PHYSICAL REVIEW B **81**, 121417(R) (2010)

General theory of Zitterbewegung

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(Received 25 January 2010; revised manuscript received 9 March 2010; published 31 March 2010)

We derive a general and simple expression for the time dependence of the position operator of a multiband Hamiltonian with arbitrary matrix elements depending only on the momentum of the quasiparticle. Our result shows that in such systems the Zitterbewegung-type term related to a trembling motion of the quasiparticle, always appears in the position operator. Moreover, the Zitterbewegung is, in general, a *multifrequency* oscillatory motion of the quasiparticle. We derive a few alternative expressions for the amplitude of the oscillatory motion including that related to the Berry connection matrix. We present several examples to demonstrate how general and versatile our result is.

DOI: 10.1103/PhysRevB.81.121417 PACS number(s): 73.22.Pr, 03.65.Pm, 03.65.Vf, 71.70.Ej

Schrödinger in his original paper has predicted a "trembling" or in other words a rapid oscillatory motion of the center of the free wave packet for relativistic electron.[1] However, the Zitterbewegung is not strictly a relativistic effect[2–6] but can be observed in spintronic systems as well.[7] This work has initiated many other works[8–32] with an aim to demonstrate the appearance of the Zitterbewegung not only for relativistic Dirac electrons. In these works a common feature is that the oscillatory motion of the free particles can be described only by one frequency.

In our previous work we showed that for a wide class of Hamiltonians related to, for example, spintronic systems and graphene, the Zitterbewegung can be treated in a unified way.[33] Here the basic idea was that the Hamiltonian of several systems can be mapped to that modeling the precession of a virtual spin in an effective magnetic field. The coupled equations for this virtual spin precession and the orbital motion of the quasiparticle can easily be solved. Thus, the Zitterbewegung is arising because the virtual spin and the orbital motion for the quasiparticle are coupled. Our work suggests as natural question whether the phenomenon of the Zitterbewegung also arises for an even more general Hamiltonian.

In the present work we extend the Zitterbewegung phenomena to a broader class of quantum Hamiltonians for free (quasi-) particles. In particularly, we derive a general and simple expression for the time dependence of the position operator $\mathbf{x}(t)$ for a multiband Hamiltonian given by

$$H = \begin{pmatrix} H_{11}(\mathbf{p}) & H_{12}(\mathbf{p}) & \dots & H_{1n}(\mathbf{p}) \\ H_{21}(\mathbf{p}) & H_{22}(\mathbf{p}) & \dots & H_{2n}(\mathbf{p}) \\ \vdots & \vdots & \ddots & \vdots \\ H_{n1}(\mathbf{p}) & H_{n2}(\mathbf{p}) & \dots & H_{nn}(\mathbf{p}) \end{pmatrix}, \tag{1}$$

where each matrix element is a differentiable function of the momentum $\mathbf{p}$ of the particle itself and $n \geq 2$ is the number of degrees of freedom of the system. From our general expression for the position operator $\mathbf{x}(t)$ we shall show that (i) the Zitterbewegung always appears for systems given by Hamiltonian (1), (ii) for $n > 2$ the Zitterbewegung is in fact a *multicomponent* oscillatory motion of the free quasiparticle, (iii) for $n=2$ we recover the results obtained earlier in the abovementioned references.

To find the time dependence of the position operator $\mathbf{x}(t)$ of the quasiparticle in Heisenberg picture one needs to calculate

$$\mathbf{x}(t) = e^{(i/\hbar)Ht}\mathbf{x}(0)e^{-(i/\hbar)Ht}, \tag{2}$$

where $\mathbf{x}(0)$ is the position operator at $t=0$, i.e., it equals to the position operator in Schrödinger picture. Because the momentum operator $\mathbf{p}$ is a constant of motion we now work in the subspace of the Hilbert space for which the momentum $\mathbf{p}$ is fixed. Calculating the right-hand side of Eq. (2) the crucial step is to decompose Hamiltonian (1) into a sum of projection operators: $H=\Sigma_a E_a Q_a$, where E_a is the ath eigenvalue of the Hamilton operator at a given momentum $\mathbf{p}$, and Q_a are projection operators satisfying the following relations: $Q_a Q_b = \delta_{ab} Q_a$ and $\Sigma_a Q_a = I_n$, where I_n is the $n \times n$ unit matrix. The position operator at time $t=0$ in Schrödinger picture and in momentum representation is $\mathbf{x}(0)=i\hbar\frac{\partial}{\partial \mathbf{p}}$. Consider the operator $U=e^{-(i/\hbar)Ht}$ which is only a function of the momentum operator $\mathbf{p}$. Then Eq. (2) can be rewritten as

$$\begin{aligned} \mathbf{x}(t) &= U^{-1}\mathbf{x}(0)U \\ &= U^{-1}[\mathbf{x}(0),U] + U^{-1}U\mathbf{x}(0) \\ &= \mathbf{x}(0) + i\hbar U^{-1}\frac{\partial U}{\partial \mathbf{p}}, \end{aligned} \tag{3}$$

where we have made use the relation $[\mathbf{x}(0),F(\mathbf{p})]=i\hbar\frac{\partial F(\mathbf{p})}{\partial \mathbf{p}}$. Decomposition of Hamiltonian (1) into a sum of projection operators makes possible to write that $e^{\pm(i/\hbar)Ht} = \Sigma_a e^{\pm(i/\hbar)E_a t} Q_a$. Now, substituting these operators into Eq. (3) and using the orthogonality relations $Q_a Q_b = \delta_{ab} Q_a$ it yields the time dependence of the position operator,

$$\mathbf{x}(t) = \mathbf{x}(0) + \sum_a \mathbf{Z}_{aa} + t\sum_a \mathbf{V}_a Q_a + \sum_a \sum_{b\neq a} e^{i\omega_{ab}t}\mathbf{Z}_{ab}, \tag{4a}$$

where

$$\mathbf{V}_a(\mathbf{p}) = \frac{\partial E_a(\mathbf{p})}{\partial \mathbf{p}}, \quad \mathbf{Z}_{ab}(\mathbf{p}) = i\hbar Q_a \frac{\partial Q_b}{\partial \mathbf{p}}, \tag{4b}$$

and $\omega_{ab}=\frac{E_a-E_b}{\hbar}$ are the so-called *beating frequencies*. Here we call $\mathbf{V}_a$ as *partial velocities* and $\mathbf{Z}_{ab}$ as *Zitterbewegung amplitudes*. This is our central result in this work.

The interpretation of the different terms in Eq. (4) is as follows. The first term is the initial position of the quasiparticle. In contrast to the usual dynamics (for systems with one degree of freedom), the second and the fourth term are entirely new. The second term is a displacement of the position operator independent of time. The third term describes the motion of the quasiparticle with constant velocity which is, in general, not equal to any of the partial velocities $\mathbf{V}_a$. Finally, the Zitterbewegung stems from the last, oscillatory term which describes the oscillatory motion of the quasiparticle. The phenomenon of Zitterbewegung is similar to the beating effect with different frequencies in the classical wave mechanics. The Zitterbewegung is a direct consequence of the coupling of different energy eigenstates for systems with more than one degree of freedom. These terms in $\mathbf{x}(t)$ are inherent of the Zitterbewegung and are expressed via the projection operator Q_a related to the given Hamiltonian.

Equation (4) is the most general form for describing the phenomenon of the Zitterbewegung. Our result shows explicitly that the oscillatory motion [the last term in Eq. (4a)] is a superposition of individual oscillatory motions with frequencies corresponding to all possible differences of the energy eigenvalues of Hamiltonian (1). Thus in the most general case the Zitterbewegung describes a *multifrequency* oscillatory motion of the quasiparticle. This multifrequency behavior of the Zitterbewegung has first been shown by Winkler *et al.* in Ref. 19 for two specific systems, namely, for the Kane model and Landau-Rashba Hamiltonian. However, the most clear manifestation of this multifrequency behavior of the Zitterbewegung for the general Hamiltonian (1) can be seen only in our main result (4). In general, the Zitterbewegung cannot be described by only one frequency (this is the case only for systems with two different eigenenergies) but all of the differences between the different energy eigenvalues corresponding to the beating frequencies appear in the time dependence of the position operator.

Sometimes in the explicit calculation of the position operator $\mathbf{x}(t)$ it is more useful to use a different form for the Zitterbewegung amplitudes $\mathbf{Z}_{ab}$ given by Eq. (4). Taking the derivative of the Hamilton operator $H=\Sigma_c E_c Q_c$ and the orthogonality relation $Q_c Q_b = \delta_{cb} Q_b$ with respect to the momentum $\mathbf{p}$ one can easily show that (for details see Ref. 34)

$$\mathbf{Z}_{ab} = i\hbar \frac{Q_a \dfrac{\partial H}{\partial \mathbf{p}} Q_b}{E_b - E_a}, \tag{5}$$

valid for $a \neq b$. Thus in the calculation of the Zitterbewegung amplitudes instead of knowing the derivative of the projection operators with respect to the momentum one needs to take only the derivative of the Hamiltonian. Another form of the position operator $\mathbf{x}(t)$ is given in Ref. 34.

We now consider several examples to demonstrate how versatile our result is to study different systems known in the literature (for more details see Ref. 34). Regarding the Zitterbewegung most of the systems studied in the literature are described by a Hamiltonian with only two different eigenvalues.[1–33] In such systems either the Hamiltonian itself is a 2×2 matrix or the dimension of the Hilbert space is more than 2 but the eigenvalues are degenerate and the Hamiltonian has only two different eigenvalues. Thus for such systems it is useful to derive an alternative form for the time dependence of the position operator given by Eq. (4). Now the Hamiltonian in terms of projectors reads $H=E_+Q_+ + E_-Q_-$, where $Q_\pm$ are the projection operators satisfying the usual relations mentioned above and $E_\pm$ are the two eigenvalues of H. Introducing the operator $T=Q_+ - Q_-$ it is obvious that $T^2=I$. Note that in the mathematical literature the operators satisfying this relation are called involutary operator related to the mirror image in geometry. The Hamiltonian can be rewritten as $H=\varepsilon I + (\hbar\omega/2)T$, where $\varepsilon=(E_+ + E_-)/2$ and $\omega=(E_+ - E_-)/\hbar$. Moreover, it is clear that $Q_\pm = (I \pm T)/2$. Then using Eq. (4) one can easily show that

$$\mathbf{x}(t) = \mathbf{x}(0) + \mathbf{W}t + \mathbf{Z}(t), \tag{6a}$$

where

$$\mathbf{W} = \frac{\partial \varepsilon}{\partial \mathbf{p}} I + \frac{1}{2}\frac{\partial \hbar\omega}{\partial \mathbf{p}} T, \tag{6b}$$

$$\mathbf{Z}(t) = \frac{\hbar}{2}\sin(\omega t)\frac{\partial T}{\partial \mathbf{p}} + \frac{i\hbar}{2}[1-\cos(\omega t)]T\frac{\partial T}{\partial \mathbf{p}}. \tag{6c}$$

From this result it is clear that in the oscillatory part of $\mathbf{x}(t)$ there is only one frequency component.

Equation (5) can easily be applied to the original Schrödinger's Zitterbewegung and we find the same results as that by Schrödinger.[34] Another example is the Luttinger Hamiltonian[35,36] given by

$$H = \frac{1}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)\mathbf{p}^2 - 2\gamma_2(\mathbf{pS})^2\right], \tag{7}$$

where $\mathbf{p}=(p_x,p_y,p_z)$ is the vector of the momentum operators, $\mathbf{S}=(S_x,S_y,S_z)$ represents the spin operator with spin 3/2, m and $\gamma_{1,2}$ are parameters of the model. Using Eq. (5) the position operator for Luttinger Hamiltonian can easily be derived (for more details see Ref. 34),

$$\begin{aligned}\mathbf{x}(t) = \mathbf{x}(0) &+ \left[\frac{\gamma_1 + \frac{5}{2}\gamma_2}{m} I_4 - \frac{2\gamma_2}{m}\frac{(\mathbf{pS})^2}{\mathbf{p}^2}\right]\mathbf{p}\, t + \sin(\omega t) \\ &\times\left[\frac{\mathbf{p}(\mathbf{pS})^2}{\mathbf{p}^4} - \frac{\mathbf{S}(\mathbf{pS}) + (\mathbf{pS})\mathbf{S}}{2\mathbf{p}^2}\right] + [1-\cos(\omega t)] \\ &\times\frac{(\mathbf{p}\times\mathbf{S})(\mathbf{pS})^2 + 2(\mathbf{pS})(\mathbf{p}\times\mathbf{S})(\mathbf{pS}) + (\mathbf{pS})^2(\mathbf{p}\times\mathbf{S})}{4\mathbf{p}^4},\end{aligned} \tag{8}$$

where $\omega=E_+ - E_- = (2\gamma_2/m)\mathbf{p}^2$. Note that this result agrees with that obtained by Winkler *et al.* in Ref. 19, and by Schliemann in a private communication using a direct calculation of the right-hand side of Eq. (2).

We also consider a nontrivial example for the Zitterbewegung not known in the literature, namely, the Zitterbewegung for bilayer graphene. The Hamiltonian for bilayer graphene in the four by four representation is given in Refs. 37 and 38. Including the trigonal warping[38–40] the position operator $\mathbf{x}(t)$ is more cumbersome but its structure and the steps of the derivation are similar to the case when the trigonal warping is omitted. Therefore, we now neglect the trigonal warping. The position operator $\mathbf{x}(t)$ can be derived using Eq. (4) but to obtain the Zitterbewegung amplitudes it is more effective to use Eq. (5). The results is quite lengthy thus here we only refer to Ref. 34 for more details. This is a nontrivial example for the Zitterbewegung. Since the Hamiltonian for bilayer graphene has four different eigenvalues, we have six values of the energy differences. However out of these six values there are only four different ones. Therefore, the number of beating frequencies is only four. In this example it is clear that the oscillatory motion of the electron is a superposition of individual oscillatory motions with *four* different frequencies.

Recently, for specific systems the connection between the Zitterbewegung and the Berry phase has been noticed and investigated by Vaishnav and Clark,[23] and Englman and Vértesi.[28] We now show that the oscillatory terms, i.e., the Zitterbewegung amplitudes in the position operator have a close relation to the *Berry connection matrix* appearing in the expression of the well-known Berry phase[41] even for a general Hamiltonian (1). To this end we present another form for position operator in terms of the eigenvectors of the Hamiltonian.

The projection operator can be expressed via the eigenvectors $|u_{a,s}(\mathbf{p})\rangle$ of the Hamiltonian operator: $Q_a(\mathbf{p})=\Sigma_s|u_{a,s}(\mathbf{p})\rangle\langle u_{a,s}(\mathbf{p})|$, where s denotes the different eigenvectors in a subspace with the same energy eigenvalue E_a. Then Eq. (4) can be rewritten as

$$\mathbf{x}(t) = \mathbf{x}(0) + t\sum_k \mathbf{V}_k|u_k(\mathbf{p})\rangle\langle u_k(\mathbf{p})| + \sum_{k,l}(e^{i\omega_{kl}t}-1)\mathbf{A}_{kl}(\mathbf{p})|u_k(\mathbf{p})\rangle\langle u_l(\mathbf{p})|, \tag{9a}$$

where

$$\mathbf{A}_{kl}(\mathbf{p}) = i\hbar\langle u_k(\mathbf{p})|\frac{\partial}{\partial \mathbf{p}}|u_l(\mathbf{p})\rangle. \tag{9b}$$

Here $\mathbf{A}_{kl}$ is the so-called *Berry connection matrix*. The index k labels the eigenvectors of the Hamiltonian with taking into account their multiplicity.

For systems with precessing spin in an effective magnetic field it turns out that to study the Zitterbewegung Eq. (9) is more appropriate than Eq. (4). This is demonstrated in Ref. 34 where we find the same result for the position operator as that we derived before using a different approach.[33]

So far we concentrate on the structure of the Zitterbewegung for general Hamiltonian (1). However, the observation of the Zitterbewegung experimentally is more difficult problem. It is well known that the spatial size of the trembling motion of the relativistic electron predicted by Schrödinger is of the order of Compton wavelength and its frequency is far beyond the present experimental possibilities.[1] The experimental observation of the Zitterbewegung in the nonrelativistic quantum regime such as in semiconductors with spin-orbit couplings[7] is much more promising. For example, Vaishnav and Clark,[23] and Merkl *et al.*[31] have proposed an experiment for observing Zitterbewegung using ultracold atoms, while Rusin and Zawadzki have proposed an experiment for observing Zitterbewegung probed by femtosecond laser pulses in graphene.[32] Very recently, Gerritsma *et al.*[42] have performed a quantum simulation of the Dirac equation using a single trapped ion and observed the Zitterbewegung.

One of the difficulty of observing the Zitterbewegung is the lack of time resolved probes. The initial state, in general, is a superposition of different momentum eigenstates: $|\Psi_0\rangle=\int d^3\mathbf{p}\Sigma_k c_k(\mathbf{p})|u_k(\mathbf{p})\rangle$. Therefore, the expectation value is $\bar{\mathbf{x}}(t)=\langle\Psi_0|\mathbf{x}(t)|\Psi_0\rangle=\int d^3\mathbf{p}\Sigma_{k,l}c_k^*(\mathbf{p})c_l(\mathbf{p})\langle u_k(\mathbf{p})|\mathbf{x}(t)|u_l(\mathbf{p})\rangle$ which involves the integration over the momentum $\mathbf{p}$. Since in Eq. (4) the beating frequencies $\omega_{kl}(\mathbf{p})$ depend on the momentum $\mathbf{p}$ the integration over the momentum $\mathbf{p}$ in $\bar{\mathbf{x}}(t)$ may result in a strong suppression of the Zitterbewegung in time. This problem can be circumvented if at least one beating frequency is independent of the momentum $\mathbf{p}$ of the quasiparticle. This is the case, for example, for bilayer graphene as shown by the authors of the present paper.[34] One beating frequency is constant and in the detectable regime $\omega=\gamma_1/\hbar\sim 0.6\ \text{fs}^{-1}$, where $\gamma_1\sim 0.4\ \text{eV}$ is the strongest interlayer coupling between two carbon atoms that are on the top of each other.[37–40] The amplitudes of the trembling motion will be investigated in the near future. Our main aim in this Rapid Communication is to establish a general theory for the Zitterbewegung. On the other hand our general theory can be a good starting point to search for systems that are realistic for experimental observation of the Zitterbewegung.

We presented a general theory for Zitterbewegung and derived a general and simple expression for the position operator $\mathbf{x}(t)$ in Heisenberg picture and in momentum representation, and for a given system it can easily be calculated. In contrast to systems studied in the literature[1–5,7–16,19–33] the Zitterbewegung is a universal phenomenon and it always appears in the quantum dynamics of a system of quasiparticle with more than one degree of freedom. Our main result (4) shows that the Zitterbewegung, in general, is a multifrequency beating effect in Heisenberg picture and has a close relation to the Berry connection. We believe that our work presented here provides a better understanding and experimental guide for the Zitterbewegung studied intensively in the literature.

We acknowledge fruitful discussions with J. Schliemann, U. Zülicke, T. Geszti, and G. Széchenyi. Supported by the Hungarian Science Foundation OTKA under the Contract No. 75529.

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