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ALLOWING FOR SPIN–CURRENT INTERACTION BY BREIT'S HAMILTONIAN IN THE HYDRODYNAMIC METHOD

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Balance equations of momentum and magnetic moment density that allow for spin–current interaction are derived for a system of quantum particles.

In examining the collective processes that take place in extended systems of many interacting particles such as wave processes [1, 2], an equation in three-dimensional physical space is needed. An equation for a system of many particles with Coulomb interaction was derived in [3]. When systems of electrically neutral interacting particles are considered, one is forced to take into account spin–spin coupling, and this was done in [4, 5]. When a system of charged particles is examined, one must take into account, in addition to the Coulomb and spin–spin interactions, the spin–current and current–current interactions, which play an important role in such systems. However, if the particles move slowly, the current–current interaction is of a higher order than the spin–current one. This allows simplifying Breit's Hamiltonian by dropping the term responsible for current–current interaction.

We begin with the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi. \tag{1}$$

Under Hermitian conjugation this equation becomes

$$-i\hbar\frac{\partial}{\partial t}\psi^\dagger = \psi^\dagger\hat{H}^\dagger, \tag{2}$$

where we have introduced the following notation: a dagger (†) on the position-derivative operator means that differentiation should be applied to the expression standing to the left of the operator rather than to the expression to the right, a † on a matrix means the simple conjugate of that matrix, and a † on a complex number means the complex conjugate of that number. In addition, such notation satisfies the following properties:

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger, \quad (\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger. \tag{3}$$

Finally, it agrees with the definition of the Hermitian conjugate of an operator common in quantum mechanics [6].

We examine the time evolution of a quantity of the following form:

$$f = \psi^\dagger\hat{f}\psi, \tag{4}$$

where $\hat{f}$ is an arbitrary operator. The time derivative of this quantity is

$$\frac{\partial}{\partial t}f = \psi^\dagger \frac{\partial \hat{f}}{\partial t}\psi + \frac{i}{\hbar}\psi^\dagger \left(\hat{H}^\dagger \hat{f} - \hat{f}\hat{H}\right)\psi. \tag{5}$$

Isolating the commutator and anticommutator explicitly yields

$$\frac{\partial}{\partial t}f = \psi^\dagger \frac{\partial \hat{f}}{\partial t}\psi + \frac{i}{\hbar}\psi^\dagger \left(\frac{1}{2}\left[(\hat{H}^\dagger - \hat{H}), \hat{f}\right]_+ + \frac{1}{2}\left[(\hat{H}^\dagger + \hat{H}), \hat{f}\right]\right)\psi, \tag{6}$$

where square brackets with a plus as subscript, $[,]_+$, indicate an anticommutator.

The following operators will also be useful:

$$\hat{A} = \hat{\partial}^\dagger + \hat{\partial}, \quad \hat{E} = \frac{1}{2}(\hat{H}^\dagger + \hat{H}). \tag{7}$$

The operator $\hat{A}$ commutes with the position and momentum operators and is what is known as the gradient operator. Below we use only Hamiltonians that satisfy the condition

$$(\hat{H}^\dagger - \hat{H}) = i\hbar \sum_{i=0}^{N} \hat{A}_i \hat{J}_i \tag{8}$$

for a set of operators $\hat{J}_1$.

In this case equation (6) transforms into

$$\frac{\partial}{\partial t}f = \psi^\dagger \frac{\partial \hat{f}}{\partial t}\psi - \sum_{i=1}^{N} \nabla_i \left(\psi^\dagger \frac{1}{2}\left[\hat{J}_i, \hat{f}\right]_+ \psi\right) + \frac{i}{\hbar}\psi^\dagger [\hat{E}, \hat{f}]\psi. \tag{9}$$

Clearly, the total derivative of a quantity consists of the partial time derivative, the flux of the quantity, and the interaction. In the particular case where for the operator $\hat{f}$ we take the identity operator, equation (9) is the continuity equation in configuration space. Projecting this equation on three-dimensional space, we get the ordinary continuity equation

$$\frac{\partial}{\partial t}n(x) + \nabla \mathbf{J}(x) = 0. \tag{10}$$

Now we examine a Hamiltonian of the form

$$\hat{H} = \sum_{i=1}^{N}\sum_{j=1}^{N} a_{ij}\hat{p}_i\hat{p}_j + \sum_{i=1}^{N} b_i\hat{p}_i + c, \tag{11}$$

where a_{ij} and b_j are real quantities that commute with $\hat{p}_i$ and, in addition, $a_{ij} = a_{ji}$. In particular, Breit's Hamiltonian has the same form to within relativistic corrections, which are small compared to the other terms in systems with many particles.

To derive an expression for the current we use the general method of quantum hydrodynamics. Obviously,

$$\hat{H}^\dagger - \hat{H} = i\hbar \sum_{i=1}^{N} \hat{A}_i \hat{J}_i, \tag{12}$$

where the current operator $\hat{J}$ can be chosen of the following form:

$$\hat{J}_i = a_{ij}(\hat{p}_j + \hat{p}_j^\dagger) + b_i. \tag{13}$$

Then we calculate the operator $\hat{E}$:

$$\hat{E} = \sum_{i=0}^{N} \hat{J}_i(\hat{p}_i^\dagger + \hat{p}_i) - \sum_{i=0}^{N} a_{ij}\hat{p}_i^\dagger \hat{p}_j + c. \tag{14}$$

Clearly, Hermitian conjugation does not change the above operators.

To allow for spin–current interaction, we examine the part of Breit's Hamiltonian [7] responsible for the kinetic energy and spin–current interaction,

$$\hat{H} = \sum_{i=1}^{N} \hat{T}(\hat{p}_i) + \sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1}{2} U(\hat{p}_i, \hat{p}_j, x_i - x_j), \tag{15}$$

where

$$\hat{T}(\hat{p}_i) = \left(\frac{\hat{p}_i^2}{2m} - \frac{\hat{p}_i^4}{8m^3c^2}\right), \tag{16}$$

and

$$U(\hat{p}_i, \hat{p}_j, \mathbf{r}) = \frac{e}{r} - \pi\left(\frac{e\hbar}{mc}\right)^2 \delta(\mathbf{r}) - \frac{e^2\hbar}{2m^2c^2r^3}(\sigma_i + 2\sigma_j)[\mathbf{r}\times\hat{p}_i] \\ + \frac{1}{4}\left(\frac{e\hbar}{mc}\right)^2\left(\frac{\sigma_i\sigma_j}{r^3} - \frac{3(\sigma_i\mathbf{r})(\sigma_j\mathbf{r})}{r^5} - \frac{8\pi}{3}\sigma_i\sigma_j\delta(\mathbf{r})\right). \tag{17}$$

To see whether condition (8) is met for this case, we calculate $(i/\hbar)(\hat{T}^\dagger - \hat{T})$,

$$\frac{i}{\hbar}(\hat{T}^\dagger(\hat{p}_i) - \hat{T}(\hat{p}_i)) = \hat{A}\left(\frac{\hat{p}_i^\dagger + \hat{p}_i}{2m} + \frac{(\hat{p}_i^\dagger)^3 + (\hat{p}_i^\dagger)^2\hat{p}_i + \hat{p}_i^\dagger\hat{p}_i^2 + \hat{p}_i^3}{8m^3c^2}\right), \tag{18}$$

and $(i/\hbar)(\hat{U}^\dagger - \hat{U})$,

$$\frac{i}{\hbar}(\hat{U}^\dagger(\hat{\mathbf{p}}_i, \hat{\mathbf{p}}_j, \mathbf{r}_i - \mathbf{r}_j) - \hat{U}(\hat{\mathbf{p}}_i, \hat{\mathbf{p}}_j, \mathbf{r}_i - \mathbf{r}_j)) = \hat{A}^\alpha\left(\frac{e^2\hbar}{2m^2c^2}\epsilon^{\alpha\beta\gamma}(\sigma_i^\beta + 2\sigma_j^\beta)\frac{r^\gamma}{r^3}\right). \tag{19}$$

Thus, we have

$$\frac{i}{\hbar}(\hat{H}^\dagger(\hat{\mathbf{p}}_i, \hat{\mathbf{p}}_j, \mathbf{r}_i - \mathbf{r}_j) - \hat{H}(\hat{\mathbf{p}}_i, \hat{\mathbf{p}}_j, \mathbf{r}_i - \mathbf{r}_j)) \\ = \hat{A}\sum_{i=1}^{N}\left(\frac{\hat{p}_i^\dagger + \hat{p}_i}{2m} + \frac{(\hat{p}_i^\dagger)^3 + (\hat{p}_i^\dagger)^2\hat{p}_i + \hat{p}_i^\dagger\hat{p}_i^2 + \hat{p}_i^3}{8m^3c^2}\right) + \hat{A}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{1}{2}\left(\frac{e^2\hbar}{2m^2c^2}\epsilon^{\alpha\beta\gamma}(\sigma_i^\beta + 2\sigma_j^\beta)\frac{r^\gamma}{r^3}\right), \tag{20}$$

which corresponds to condition (8) and makes it possible to use the method. For systems of many particles examined at normal temperatures, the relativistic corrections, whose order is that of c^{-2} are usually small compared to the other terms in the Hamiltonian. The main reason for this is the linear dependence of the relativistic corrections on the number of particles in the system. Hence, ignoring the relativistic corrections, we can think of Breit's Hamiltonian as a particular case of a quadratic Hamiltonian.

To simplify matters we introduce a number of approximations. We ignore the relativistic corrections, which can be done at normal temperatures. Since our aim is to derive corrections representing spin–current interaction, we can assume that the matrix a_{ij} in equation (11) is diagonal, which means we ignore the current–current interaction between particles. Finally, in the part responsible for spin–current interaction we replace $\hat{\sigma}$ with $2\hat{\sigma}$, which corresponds to the symmetric case. We then have

$$\hat{E} = \frac{1}{4m}\sum_{i=1}^{N}(\hat{\mathbf{p}}_i\hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i^\dagger\hat{\mathbf{p}}_i^\dagger) + \frac{1}{2}\sum_{i=1}^{N} b_i(\hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i^\dagger) + c, \tag{21}$$

$$\hat{\mathbf{J}}_i = \frac{1}{2m}(\hat{\mathbf{p}}_i + \hat{\mathbf{p}}_i) + \mathbf{b}_i, \tag{22}$$

where

$$b_i^\alpha = -\frac{e^2\hbar}{4m^2c^2}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{x_i^\beta - x_j^\beta}{|\mathbf{x}_i - \mathbf{x}_j|^3}\epsilon^{\alpha\beta\gamma}(2\hat{\sigma}_i^\gamma + 2\sigma_j^\gamma), \tag{23}$$

$$c = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\left(\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} - \frac{\pi e^2\hbar^2}{m^2c^2}\delta(\mathbf{x}_i - \mathbf{x}_j) + \frac{e^2\hbar^2}{4m^2c^2}\hat{\sigma}_i^\alpha\hat{\sigma}_j^\beta\left(-\frac{\partial}{\partial x_i^\alpha}\frac{\partial}{\partial x_j^\beta}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} - 4\pi\delta^{\alpha\beta}\delta(\mathbf{r}_i - \mathbf{r}_j)\right)\right). \tag{24}$$

The commutator of $\hat{E}$ and the current operator is

$$[\hat{E}, \hat{J}_i] = \frac{1}{4m}\sum_{j=1}^{N}[(\hat{p}_j\hat{p}_j + \hat{p}_j^\dagger\hat{p}_j^\dagger), b_i] + \frac{1}{2}\sum_{j=1}^{N} b_j[\hat{p}_j + \hat{p}_j^\dagger, b_i] + \frac{1}{4m}\sum_{j=1}^{N}[b_j, \hat{p}_i + \hat{p}_i^\dagger](\hat{p}_j + \hat{p}_j^\dagger) + \frac{1}{2}[c, \hat{p}_i + \hat{p}_i^\dagger]. \tag{25}$$

In the case at hand the result of calculating the commutator is

$$\frac{i}{\hbar}[\hat{E}, \hat{J}_i] = \sum_{j=1}^{N}\frac{1}{2}\left[\frac{\partial b_i^\alpha}{\partial x_j^\beta} - \frac{\partial b_j^\beta}{\partial x_i^\alpha}, \hat{J}_j^\beta\right]_+ - \frac{1}{m}\frac{\partial c}{\partial x_i^\alpha}. \tag{26}$$

The last term on the right-hand side of this expression is responsible for the Coulomb and spin–spin interactions and was calculated in [4, 5], while the first term is responsible for spin–current interaction, which is of interest to us:

$$\frac{\partial b_i^\alpha}{\partial x_j^\beta} - \frac{\partial b_j^\beta}{\partial x_i^\alpha} = \frac{e^2\hbar}{4m^2c^2}\left[\sum_{\substack{k=1\\ k\neq i}}^{N}\frac{\partial}{\partial x_j^\beta}\frac{\partial}{\partial x_i^\mu}\frac{1}{|\mathbf{x}_i - \mathbf{x}_k|}\epsilon^{\alpha\mu\nu}(2\hat{\sigma}_i^\nu + 2\hat{\sigma}_k^\nu) - \sum_{\substack{k=1\\ k\neq j}}^{N}\frac{\partial}{\partial x_i^\alpha}\frac{\partial}{\partial x_j^\mu}\frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}\epsilon^{\beta\mu\nu}(2\hat{\sigma}_j^\nu + 2\hat{\sigma}_k^\nu)\right]. \tag{27}$$

We calculate the above expression for two cases, $i = j$ and $i \neq j$. When $i = j$, we have

$$\frac{\partial b_i^\alpha}{\partial x_i^\beta} - \frac{\partial b_i^\beta}{\partial x_i^\alpha} = \frac{e^2\hbar}{4m^2c^2}\sum_{\substack{k=1\\ k\neq i}}^{N}(2\hat{\sigma}_i^\nu + 2\hat{\sigma}_k^\nu)\frac{\partial}{\partial x_i^\mu}\left(\epsilon^{\alpha\mu\nu}\frac{\partial}{\partial x_i^\beta} - \epsilon^{\beta\mu\nu}\frac{\partial}{\partial x_i^\alpha}\right)\frac{1}{|\mathbf{x}_i - \mathbf{x}_k|}. \tag{28}$$

Using the relation

$$\epsilon^{\alpha\mu\nu}\nabla^\beta - \epsilon^{\beta\mu\nu}\nabla^\alpha = \epsilon^{\alpha\beta\nu}\nabla^\mu - \epsilon^{\alpha\beta\mu}\nabla^\nu, \tag{29}$$

we get

$$\frac{\partial b_i^\alpha}{\partial x_i^\beta} - \frac{\partial b_i^\beta}{\partial x_i^\alpha} = \frac{e^2\hbar}{4m^2c^2}\sum_{\substack{k=1\\ k\neq i}}^{N}\left(4\pi\delta^{\mu\nu}\delta(\mathbf{x}_i - \mathbf{x}_k) - \frac{\partial}{\partial x_i^\mu}\frac{\partial}{\partial x_i^\nu}\frac{1}{|\mathbf{x}_i - \mathbf{x}_k|}\right)\epsilon^{\alpha\beta\mu}(2\hat{\sigma}_i^\nu + 2\hat{\sigma}_k^\nu). \tag{30}$$

Reasoning along similar lines, for $i \neq j$ we get

$$\frac{\partial b_i^\alpha}{\partial x_j^\beta} - \frac{\partial b_j^\beta}{\partial x_i^\alpha} = \frac{e^2\hbar}{4m^2c^2}\epsilon^{\alpha\beta\mu}\left(-4\pi\delta^{\mu\nu}\delta(\mathbf{x}_i - \mathbf{x}_j) + \frac{\partial}{\partial x_i^\mu}\frac{\partial}{\partial x_i^\nu}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}\right)(2\hat{\sigma}_j^\nu + 2\hat{\sigma}_i^\nu). \tag{31}$$

Plugging (30) and (31) into (27) yields

$$\sum_{j=1}^{N}\frac{1}{2}\left[\frac{\partial b_i^\alpha}{\partial x_j^\beta}-\frac{\partial b_j^\beta}{\partial x_i^\alpha},\hat{j}_j^\beta\right]_+$$
$$=\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{1}{2}\left[\frac{e^2\hbar}{4m^2c^2}\epsilon^{\alpha\beta\mu}\left(4\pi\delta^{\mu\nu}\delta(\mathbf{x}_i-\mathbf{x}_j)-\frac{\partial}{\partial x_i^\mu}\frac{\partial}{\partial x_i^\nu}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\right)(2\hat{\sigma}_j^\nu+2\hat{\sigma}_i^\nu),\hat{j}_i^\beta-\hat{j}_j^\beta\right]_+. \quad (32)$$

We must also know how to calculate commutators with the magnetic moment operator

$$\hat{M}^\alpha=\frac{e\hbar}{2mc}\hat{\sigma}^\alpha. \quad (33)$$

For the commutator of the energy operator and $\hat{M}$ we obtain

$$[\hat{E},\hat{M}_i^\mu]=\frac{1}{2}\sum_{j=1}^{N}[b_j^\alpha,\hat{M}_i^\mu]\left(\hat{p}_j^\alpha+(\hat{p}_j^\alpha)^\dagger\right)[c,\hat{M}_i^\mu]. \quad (34)$$

The last term on the right-hand side reflects the spin–spin interaction and was calculated in [4, 5]. Hence, we will limit ourselves to calculating the first term:

$$\frac{1}{2}\sum_{j=1}^{N}[b_j^\alpha,\hat{M}_i^\mu]\left(\hat{p}_j^\alpha+(\hat{p}_j^\alpha)^\dagger\right)$$
$$=\frac{e}{mc}\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{e}{c}\frac{x_i^\beta-x_j^\beta}{|\mathbf{x}_i-\mathbf{x}_j|^3}\epsilon^{\alpha\beta\gamma}\epsilon^{\gamma\mu\nu}\frac{1}{2}\left[\hat{M}_i^\nu\hat{J}_j^\alpha\right]_+ +\frac{e}{mc}\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{1}{c}\frac{x_j^\beta-x_i^\beta}{|\mathbf{x}_j-\mathbf{x}_i|^3}\epsilon^{\alpha\beta\gamma}\epsilon^{\gamma\mu\nu}\frac{e}{2}\left[\hat{M}_i^\nu\hat{J}_j^\alpha\right]_+. \quad (35)$$

To obtain equations that operate in three-dimensional space one must integrate the equation written for functions in three-dimensional configuration space over all the coordinates except the three coordinates of the particle under investigation. The choice of a particle is unimportant in view of the principle of symmetry of the wave function for identical particles. Such an operation is equivalent to integrating the equation that has been multiplied by the delta-function over all $3N$ coordinates.

Integrating equations (32) and (35) together with the delta-function and ignoring correlations, we arrive at the following equations:

$$\left(\frac{d\mathbf{M}(\mathbf{x})}{dt}\right)_{MJ}=\frac{e}{mc}\left[\mathbf{M}(\mathbf{x})\times\mathbf{B}^J(\mathbf{x})\right]-\frac{e}{mc}\left[\mathbf{M}(\mathbf{x})\times\left[\frac{\mathbf{v}(\mathbf{x})}{c}\times\mathbf{E}(\mathbf{x})\right]\right], \quad (36)$$

$$\left(\frac{d\mathbf{J}(\mathbf{x})}{dt}\right)_{MJ}=\frac{e}{mc}\left[\mathbf{J}(\mathbf{x})\times\mathbf{B}^S(\mathbf{x})\right]+\frac{e}{m}n\mathbf{E}^S(\mathbf{x})+\frac{1}{m}\left[\mathbf{M}(\mathbf{x})\cdot\nabla\right]\mathbf{B}^J(\mathbf{x})-\frac{1}{m}\left[\frac{\mathbf{v}(\mathbf{x})}{c}\times\left(\mathbf{M}(\mathbf{x})\cdot\nabla\right)\mathbf{E}(\mathbf{x})\right], \quad (37)$$

where

$$\left[\nabla\times\mathbf{B}^J(\mathbf{x})\right]=\frac{4\pi}{c}e\mathbf{J}(\mathbf{x}), \quad (38)$$

$$\left[\nabla\times\left(\mathbf{B}^S(\mathbf{x})+4\pi\mathbf{M}(\mathbf{x})\right)\right]=0, \quad (39)$$

$$(\nabla\mathbf{E}(\mathbf{x}))=4\pi en(\mathbf{x}), \quad (40)$$

$$\left[\nabla\times\mathbf{E}^S(\mathbf{x})\right]=-\frac{1}{c}\left(\frac{\partial\mathbf{B}^S(\mathbf{x})}{\partial t}\right)_J. \quad (41)$$

In equation (41), the curl of the electric field generated by the moving magnetic moments depends on the variation of the spin magnetic field caused by the transport of the magnetic moments.

Thus, we have derived equations that describe the balance of momentum and magnetic moment density and allow for the interaction of the current and the intrinsic magnetic moment of the particles.

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REFERENCES

1. L.S. Kuz'menkov and D.E. Kharabadze, *Izv. Vyssh. Uchebn. Zaved. Fiz.*, no. 4, p. 87, 2004.
2. L.S. Kuz'menkov, S.G. Maksimov, and D.E. Kharabadze, in: *Summaries of Reports Presented at the 12th International Conf. on Spin Electronics and Gyrovector Electrodynamics* (in Russian), p. 333, Moscow (Firsanovka), November 14–16, 2003.
3. L.S. Kuz'menkov and S.G. Maksimov, *Teor. Mat. Fiz.*, vol. 118, no. 2, p. 287, 1999.
4. L.S. Kuz'menkov, S.G. Maksimov, and V.V. Fedoseev, *Teor. Mat. Fiz.*, vol. 126, no. 1, p. 136, 2001.
5. L.S. Kuz'menkov, S.G. Maksimov, and V.V. Fedoseev, *Teor. Mat. Fiz.*, vol. 126, no. 2. p. 258, 2001.
6. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: Non-relativistic Theory*, 3rd. edn., Boston, 1996.
7. V.B. Berestetskii, E.M. Lifshitz, and L.P. Pitaevskii, *Quantum Electrodynamics*, Oxford, 1982.

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