Hamiltonian formulation, his derivation lacked any rigor and cannot be quantized, nevertheless it contains a grain of truth and was considered later also by Landau and Lifshitz [2].

Actually, one needs a new analysis of the problem in the frame of the non-relativistic QED of electrons we describe in Section 2. By restricting the discussion to the states without photons and neglecting the retardation in the photon propagator we give in Section 3 a derivation of the electronic Hamiltonian containing the diamagnetic interaction between the transverse currents (microscopic Biot-Savart law !). This proof was first published in a preprint [3] and included in a recent book [4]. A short exposure is contained also in [5]. We try here a better presentation for a wider public, taking into account also discussions, with emphasis on the general problem of diamagnetism. Thereafter, in Section 4 we derive the classical version of this Hamiltonian within the Darwin-Landau-Lifschitz reasoning, however within the physical Coulomb gauge. This shows, that the difference to Darwin's Hamiltonian lies in his implicit choice of an unsuitable gauge implying constraints on the velocities. Our Hamiltonian in its mean field version [5] leads to the same linear linear response to an external magnetic field as the standard mean field BCS theory of superconductivity [6], [7],[8] predicting ideal diamagnetism in the bulk, whereas being essentially different beyond this reduced frame.

2 Non-relativistic QED

The basic idea underlying the solid state theory is that one may describe solids as a system of interacting electrons and ions. These charged particles should obey the rules of the electromagnetic theory. Since these are not the ultimate elementary particles one cannot resort directly to the relativistic quantum field theory. One has to build up a non-relativistic Quantum Electrodynamics for arbitrary charged non-relativistic particles (fermions and bosons). Such a theory may be constructed following the scheme of the relativistic QED, starting from the classical field theory based on the coupled Maxwell and the Schrödinger equations (instead Dirac's) followed by the quantization of the fields. Such an approach was described recently [9], [10]. The standard presentation however starts from the Hamiltonian of a quantum mechanical charged particle in external electromagnetic field, quantizes both the wave function and the vector potential in the Coulomb gauge, while replacing the scalar potential with the standard quantized Coulomb interaction. Thereafter one has still to add the Hamiltonian of the radiation field. Both ways have to be formulated in the Coulomb gauge, the only one without spurious degrees of freedom for the photons. The two ways lead to the same result however the field-theoretical one omits several sharp jumps by avoiding the inconsistent classical electromagnetic theory of charged point-like particles.

This non-relativistic QED is defined by the Hamiltonian (here just for electrons and photons) in the presence of time-dependent external electric and magnetic potentials

$$H^{QED}(t) = \sum_{\vec{q}, \lambda} \hbar \omega_q b_{\vec{q}, \lambda}^{\dagger} b_{\vec{q}, \lambda} + \quad (1)$$

$$\begin{aligned}
& \int d\vec{x} \mathcal{N} \left[\frac{1}{2m} \left(i\hbar \nabla \psi^+(\vec{x}) + \frac{e}{c} (\vec{A}_\perp(\vec{x}) + \vec{A}_{ext}(\vec{x}, t)) \psi^+(\vec{x}) \right) \right. \\
& \quad \times \left. \left(-i\hbar \nabla \psi(\vec{x}, t) + \frac{e}{c} (\vec{A}_\perp(\vec{x}) + \vec{A}_{ext}(\vec{x}, t)) \psi(\vec{x}) \right) \right] \\
& + \frac{1}{2} \int d\vec{x} \int d\vec{x}' \psi^+(\vec{x}) \psi^+(\vec{x}') \frac{e^2}{|\vec{x} - \vec{x}'|} \psi(\vec{x}') \psi(\vec{x}) + e \int d\vec{x} V_{ext}(\vec{x}, t) \psi^+(\vec{x}) \psi(\vec{x}) .
\end{aligned} \tag{2}$$

with the transverse radiation field being (Ω is the volume of the system)

$$\vec{A}_\perp(\vec{x}) = \sum_{\lambda=1,2} \sqrt{\frac{\hbar c}{\Omega}} \sum_{\vec{q}} \frac{1}{\sqrt{|\vec{q}|}} \vec{e}_{\vec{q}}^{(\lambda)} e^{-i\vec{q}\vec{x}} \left(b_{\vec{q},\lambda} + b_{-\vec{q},\lambda}^+ \right) , \tag{3}$$

while $\vec{A}_{ext}(\vec{x}, t)$ and $V_{ext}(\vec{x}, t)$ are classical external vector and scalar potentials. The unit vectors $\vec{e}_{\vec{q}}^{(\lambda)}$ are orthogonal to the wave vector \vec{q} as well as to each other and according to the general recipe of second quantization a normal ordering $\mathcal{N}[\dots]$ has to be introduced also with respect to the photon creation and annihilation operators $b_{\vec{q},\lambda}^+$, $b_{\vec{q},\lambda}$ in the Hamiltonian and the photon frequency is $\omega_q = c|q|$.

One may check, that the equations of motion derived from this Hamiltonian lead to the coupled Maxwell and Schrödinger operator equations.

As usual in many body theories of solid-state, the non-relativistic QED, contrary to the fundamental relativistic QED, is understood as a cut-off theory, where the bare parameters coincide with the physical ones.

This non-relativistic QED has been widely and successfully used since the mid of the last century in the quantum optics of atoms and solids. See a recent book [11] about.

Although in their basic paper "de Haas-van Alphen Effect and the Specific Heat of an Electron Gas", T. Holstein, R. E. Norton and P. Pincus [12] already have shown, that the current-current interaction in the non-relativistic QED is the basic piece for understanding diamagnetism, their ideas and proofs are ignored up to date. Its essence is that transverse photons transmit the diamagnetic interaction!

3 The restricted electronic Hamiltonian.

In order to obtain a pure electronic Hamiltonian suitable for solid state theory one must restrict the discussion to the subspace of states without photons. (To simplify the discussion we omit here the external fields and reintroduce them again at the end according to the "minimal rule".) This task cannot be done without neglecting at least terms of higher order than $1/c^2$. First of all, the normal ordered "seagull" term $\frac{e^2}{2mc^2} \psi^+ \psi A^2$ being already of order $1/c^2$ may be ignored. Being itself of order $1/c^2$ it may have only higher order non-vanishing matrix elements in this subspace.

The next step has to be neglecting any retardation in time induced by the photon propagator. Otherwise one cannot obtain a Hamilton operator local in

time. In the 4-dimensional Fourier space it amounts to neglect the term $-\omega^2/c^2$ in the denominator of the photon propagator

$$\frac{1}{q^2 - \omega^2/c^2 - i0}(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{q^2}); \quad (\mu, \nu = 1, 2, 3) \quad (4)$$

thus retaining only

$$\frac{i\hbar}{q^2}(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{q^2}); \quad (\mu, \nu = 1, 2, 3) \quad (5)$$

Since no pole survived, the $-i0$ term could have been also ignored and $4\pi/q^2$ is just the Fourier transform of the Coulomb potential.

To proceed further one can consider either the S-matrix, or the theory of Green functions in terms of the Feynman diagrams [3, 4] built with the standard Coulomb term and the photon-current interaction $-\frac{1}{c} \int i_{\perp} A$. It is easy to see that after the previous steps all the Feynman diagrams of the reduced S-matrix (having only external electron legs) may be constructed from the two basic graphs shown in the Fig. 1 having four electron legs, where in both cases the wavy line represents the Coulomb potential. The vertex " ρ " is a scalar, while the vertex " j_{\perp}^{μ} " is a vector one.

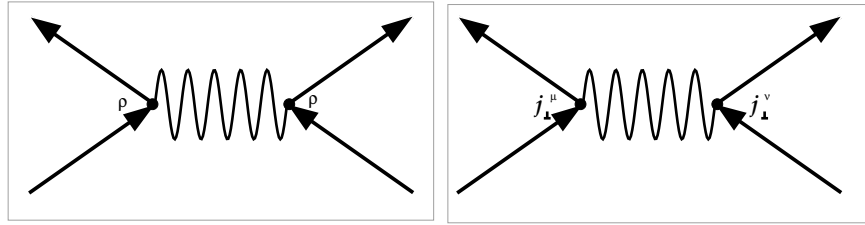


Figure 1: The basic four-leg graphs in the reduced S-matrix.

Therefore, we may conclude, that the quantum mechanical $1/c^2$ electron Hamiltonian that generates these diagrams is just

$$\begin{aligned} \mathbf{H}(t) = & \int d\vec{x} \psi^+(\vec{x}) \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}_{ext}(\vec{x}, t) \right)^2 + V_{ext}(\vec{x}, t) \right] \psi(\vec{x}) \\ & + \frac{1}{2} \int d\vec{x} \int d\vec{x}' \frac{\mathcal{N}[\rho(\vec{x})\rho(\vec{x}')] }{|\vec{x} - \vec{x}'|} - \frac{1}{2} \int d\vec{x} \int d\vec{x}' \frac{\mathcal{N}[\vec{j}_{\perp}(\vec{x}, t)\vec{j}_{\perp}(\vec{x}', t)]}{c^2|\vec{x} - \vec{x}'|} . \end{aligned} \quad (6)$$

Here $\rho(\vec{x})$ denotes the charge density operator

$$\rho(\vec{x}) = e\psi^+(\vec{x})\psi(\vec{x}), \quad (7)$$

while $\vec{j}_{\perp}(\vec{x}, t)$ denotes the transverse part of the current density operator

$$\vec{j}(\vec{x}, t) = \frac{e}{2m} \left(\psi^+(\vec{x}) \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}_{ext}(\vec{x}, t) \right) \psi(\vec{x}) + h.c. \right). \quad (8)$$

For sake of completeness we reintroduced here the time-dependent external fields according to the minimal principle of Yang-Mills theories.

The generalization of these results for a system of electrons and ions as constituents of the solid state is obvious.

The current-current term is nothing else but the well-known Biot-Savart law resulting from the exchange of transverse photons responsible for diamagnetic forces. One may argue that due to the smallness of the velocities in the condensed matter such an $1/c^2$ term may be neglected. This is obviously false. Our everyday experience teaches us, that a macroscopic number of slow electrons may create enormous magnetic fields.

For a better understanding of the underlying physics, let us consider now the Hartree approximation of this Hamiltonian. It looks as

$$\begin{aligned} \mathbf{H}_{Hartree}(t) = & \int d\vec{x} \psi^\dagger(\vec{x}) \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}_{ext}(\vec{x}, t) \right)^2 + V_{ext}(\vec{x}, t) \right] \psi(\vec{x}) \\ & + \int d\vec{x} \int d\vec{x}' \frac{\rho(\vec{x}) \langle \rho(\vec{x}', t) \rangle}{|\vec{x} - \vec{x}'|} - \int d\vec{x} \int d\vec{x}' \frac{\vec{j}_\perp(\vec{x}, t) \langle \vec{j}_\perp(\vec{x}', t) \rangle}{c^2 |\vec{x} - \vec{x}'|} . \end{aligned} \quad (9)$$

where $\langle \rho(\vec{x}, t) \rangle$ and $\langle \vec{j}_\perp(\vec{x}, t) \rangle$ are the (chosen) ensemble averages of the charge and transverse current densities.

One may here identify the s.c. internal scalar and vector potentials

$$V_{int}(\vec{x}, t) = \int d\vec{x}' \frac{\rho(\vec{x}', t)}{|\vec{x} - \vec{x}'|}; \quad \vec{A}_{int}(\vec{x}, t) = \int d\vec{x}' \frac{\vec{j}_\perp(\vec{x}', t)}{|\vec{x} - \vec{x}'|} . \quad (10)$$

Of course, here in the definition of the internal vector potential the retardation is missing!

Eq.6 and Eq.9 together with the identifications of Eq.10 show, that the average Coulomb field created by the electron results from the charge-charge interaction and the average (dia-) magnetic field created by the velocity of the electron results from the current-current interactions. This is analogous to the (ferro-) magnetic field of localized spins resulting from their mutual interaction in the Heisenberg spin model.

It is important also to remark, that this mean-field Hamiltonian resulting from the non-relativistic QED differs from the electromagnetic part of the mean-field Hamiltonian used in the equilibrium theory of the BCS superconductivity [7, 8]

$$\mathcal{H} = \int d\vec{x} \psi^\dagger(\vec{x}) \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \frac{e}{c} \vec{A}(\vec{x}) \right)^2 + V(\vec{x}) \right] \psi(\vec{x}) , \quad (11)$$

where the time independent potentials are interpreted as being the total ones

$$V(\vec{x}) = V_{ext}(\vec{x}) + V_{int}(\vec{x}); \quad \vec{A}(\vec{x}) = \vec{A}_{ext}(\vec{x}) + \vec{A}_{int}(\vec{x}) . \quad (12)$$

Though, the terms linear in the vector potentials are correct and therefore the equilibrium linear responses of the two Hamiltonians to an external magnetic field are also identical [5].

4 Darwin's classical approach revisited.

In this Section we show that Darwin's reasoning within the classical electromagnetic theory of point-like charges, if properly formulated in the Coulomb gauge, thus considering only the true physical degrees of freedom of the magnetic field, leads to a classical Hamiltonian analogous to the one we got in the previous Section.

One can not formulate a Lagrangian theory of classical point-like charged particles interacting with the electromagnetic field due to the divergent self-interaction. (From the Lorentz force one has to omit the action of the field created by each charged particle on itself!) This impedes also the derivation of the appropriate Hamiltonian.

Almost one hundred years ago Darwin [1] proposed a closed classical Lagrangian for N point-like charges e_i and mass m_i ($i, j = 1, \dots, N$) including terms up to order $1/c^2$ avoiding self-interaction and constructed the following Hamiltonian

$$\begin{aligned} \mathcal{H} = & \sum_i \frac{m_i}{2} \vec{p}_i^2 + \sum_{i>j} \frac{e_i e_j}{|\vec{r}_i - \vec{r}_j|} \\ & - \sum_{i>j} \frac{e_i e_j}{2c^2 m_i m_j |\vec{r}_i - \vec{r}_j|} [\vec{p}_i \cdot \vec{p}_j + (\vec{p}_i \cdot \vec{n}_{ij})(\vec{p}_j \cdot \vec{n}_{ij})], \end{aligned} \quad (13)$$

where $\vec{n}_{ij} \equiv \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|}$. His derivation is based on the expansion of the Liénard-Wiechert potentials to second order in $1/c$. Jackson in his derivation [13] uses the correct Coulomb gauge, but he wants to get Darwin's result and is forced to make one more not justified approximation to get it.

Landau-Lifshitz [2] have shown that Eq. 13 actually implies a very unusual choice of gauge, not the usual Coulomb one. The choice of the gauge is however essential, since the physical magnetic field \vec{B} , as well as the photon in quantum electrodynamics (QED), have only two transverse degrees of freedom and only in the Coulomb gauge (often called as the "physical" or "unitary" gauge) one is left just with these two degrees of freedom for the radiation field. The constraint on the vector potential (implied by Landau-Lifshitz's choice), after its elimination through the velocities, propagates on the velocities. It is worth to recall here for example, that in the relativistic QED, in the Lorentz gauge, restrictions on the allowed physical states have to be imposed to eliminate the longitudinal and temporal photons!

We follow here the way chosen by Landau-Lifshitz [2] to construct a classical Hamiltonian up to terms of order $1/c^2$, however not in their choice of gauge, but consequently in the Coulomb one. One starts with the Lagrangian of a single electron in an external field (here in a non-relativistic approach!) produced by some external sources ρ^{ext} and \vec{j}^{ext}

$$L(\vec{r}, \dot{\vec{r}}) = \frac{m \dot{\vec{r}}^2}{2} - e\phi^{ext}(\vec{r}, t) + \frac{e}{c} \vec{A}^{ext}(\vec{r}, t) \dot{\vec{r}}. \quad (14)$$

In the Coulomb gauge

$$\nabla \vec{\mathcal{A}}^{ext}(\vec{r}, t) = 0 \quad (15)$$

the potentials are

$$\phi(\vec{r}, t)^{ext} = \int d\vec{x} \frac{\rho^{ext}(\vec{x}, t)}{|\vec{r} - \vec{x}|}; \quad \vec{\mathcal{A}}^{ext}(\vec{r}, t) = \int d\vec{x} \frac{\vec{i}_{\perp}^{ext}(\vec{x}, t - |\vec{r} - \vec{x}|/c)}{c|\vec{r} - \vec{x}|}, \quad (16)$$

where $\rho^{ex}(\vec{x}, t)$ is the external charge density, while $\vec{i}_{\perp}^{ext}(\vec{x}, t)$ is the external transverse ($\nabla \vec{i}_{\perp}^{ext} = 0$) current density

$$\vec{i}_{\perp}^{ext}(\vec{x}, t) \equiv \vec{i}^{ext}(\vec{x}, t) + \frac{1}{4\pi} \nabla \int d\vec{x}' \frac{\nabla' \vec{i}^{ext}(\vec{x}', t)}{|\vec{x} - \vec{x}'|}. \quad (17)$$

As Landau-Lifshitz do it, one has to expand the retarded current density in powers of $1/c$, however here we need only the lowest approximation due to the already existent $1/c$ factor in the Lagrangian i.e.

$$\vec{\mathcal{A}}^{ext}(\vec{r}, t) \approx \int d\vec{x} \frac{\vec{i}_{\perp}^{ext}(\vec{x}, t)}{c|\vec{r} - \vec{x}|}. \quad (18)$$

If the source of the fields is a single point particle of charge e' at $\vec{x}(t)$ having the velocity $\dot{\vec{x}}(t)$ then

$$\rho^{ext}(\vec{x}, t) = e' \delta(\vec{x} - \vec{x}(t)), \quad \vec{i}^{ext}(\vec{x}, t) = e' \dot{\vec{x}}(t) \delta(\vec{x} - \vec{x}(t)), \quad (19)$$

with

$$\phi^{ext}(\vec{r}, t) = \frac{e'}{|\vec{r} - \vec{x}(t)|} \quad (20)$$

and

$$\vec{\mathcal{A}}^{ext}(\vec{r}, t) = \frac{e'}{c} \left[\frac{\dot{\vec{x}}(t)}{|\vec{r} - \vec{x}(t)|} - \frac{1}{4\pi} \int d\vec{x} \frac{1}{|\vec{r} - \vec{x}|} \nabla \left(\dot{\vec{x}}(t) \nabla \frac{1}{|\vec{x} - \vec{x}(t)|} \right) \right]. \quad (21)$$

Therefore the Lagrangian of the electron in the field of the another electron, in this approximation, is

$$\begin{aligned} \mathcal{L}(\vec{r}, \dot{\vec{r}}; \vec{x}, \dot{\vec{x}}) &= \frac{m_i \dot{\vec{r}}^2}{2} - \frac{ee'}{|\vec{r} - \vec{x}(t)|} \\ &+ \frac{ee' \dot{\vec{r}}}{c^2} \left[\frac{\dot{\vec{x}}(t)}{|\vec{r} - \vec{x}(t)|} - \frac{1}{4\pi} \int d\vec{x} \frac{1}{|\vec{r} - \vec{x}|} \nabla \left(\dot{\vec{x}}(t) \nabla \frac{1}{|\vec{x} - \vec{x}(t)|} \right) \right]. \end{aligned} \quad (22)$$

By generalization one obtains for a system of N charged particles the total Lagrange function

$$\begin{aligned} L &= \sum_i \frac{m_i}{2} \dot{\vec{v}}_i^2 - \sum_{i>j} \frac{e_i e_j}{|\vec{r}_i - \vec{r}_j|} \\ &+ \sum_{i>j} \frac{e_i e_j}{c^2} \dot{\vec{v}}_i \left[\frac{\dot{\vec{v}}_j}{|\vec{r}_i - \vec{r}_j|} - \frac{1}{4\pi} \int d\vec{x} \frac{1}{|\vec{r}_i - \vec{x}|} \nabla \left(\dot{\vec{v}}_j \nabla \frac{1}{|\vec{x} - \vec{r}_j|} \right) \right]. \end{aligned} \quad (23)$$

Actually one has to use here Dirac's canonical formalism [14, 15], since due to the velocity dependent terms, there is a relationship between the canonical momenta, However, to lowest order in $1/c$ we have

$$\vec{p}_i = \frac{\delta L}{\delta \dot{\vec{r}}_i} \approx m \dot{\vec{r}}_i \quad (24)$$

and therefore (according to Landau-Lifshitz), we may still remain in the frame of the standard canonical formalism. The resulting classical Hamiltonian including $1/c^2$ terms is

$$H = \sum_i \frac{\vec{p}_i^2}{2m_i} + \sum_{i>j} \frac{e_i e_j}{|\vec{r}_i - \vec{r}_j|} - \sum_{i>j} \frac{e_i e_j}{c^2 m_i m_j} \vec{p}_i \left[\frac{\vec{p}_j}{|\vec{r}_i - \vec{r}_j|} - \frac{1}{4\pi} \int d\vec{x} \frac{1}{|\vec{r}_i - \vec{x}|} \nabla \left(\vec{p}_j \nabla \frac{1}{|\vec{x} - \vec{r}_j|} \right) \right]. \quad (25)$$

This Hamiltonian is not identical with the Darwin Hamiltonian Eq.13! By introducing the charge and current densities:

$$\rho(\vec{x}) = \sum_i e \delta(\vec{x} - \vec{r}_i); \quad \vec{i}(\vec{x}) = \sum_i \frac{e}{m} \vec{p}_i \delta(\vec{x} - \vec{r}_i) \quad (26)$$

one would be tempted to rewrite the classical Hamiltonia Eq.25 as

$$\sum_i \frac{1}{2m} \vec{p}_i^2 + \frac{1}{2} \int d\vec{x} \int d\vec{x}' \frac{\rho(\vec{x}) \rho(\vec{x}')}{|\vec{x} - \vec{x}'|} - \frac{1}{2} \int d\vec{x} \int d\vec{x}' \frac{\vec{i}_\perp(\vec{x}) \vec{i}_\perp(\vec{x}')}{c^2 |\vec{x} - \vec{x}'|}, \quad (27)$$

where $\vec{i}_\perp(\vec{x})$ is the transverse part of the current density

$$\vec{i}_\perp(\vec{r}, t) \equiv \vec{i}(\vec{r}, t) + \frac{1}{4\pi} \nabla \int d\vec{r}' \frac{\nabla' \cdot \vec{i}(\vec{r}', t)}{|\vec{r} - \vec{r}'|}. \quad (28)$$

The above expression is similar to the result we obtained before (in the absence of external fields). However, due to the divergent self-interaction of point-like classical particles it is not meaningful in this form, even without the $1/c^2$ terms. Nevertheless, in the mean-field approximation, where the singularity is smeared out, it looks identical.

5 Conclusions

We derived from the non-relativistic QED the (transverse) current-current interaction term to be included in the solid state Hamiltonian in order to take into account the diamagnetic field created by the moving charges. We have shown

also, that the classical reasoning of Darwin [1], when properly treated in the Coulomb gauge, leads to a similar result.

The mean-field version of this $1/c^2$ Hamiltonian differs from the electromagnetic part of the Hamiltonian used in the mean field theory of superconductivity [8], based just on physical intuition. However, the difference occurs only in the terms non-linear in the vector potential. The correct variant may have important implications for higher magnetic fields, as well as beyond the mean-field approximation. The corrected classical Darwin Hamiltonian may have implications in the plasma theory.

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