

Unified description of *Zitterbewegung* for spintronic, graphene, and superconducting systems

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We present a unified treatment of *Zitterbewegung* phenomena for a wide class of systems including spintronic, graphene, and superconducting systems. We derive an explicit expression for the time dependence of the position operator of the quasiparticles which can be decomposed into a mean part and an oscillatory term. The latter corresponds to the *Zitterbewegung*. To apply our result for different systems, one needs to use only vector algebra instead of the more complicated operator algebra.

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The *Zitterbewegung* (ZB) was first regarded as a relativistic effect rooted in the Dirac equation and related to a “trembling” or oscillatory motion of the center of a free wave packet.^{1,2} The ZB is caused by the interference between the positive and negative energy states in the wave packet; the characteristic frequency of this motion is determined by the gap between the two states. It was believed that the experimental observation of the effect is impossible since one would confine the electron to a scale of the Compton wavelength \hbar/m_0c , where m_0 is the bare mass of the electron.² However, the ZB is not a strictly relativistic effect: It can appear even for a nonrelativistic particle moving in a crystal³ or for quasiparticles governed by the Bogoliubov–de Gennes equations in superconductors.⁴

Most recently, Schliemann *et al.*^{5,6} predicted the ZB in spintronic systems where the experimental observation of the effect is more realistic due to the much smaller frequency of the oscillatory motion. In these semiconductor nanostructures⁷ spin-orbit coupling generates an oscillatory motion of the wave packet. The semiclassical time evolution of holes was investigated numerically for the Luttinger Hamiltonian by Jiang *et al.*⁸ The relation between the ZB and the spin transverse force was studied by Shen.⁹ In a numerical work, Lee and Bruder observed an oscillatory behavior in the charge and spin densities of quantum wires with Rashba and Dresselhaus types of spin-orbit coupling.¹⁰ With a spin-polarized electron injected into a waveguide, Nikolić *et al.*¹¹ found an oscillatory motion of the wave packet numerically, and the ZB pattern was also predicted numerically by Brushheim and Xu.¹² Similarly, Zawadzki studied the ZB in narrow gap semiconductors,¹³ in single-wall semiconducting carbon nanotubes,¹⁴ and in crystals using the nearly-free electron approximation,¹⁵ which is essentially the same as the two-band model in Ref. 3.

Two-dimensional carbon sheets, known as graphene, have been studied theoretically^{16,17} for many decades, since their band structure, a gapless Dirac-type spectrum, is unique.¹⁸ However, the experimental consequences of such a relativistic electron dynamics were observed only recently in Hall conductivity measurements.^{19,20} In bilayer graphene a more peculiar behavior of the Hall effect was observed experimentally,²¹ and explained in terms of the chiral Hamiltonian first derived by McChann and Fal’ko.²² Both in single and bilayer graphene the appearance of the oscillatory motion of the electron related to the ZB was pointed out by

Katsnelson.²³ Most recently, Tworzydło *et al.* associated the shot noise with the interference of electron-hole pairs at the Dirac point in graphene.²⁴ As an experimental observation of the ZB Trauzettel *et al.* proposed measuring the photon-assisted electron transport in graphene.²⁵

In this work, we present a unified description of the ZB in the systems mentioned above. Our approach makes it possible to calculate with simple algebra (without using operator algebra) the time dependence of the position operator of the particle for a wide class of systems. We also easily verify the results first obtained by Schliemann *et al.*^{5,6} for spintronic systems. Our result directly shows that the ZB is not necessarily a relativistic effect but it is related to the coupling between the components of the eigenstates of the system. This phenomenon is thus the direct consequence of the pseudospin degree of freedom.

The time dependence of the position operator in the Heisenberg picture is given by $\mathbf{r}(t) = e^{iHt/\hbar} \mathbf{r}(0) e^{-iHt/\hbar}$, where H is the Hamiltonian of the system. To calculate the operator $\mathbf{r}(t)$ one can work with the eigenstates of H . However, a further insight into the nature of the ZB can be gained by solving the equations of motion. We start with a quite general form of the Hamiltonian that is suitable to describe spintronic, graphene, and superconducting systems:

$$H = \varepsilon(\mathbf{p})\mathbb{1} + \boldsymbol{\Omega}^T \mathbf{S}, \quad (1)$$

where the system is characterized by the one-particle energy dispersion $\varepsilon(\mathbf{p})$ and the effective magnetic field $\boldsymbol{\Omega}(\mathbf{p})$ coupled to the spin \mathbf{S} . Here we assume that $\varepsilon(\mathbf{p})$ and $\boldsymbol{\Omega}(\mathbf{p})$ are differentiable functions of the momentum $\mathbf{p} = (p_x, p_y, p_z)$. Here T stands for the transpose of a vector, while $\mathbb{1}$ is the unit matrix in spin space, which will be omitted hereafter. In the absence of an electrostatic potential $V(\mathbf{r})$, the momentum \mathbf{p} and, consequently, $\boldsymbol{\Omega}(\mathbf{p})$ are constants of motion. In Table I we listed a few systems [together with the effective magnetic field $\boldsymbol{\Omega}(\mathbf{p})$] that are currently intensely studied in spintronics and in the research of graphene and superconductors.

It should be emphasized that although in Table I the Hamiltonian for all systems is given in terms of the Pauli matrices corresponding to a spin $S = \frac{1}{2}$, in our general consideration, the spin operator \mathbf{S} in Eq. (1) can represent a quasiparticle with an arbitrary spin $S \geq \frac{1}{2}$.

TABLE I. The Hamiltonian of different systems can be expressed as in Eq. (1). Here D is the dimension of the system, $p_{\pm}=p_x \pm ip_y$, $\sigma_{\pm}=\sigma_x \pm i\sigma_y$, and the spin operator is $\mathbf{S}=(\hbar/2)\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}=(\sigma_x, \sigma_y, \sigma_z)$ is the set of Pauli matrices. For Cooper pairs we assume (for simplicity) that the pair potential Δ is real and independent of \mathbf{r} , and that the energy is measured from the Fermi energy E_F . In the last row, $\epsilon_{\mathbf{p}}=\hbar^2\mathbf{k}^2/(2m)$, where $\mathbf{p}=\hbar\mathbf{k}$, \mathbf{q} is fixed, and $V_{\mathbf{q}}$ is the Fourier transform of the periodic potential treated as a perturbation in the crystal. Here $\text{Re}\{\cdot\}$ and $\text{Im}\{\cdot\}$ are the real and imaginary parts of the argument. More details of these systems can be found in the references listed in the last column.

System	D	H	$\boldsymbol{\Omega}$	$\varepsilon(\mathbf{p})$	References
Rashba-Dresselhaus	2	$\frac{\mathbf{p}^2}{2m} + \frac{\alpha}{\hbar}(p_x\sigma_y - p_y\sigma_x) + \frac{\beta}{\hbar}(p_y\sigma_y - p_x\sigma_x)$	$\frac{2}{\hbar^2} \begin{pmatrix} -\alpha p_y - \beta p_x \\ \alpha p_x + \beta p_y \\ 0 \end{pmatrix}$	$\frac{\mathbf{p}^2}{2m}$	5,6,7,26
Heavy holes in a quantum well	2	$\frac{\mathbf{p}^2}{2m} + i\frac{\tilde{\alpha}}{2\hbar^3}(p_x^3\sigma_+ - p_x^3\sigma_-)$	$\frac{2\tilde{\alpha}}{\hbar^4} \begin{pmatrix} p_y(3p_x^2 - p_y^2) \\ p_x(3p_y^2 - p_x^2) \\ 0 \end{pmatrix}$	$\frac{\mathbf{p}^2}{2m}$	6,26,27
Bulk Dresselhaus	3	$\frac{\gamma_D}{\hbar^3}[\sigma_x p_x(p_y^2 - p_z^2) + \sigma_y p_y(p_z^2 - p_x^2) + \sigma_z p_z(p_x^2 - p_y^2)]$	$\frac{2\gamma_D}{\hbar^4} \begin{pmatrix} p_x(p_y^2 - p_z^2) \\ p_y(p_z^2 - p_x^2) \\ p_z(p_x^2 - p_y^2) \end{pmatrix}$	0	7,26
Single-layer graphene	2	$v(p_x\sigma_x + p_y\sigma_y)$	$\frac{2v}{\hbar} \begin{pmatrix} p_x \\ p_y \\ 0 \end{pmatrix}$	0	16,17,19,20,23
Bilayer graphene	2	$\frac{1}{2m} \left(\frac{p_+^2 + p_-^2}{2} \sigma_x - \frac{p_-^2 - p_+^2}{2i} \sigma_y \right)$	$\frac{1}{m\hbar} \begin{pmatrix} p_x^2 - p_y^2 \\ 2p_x p_y \\ 0 \end{pmatrix}$	0	21–23
Cooper pairs	3	$\left(\frac{\mathbf{p}^2}{2m} - E_F \right) \sigma_z + \Delta \sigma_x$	$\frac{2}{\hbar} \begin{pmatrix} \Delta \\ 0 \\ p_x^2 + p_y^2 + p_z^2 - E_F \end{pmatrix}$	0	4,28
Nearly free electrons	3	$H = \begin{pmatrix} \epsilon_{\mathbf{k}+\mathbf{q}} & V_{\mathbf{q}} \\ V_{\mathbf{q}}^* & \epsilon_{\mathbf{k}} \end{pmatrix}$	$\begin{pmatrix} \text{Re}\{V_{\mathbf{q}}\} \\ -\text{Im}\{V_{\mathbf{q}}\} \\ \frac{1}{2}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) \end{pmatrix}$	$\frac{1}{2}(\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}})$	3,15

The equations of motion of the position operator $\mathbf{r}(t)$ and the spin operator $\mathbf{S}(t)$ in the Heisenberg picture for the Hamiltonian (1) read

$$\frac{d}{dt}\mathbf{r}(t) = \frac{i}{\hbar}[H, \mathbf{r}] = \frac{d\varepsilon(\mathbf{p})}{d\mathbf{p}} + \mathbf{K}\mathbf{S}(t), \quad (2a)$$

$$\frac{d}{dt}\mathbf{S}(t) = \frac{i}{\hbar}[H, \mathbf{S}] = \boldsymbol{\Omega}(\mathbf{p}) \times \mathbf{S}(t), \quad (2b)$$

where

$$K_{ik} = -\frac{i}{\hbar}[x_i, \Omega_k(\mathbf{p})] = \frac{\partial \Omega_k}{\partial p_i}. \quad (2c)$$

Note that Eqs. (2) are coupled equations of all three components of $\mathbf{S}(t)$ and $\mathbf{r}(t)$. However, in the case of two-

dimensional systems only the x and y components of $\mathbf{r}(t)$ are involved in Eq. (2a).

It is clear from Eq. (2b) that the spin vector $\mathbf{S}(t)$ precesses around the vector $\boldsymbol{\Omega}$. The solution of Eq. (2b) with the initial condition $\mathbf{S}(0)=\mathbf{S}_0$ can be written as

$$\mathbf{S}(t) = [\mathbf{n} \circ \mathbf{n} + (\mathbf{I} - \mathbf{n} \circ \mathbf{n}) \cos \Omega t + \sin \Omega t \mathbf{n} \times] \mathbf{S}_0, \quad (3)$$

where \mathbf{I} is the 3×3 unit matrix, $\boldsymbol{\Omega} = \Omega \mathbf{n}$, \mathbf{n} is a unit vector, $\Omega^2 = \boldsymbol{\Omega}^T \boldsymbol{\Omega}$, and $\mathbf{n} \circ \mathbf{n}$ denotes the outer or direct product, i.e., $(\mathbf{n} \circ \mathbf{n})_{ik} = n_i n_k$. Here the operator \mathbf{S}_0 on the right-hand side is in the Schrödinger picture, i.e., it is time independent. One can show that the usual commutation relations still hold: $[S_i(t), S_j(t)] = i\hbar \varepsilon_{ijk} S_k(t)$.

Inserting Eq. (3) into Eq. (2a) and solving the differential equation one finds

$$\mathbf{r}(t) = \mathbf{r}_0 + \frac{1}{\Omega} \mathbf{K}(\mathbf{n} \times \mathbf{S}_0) + \frac{d\varepsilon(\mathbf{p})}{d\mathbf{p}} t + (\mathbf{K}\mathbf{n})(\mathbf{n} \cdot \mathbf{S}_0) t + \frac{\sin \Omega t}{\Omega} \mathbf{K}(\mathbf{I} - \mathbf{n} \circ \mathbf{n}) \mathbf{S}_0 - \frac{\cos \Omega t}{\Omega} \mathbf{K}(\mathbf{n} \times \mathbf{S}_0), \quad (4)$$

with the initial condition $\mathbf{r}(0) = \mathbf{r}_0$. This is our central result. The interpretation of the different terms in Eq. (4) is as follows. The ZB stems from the oscillatory terms (cosine and sine terms). In contrast to the usual dynamics (first and third terms), two new terms appear in the nonoscillatory part: The transverse displacement, which is independent of time (second term), and a term that corresponds to a particle motion with constant anomalous velocity (fourth term). In addition to the oscillatory part, these two terms in $\mathbf{r}(t)$ are inherent of the ZB. The anomalous velocity plays a crucial role in the anomalous and spin Hall effects in semiconductors.²⁹

To evaluate the time-dependent position operator $\mathbf{r}(t)$ within a Gaussian wave packet, one can follow, e.g., the calculation presented in Refs. 5 and 6.

We are now in a position to apply our results to the systems listed in Table I. Using Eqs. (2c) and (4), some simple algebra yields the same results as given by Eqs. (7) and (8) in Ref. 6 for the Rashba-Dresselhaus system. Similarly, it is easy to verify the results Eqs. (41) and (42) in Ref. 6 for systems of heavy holes in a quantum well.³⁰

The current operator in graphene systems splits into three terms of which the last one can be associated with the ZB phenomenon.²³ Our general approach can also be applied to graphene layers to find the time evolution of the position operator $\mathbf{r}(t)$. We now present explicit results for the position operator $\mathbf{r}(t)$ from which the trembling (oscillatory) motion of the electron in graphene systems is clearly seen. For single-layer and bilayer graphene, the explicit formulas for $x(t)$ and $y(t)$ can again be easily obtained using Table I and Eqs. (2c) and (4). The results for single-layer graphene are

$$x(t) = x_0 + v\sigma_x t + \frac{p_y \hbar}{p^2 2} \sigma_z \left[1 - \cos\left(\frac{2pv}{\hbar} t\right) \right] + \frac{p_y \hbar}{p^3 2} (p_x \sigma_y - p_y \sigma_x) \left[\frac{2pv}{\hbar} t - \sin\left(\frac{2pv}{\hbar} t\right) \right], \quad (5a)$$

$$y(t) = y_0 + v\sigma_y t - \frac{p_x \hbar}{p^2 2} \sigma_z \left[1 - \cos\left(\frac{2pv}{\hbar} t\right) \right] - \frac{p_x \hbar}{p^3 2} (p_x \sigma_y - p_y \sigma_x) \left[\frac{2pv}{\hbar} t - \sin\left(\frac{2pv}{\hbar} t\right) \right], \quad (5b)$$

and for bilayer graphene

$$x(t) = x_0 + \frac{p_x \sigma_x + p_y \sigma_y}{m} t + \frac{p_y \hbar}{p^2} \sigma_z (1 - \cos \Omega t) - \frac{p_y \Sigma_G}{p^4} (\Omega t - \sin \Omega t), \quad (6a)$$

$$y(t) = y_0 + \frac{-p_y \sigma_x + p_x \sigma_y}{m} t - \frac{p_x \hbar}{p^2} \sigma_z (1 - \cos \Omega t) + \frac{p_x \Sigma_G}{p^4} (\Omega t - \sin \Omega t), \quad (6b)$$

$$\Sigma_G = \hbar [2p_x p_y \sigma_x - (p_x^2 - p_y^2) \sigma_y], \quad \Omega = \frac{p^2}{\hbar m}. \quad (6c)$$

Here σ_i are the Pauli matrices and $p^2 = p_x^2 + p_y^2$.

Similarly, using the Hamiltonian for Cooper pairs given in Table I, the following results are obtained:

$$\mathbf{r}(t) = \mathbf{r}_0 + \frac{\mathbf{p}}{m} \sigma_x t + \frac{\mathbf{p}}{m} \Sigma_C (\Omega t - \sin \Omega t) + \frac{\mathbf{p}}{m} \frac{\Delta}{E^2(p)} \frac{\hbar}{2} \sigma_y (1 - \cos \Omega t), \quad (7a)$$

$$E(p) = \sqrt{\left(\frac{p^2}{2m} - E_F\right)^2 + \Delta^2}, \quad \Omega = \frac{2E(p)}{\hbar}, \quad (7b)$$

$$\Sigma_C = \frac{\hbar}{2} \frac{\Delta}{E^3(p)} \left[\left(\frac{p^2}{2m} - E_F\right) \sigma_x - \Delta \sigma_z \right]. \quad (7c)$$

Here $p^2 = p_x^2 + p_y^2 + p_z^2$. One can show that these results agree with those presented in Ref. 4.

Similarly, some simple algebra yields the same results as in Refs. 3 and 15 for nearly free electrons listed in Table I (except that the off-diagonal elements are swapped in the latter reference). For bulk Dresselhaus systems (third row in Table I) the calculation is again straightforward but the results are rather cumbersome and not presented here.

Discussion. As mentioned above, the position operator $\mathbf{r}(t)$ in Eq. (4) is decomposed into a mean part and an oscillatory term. If one derives the position operator $\mathbf{r}(t)$ directly from $\mathbf{r}(t) = e^{iHt/\hbar} \mathbf{r}(0) e^{-iHt/\hbar}$ then such a decomposition can only be obtained using the Foldy-Wouthuysen transformation.^{4,31} In this transformation the operator $\mathbf{r}(t)$ is calculated in the basis of the eigenstates of Hamiltonian (1). It can be shown that for $S = \frac{1}{2}$ (with Pauli matrices) the eigenenergies $E_{\pm}(\mathbf{k})$ and the eigenstates $|\chi_{\pm}\rangle = |\chi_{\pm}\rangle e^{i\mathbf{k}\cdot\mathbf{r}}$ are given by

$$E_{\pm}(\mathbf{k}) = \varepsilon(\hbar\mathbf{k}) \pm \frac{\hbar}{2} |\boldsymbol{\Omega}(\hbar\mathbf{k})|, \quad (8a)$$

$$|\chi_{+}\rangle = \begin{pmatrix} \cos \frac{\Theta}{2} e^{-i\Phi/2} \\ \sin \frac{\Theta}{2} e^{i\Phi/2} \end{pmatrix}, \quad |\chi_{-}\rangle = \begin{pmatrix} -\sin \frac{\Theta}{2} e^{-i\Phi/2} \\ \cos \frac{\Theta}{2} e^{i\Phi/2} \end{pmatrix}, \quad (8b)$$

where Θ and Φ are the spherical polar angles of the vector $\boldsymbol{\Omega}(\hbar\mathbf{k})$ in \mathbf{k} space, and $|\mathbf{a}|$ is the magnitude of vector \mathbf{a} . However, for $S > \frac{1}{2}$, the Foldy-Wouthuysen transformation is more complicated. The advantage of our approach is that it

leads directly to the desired decomposition of the position operator $\mathbf{r}(t)$.

For pure Rashba coupling and for single-layer graphene the ZB can be interpreted as a consequence of the conservation of the total angular momentum $J_z = L_z + S_z$, where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum (see Ref. 6). However, in general, J_z is not a constant of motion, i.e., $[H, J] = \boldsymbol{\Omega} \times \mathbf{S} - \mathbf{p} \times \mathbf{KS} \neq 0$. As can be readily seen, this is the case, for example, for Rashba-Dresselhaus systems where $\alpha \neq 0$ and $\beta \neq 0$, or for heavy holes in a quantum well.

Finally, it should be mentioned that the ZB is related to the nontrivial behavior of the conductivity of single and bilayer graphenes²³ since the velocity operator (2a) does not commute with the Hamiltonian (1). The peculiar behavior of the spin Hall effect may also be related to the ZB.⁹

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