

Zitterbewegung of electrons and holes in III–V semiconductor quantum wellsJohn Schliemann,^{1,2} Daniel Loss,² and R. M. Westervelt³¹*Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany*²*Department of Physics and Astronomy, University of Basel, CH-4056 Basel, Switzerland*³*Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA*

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The notion of *zitterbewegung* is a long-standing prediction of relativistic quantum mechanics. Here we extend earlier theoretical studies on this phenomenon for the case of III–V zinc-blende semiconductors which exhibit particularly strong spin-orbit coupling. This property makes nanostructures made of these materials very favorable systems for possible experimental observations of *zitterbewegung*. Our investigations include electrons in *n*-doped quantum wells under the influence of both Rashba and Dresselhaus spin-orbit interactions, and also the two-dimensional hole gas. Moreover, we give a detailed analysis of electron *zitterbewegung* in quantum wires which appear to be particularly suited for experimentally observing this effect.

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I. INTRODUCTION

The spin degree of freedom of electrons in semiconductor nanostructures is one of the central subjects in the growing field of spin electronics.¹ The latter keyword describes the whole variety of efforts and proposals for using the electron spin instead of, or in combination with, its charge for information processing, or, even more ambitious, quantum information processing. A central issue is the possibility of *electrical* control electron spins, which avoids many difficulties arising from applying and gating magnetic fields. Zinc-blende III–V semiconductors show a particularly strong spin-orbit interaction and are therefore natural candidates with respect to the above goals.

In the present paper we extend earlier results on the relativistic effect of *zitterbewegung* in systems of the above type.² In this context we also discuss related recent work by other authors.^{3–8} Our investigations include electrons in *n*-doped quantum wells under the influence of both Rashba and Dresselhaus spin-orbit interactions, and holes in two-dimensional geometry. Phenomena related to spin-orbit coupling in such systems are presently studied very intensively also in the context of the intrinsic spin-Hall effect.^{9–11} Particular attention is paid to the case of electron *zitterbewegung* in quantum wires which appear to be good candidates for experimental investigations of this effect.

The coupling between the orbital and the spin degree of freedom of electrons is a relativistic effect described by the Dirac equation and its nonrelativistic expansion in powers of the inverse speed of light c .¹² In second order, one obtains, apart from two spin-independent contributions, the following well-known spin-orbit coupling term,

$$\mathcal{H}_{so} = \frac{1}{2m_0c^2} \vec{s} \cdot \left(\nabla V \times \frac{\vec{p}}{m_0} \right), \quad (1)$$

where m_0 is the bare mass of the electron, \vec{s} , \vec{p} its spin and momentum, respectively, and V is some applied external potential. On the other hand, the free Dirac equation, $V=0$, has two dispersion branches with positive and negative energy,

$$\varepsilon(\vec{p}) = \pm \sqrt{m_0^2c^4 + c^2p^2}, \quad (2)$$

which are separated by an energy gap of $2m_0c^2 \approx 1$ MeV. In particular, the nonrelativistic expansion of the Dirac equation quoted above can be seen as a method of systematically including the effects of the negative-energy solutions on the states of positive energy starting from their nonrelativistic limit.¹² Moreover, the large energy gap $2m_0c^2$ appears in the denominator of the right-hand side of Eq. (1), suppressing the effects of spin-orbit coupling for weakly bound electrons.

On the other hand, the band structure of zinc-blende III–V semiconductors shows many formal similarities to the situation of free relativistic electrons, while the relevant energy scales are grossly different.^{13–15} For not too large doping of such semiconductors, one can concentrate on the band structure around the Γ point. Here one has a parabolic *s*-type conduction band and a *p*-type valence band consisting of the well-known dispersion branches for heavy and light holes, and the split-off band. However, the gap between conduction and valence band is of order 1 eV or smaller. This heuristic argument makes plausible that spin-orbit coupling is an important effect in III–V semiconductors which actually lies at the very heart of the field of semiconductor spintronics.

Dating back to a seminal paper by Schrödinger^{16,17} from 1930, the notion of *zitterbewegung* has been a long-standing theoretical prediction of relativistic quantum mechanics. In the free Dirac equation, this oscillatory quantum motion occurs for particle wave packets which are superpositions of both solutions of positive and negative energy. Thus, the dominant frequency of this dynamics is given by $2m_0c^2/\hbar$ which is of order 10^{20} Hz. Moreover, the length scale of this motion is given by the Compton wavelength \hbar/m_0c of the free electron. Therefore, in order to experimentally observe the *zitterbewegung* of free electrons, one would need to confine these objects on a length scale of a few picometers. Now it follows from general uncertainty arguments that such a spatial confinement leads to an energy scale where electron-positron pair production plays a serious and detrimental role. These arguments have led many authors to the opinion that

the *zitterbewegung* of electrons is impossible to observe; see, e.g., Ref. 18.

Most recently, we have theoretically investigated *zitterbewegung* in III–V zinc-blende semiconductors and developed a proposal for its experimental observation. As already mentioned, the mathematical treatment of effective band structure models relevant to such systems on the one hand, and the nonrelativistic expansion of the Dirac equation on the other hand, show many formal similarities.^{13–15} In fact, under certain aspects, the low-energy band structure of such semiconductors around the Fermi level can be viewed as a model for truly relativistic electrons, but with energy and length scales which are much more favorable for observing effects like *zitterbewegung*.

This paper is organized as follows. In Sec. II we study *zitterbewegung* in the two-dimensional electron gas. We extend previous results² to the situation where spin-orbit coupling of both the Rashba and Dresselhaus types is present. Moreover, we give a deeper discussion of *zitterbewegung* in quantum wires and our related experimental proposal. Section III is devoted to the same phenomenon for heavy holes in two-dimensional quantum wells. We close with conclusions in Sec. IV.

II. ZITTERBEWEGUNG IN THE TWO-DIMENSIONAL ELECTRON GAS AND IN QUANTUM WIRES

A. The two-dimensional electron gas

For conduction band electrons in n -doped quantum wells of zinc-blende semiconductor structures, the dominant effects of spin-orbit interaction can be described in terms of two effective contributions to the Hamiltonian. One of them is the Rashba spin-orbit term¹⁹ which is due to the inversion-asymmetry of the confining potential and has the form

$$\mathcal{H}_R = \frac{\alpha}{\hbar}(p_x\sigma^y - p_y\sigma^x), \quad (3)$$

where \vec{p} is the momentum of the electron confined in a two-dimensional geometry, and $\vec{\sigma}$ the vector of Pauli matrices. The coefficient α is tunable in strength by the external gate perpendicular to the plane of the two-dimensional electron gas. The other contribution is the Dresselhaus spin-orbit term which is present in semiconductors lacking bulk inversion symmetry.²⁰ When restricted to a two-dimensional semiconductor nanostructure grown along the [001] direction this coupling is of the form^{21,22}

$$\mathcal{H}_D = \frac{\beta}{\hbar}(p_y\sigma^y - p_x\sigma^x), \quad (4)$$

where the coefficient β is determined by the semiconductor material and the geometry of the sample. These two contributions to the effective Hamiltonian have also an interesting interplay.^{23,24}

We now consider the single-particle Hamiltonian of a free electron under the influence of spin-orbit coupling of both the Rashba and the Dresselhaus types,

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + \mathcal{H}_R + \mathcal{H}_D, \quad (5)$$

where m is the effective band mass. The components of the time-dependent position operator

$$\vec{r}_H(t) = e^{i\mathcal{H}t/\hbar}\vec{r}(0)e^{-i\mathcal{H}t/\hbar} \quad (6)$$

in the Heisenberg picture read explicitly

$$\begin{aligned} x_H(t) = & x(0) + \frac{p_x}{m}t + \left(\frac{\alpha}{\hbar}\sigma^y - \frac{\beta}{\hbar}\sigma^x\right)t \\ & + \frac{\alpha^2 - \beta^2}{\Lambda^2}p_y \left[1 - \cos\left(\frac{2}{\hbar^2}\Lambda t\right)\right] \frac{\hbar}{2}\sigma^z \\ & - \frac{\alpha^2 - \beta^2}{\Lambda^3}p_y \left[\frac{2}{\hbar^2}\Lambda t - \sin\left(\frac{2}{\hbar^2}\Lambda t\right)\right] \Sigma, \end{aligned} \quad (7)$$

$$\begin{aligned} y_H(t) = & x(0) + \frac{p_y}{m}t - \left(\frac{\alpha}{\hbar}\sigma^x - \frac{\beta}{\hbar}\sigma^y\right)t \\ & - \frac{\alpha^2 - \beta^2}{\Lambda^2}p_x \left[1 - \cos\left(\frac{2}{\hbar^2}\Lambda t\right)\right] \frac{\hbar}{2}\sigma^z \\ & + \frac{\alpha^2 - \beta^2}{\Lambda^3}p_x \left[\frac{2}{\hbar^2}\Lambda t - \sin\left(\frac{2}{\hbar^2}\Lambda t\right)\right] \Sigma, \end{aligned} \quad (8)$$

with

$$\Lambda^2(\vec{p}; \alpha, \beta) = (\alpha^2 + \beta^2)p^2 + 4\alpha\beta p_x p_y \quad (9)$$

and

$$\Sigma(\vec{p}, \vec{\sigma}; \alpha, \beta) = \frac{\hbar}{2}(\alpha(p_x\sigma^x + p_y\sigma^y) + \beta(p_x\sigma^y + p_y\sigma^x)). \quad (10)$$

Here the operators \vec{p} and $\vec{\sigma}$ on the right-hand sides are in the Schrödinger picture and therefore time independent.

The oscillatory terms on the right-hand sides of Eqs. (7) and (8) can be viewed as the *zitterbewegung* the electron performs under the influence of spin-orbit coupling. This oscillatory quantum motion vanishes if relativistic effects are absent, $\alpha = \beta = 0$. The contributions linear in time t in the first lines in Eqs. (7) and (8) are just proportional to the velocity

$$\vec{v} = \frac{i}{\hbar}[\mathcal{H}, \vec{r}], \quad (11)$$

which is in the presence of spin-orbit coupling a spin-dependent operator. The expressions (7) and (8) contain the results given in Ref. 2 for pure Rashba or Dresselhaus coupling as special cases. For instance, if only Rashba coupling is present ($\beta = 0$), one can express the position operator in the Heisenberg picture as

$$\begin{aligned}
x_H(t) = & x(0) + \frac{p_x}{m}t + \frac{p_y}{p^2} \frac{\hbar}{2} \sigma^z \left[1 - \cos\left(\frac{2\alpha p}{\hbar^2}t\right) \right] \\
& + \frac{p_x}{p^3} \frac{\hbar}{2} (p_x \sigma^y - p_y \sigma^x) \left[\frac{2\alpha p}{\hbar^2}t - \sin\left(\frac{2\alpha p}{\hbar^2}t\right) \right] \\
& + \frac{1}{p} \frac{\hbar}{2} \sigma^y \sin\left(\frac{2\alpha p}{\hbar^2}t\right), \quad (12)
\end{aligned}$$

$$\begin{aligned}
y_H(t) = & y(0) + \frac{p_y}{m}t - \frac{p_x}{p^2} \frac{\hbar}{2} \sigma^z \left[1 - \cos\left(\frac{2\alpha p}{\hbar^2}t\right) \right] \\
& + \frac{p_y}{p^3} \frac{\hbar}{2} (p_x \sigma^y - p_y \sigma^x) \left[\frac{2\alpha p}{\hbar^2}t - \sin\left(\frac{2\alpha p}{\hbar^2}t\right) \right] \\
& - \frac{1}{p} \frac{\hbar}{2} \sigma^x \sin\left(\frac{2\alpha p}{\hbar^2}t\right). \quad (13)
\end{aligned}$$

The case $\alpha = \pm\beta$ is particular.^{23,24} As seen from Eqs. (7) and (8), the oscillatory part of the time-dependent position operator, i.e., the *zitterbewegung*, vanishes due to the prefactor $(\alpha^2 - \beta^2)$. Physically, this observation results from an additional conserved quantity arising at this point.^{23,24}

It is straightforward to evaluate the above time-dependent position operators within Gaussian wave packets. For simplicity we concentrate on the case of pure Rashba coupling described by Eqs. (12) and (13). We consider a Gaussian wave packet with initial spin polarization along the z direction perpendicular to the quantum well,

$$\langle \vec{r} | \psi \rangle = \frac{1}{2\pi} \frac{d}{\sqrt{\pi}} \int d^2k e^{-(1/2)d^2(\vec{k} - \vec{k}_0)^2} e^{i\vec{k}\vec{r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (14)$$

Clearly we have $\langle \psi | \vec{r} | \psi \rangle = 0$, $\langle \psi | \vec{p} | \psi \rangle = \hbar \vec{k}_0$, and the variances of the position and momentum operators are $(\Delta x)^2 = (\Delta y)^2 = d^2/2$, $(\Delta p_x)^2 = (\Delta p_y)^2 = \hbar^2/2d^2$. Thus, the group velocity of the wave packet is given by $\hbar \vec{k}_0/m$, while its spatial width is described by the parameter d with the minimum uncertainty product typical for Gaussian wave packets, $\Delta p_x \Delta x = \Delta p_y \Delta y = \hbar/2$.

A direct calculation gives

$$\begin{aligned}
\langle \psi | x_H(t) | \psi \rangle = & \frac{\hbar k_{0x}}{m} + \frac{d}{2\pi} e^{-d^2 k_0^2} \int_0^{2\pi} d\varphi \sin \varphi \\
& \times \int_0^\infty dq e^{-q^2 + 2dq(k_{0x} \cos \varphi + k_{0y} \sin \varphi)} \\
& \times \left[1 - \cos\left(\frac{2\alpha q}{\hbar d}t\right) \right]. \quad (15)
\end{aligned}$$

In the above expression q is a dimensionless integration variable. The remaining integration over the polar angle φ gives a vanishing result if $k_{0y} = 0$, i.e., if the group velocity is along the x direction. More generally, one finds that

$$\langle \psi | \vec{k}_0 \cdot \vec{r}_H(t) / k_0 | \psi \rangle = \frac{\hbar k_0}{m} t, \quad (16)$$

which means that the *zitterbewegung* is always perpendicular to the group velocity of the wave packet. The same observa-

tion is made for the case of pure Dresselhaus coupling, $\alpha = 0$. Note that for pure Rashba coupling the sum of the z component of the orbital angular momentum $\vec{l} = \vec{r} \times \vec{p}$ and the z component of the spin $\vec{s} = \hbar \vec{\sigma}/2$ is a conserved quantity, $[\mathcal{H}, l^z + s^z] = 0$, while for pure Dresselhaus coupling we have $[\mathcal{H}, l^z - s^z] = 0$. In the presence of these conservation laws, the *zitterbewegung* can also be interpreted as a consequence of spin rotation due to spin-orbit coupling. Consider, for instance, an electron moving along the y direction with its spin being initially aligned with the z direction. In the time evolution of the particle, the spin will then be rotated due to spin-orbit coupling which requires, by virtue of the conservation law, also a finite component l^z to develop, i.e., the electron has to perform also a movement perpendicular to its group velocity. In the general case $\alpha \neq 0 \neq \beta$, such an interpretation does not seem to be possible since a conserved quantity of the above kind does not exist.

Let us turn back to the case of pure Rashba coupling. Without loss of generality we consider an electron wave packet moving along the y direction, $k_{0x} = 0$. By expanding the exponential containing the trigonometric functions in Eq. (15), one derives²⁵

$$\begin{aligned}
\langle \psi | x_H(t) | \psi \rangle = & \frac{1}{2k_{0y}} (1 - e^{-d^2 k_{0y}^2}) - \frac{1}{k_{0y}} e^{-d^2 k_{0y}^2} \\
& \times \sum_{n=0}^{\infty} \left[\frac{(dk_{0y})^{2(n+1)}}{n!(n+1)!} \int_0^\infty dq q^{2n+1} e^{-q^2} \cos\left(\frac{2\alpha q}{\hbar d}t\right) \right]. \quad (17)
\end{aligned}$$

Thus, the amplitude of the *zitterbewegung* is proportional to the wavelength $\lambda_{0y} = 2\pi/k_{0y}$ of the electron motion perpendicular to it. In a semiconductor quantum well, this length can be of order of a few ten nanometers, which is several orders of magnitude larger than the length scale of the *zitterbewegung* of free electrons given by the Compton wavelength. Note also that the oscillatory *zitterbewegung* changes its sign if the translational motion is reversed.

If the product dk_{0y} is not too large, $dk_{0y} \lesssim 1$, only low values of the summation index n in Eq. (17) lead to substantial contributions, and the Gaussian factor in the integrand suppresses contributions from large values of q . Thus, a typical scale of this integration variable is leading to sizable contributions is $q \approx 1/\sqrt{2}$. Thus, a typical time scale in the integrand is $T = \sqrt{2}\pi\hbar d/\alpha$, and when averaging the *zitterbewegung* over time scales significantly larger than T , the cosine term drops, giving

$$\overline{\langle \psi | x_H(t) | \psi \rangle} = \frac{1}{2k_{0y}} (1 - e^{-d^2 k_{0y}^2}), \quad (18)$$

i.e., the time-averaged guiding center of the wave packet is shifted perpendicular to its direction of motion. Note that the *zitterbewegung* is absent for $k_{0y} = 0$.¹⁸

In the opposite case $dk_{0y} \gg 1$ the Gaussian approaches a δ function. In this limit one finds (for $k_{0x} = 0$)

$$\langle \psi | x_H(t) | \psi \rangle = \frac{1}{2k_{0y}} \left[1 - \cos\left(\frac{2\alpha k_{0y}}{\hbar}t\right) \right]. \quad (19)$$

Here the frequency of the *zitterbewegung* is $\Omega=2ak_{0y}/\hbar$, and the guiding center of the wave packet is also shifted in the direction perpendicular to its group velocity. Note that $\hbar\Omega$ is the excitation energy between the two branches of the Rashba Hamiltonian \mathcal{H} at a given momentum $\vec{k}=k_{0y}\vec{e}_y$. Rashba spin-orbit coupling is particularly strong in InAs where values for the parameter α of a few 10^{-11} eV m can be reached,^{26–32} leading to frequencies Ω in the terahertz regime. This is much smaller than the typical frequency of the *zitterbewegung* of free electrons which is of order 10^{20} Hz. For GaAs, the Rashba coefficient is typically an order of magnitude smaller than in InAs (Ref. 33) and the Dresselhaus coupling plays a more important role.^{34–36} In summary, the *zitterbewegung* of electronic wave packets in semiconductor quantum wells as discussed above is characterized by amplitudes and frequencies which are by orders of magnitude larger and smaller, respectively, than it is the case for free electrons. This opens the perspective to experimentally observe the electron *zitterbewegung* in semiconductor nanostructures via terahertz methods, or using high-resolution scanning-probe microscopy imaging techniques as developed and discussed in Refs. 37 and 38. The latter approach will be described in more detail in Sec. II B.

The issue of *zitterbewegung* of electrons in III–V semiconductors was also discussed recently by Zawadzki where the three-dimensional bulk case was considered.⁴ The author starts from an 8×8 Kane model for conduction and with the valence band being diagonal in the hole sector.^{14,39} Specializing on particles moving along the z direction in real space and neglecting the split-off band, the author obtains an effective Hamiltonian coupling only light holes and conduction band electron states. Moreover, for an appropriate choice of basis this Hamiltonian matrix mimics the Hamiltonian of the free Dirac equation, which enables one to derive a *zitterbewegung* directly following Schrödinger’s original approach.^{16,17} However, when reducing the underlying 8×8 Kane model in a systematic way to an effective 2×2 Hamiltonian for conduction band electrons only, one obtains in the absence of an additional potential and magnetic fields to second order in the gap energy only a kinetic term involving an effective mass depending on band structure parameters.¹⁴ This is analogous to the situation of the free Dirac equation where, again in the absence of external fields, the lowest order relativistic correction is an additional contribution to the kinetic energy which does not lead to *zitterbewegung*.¹² The *zitterbewegung* studied in the present work occurs, for the case of Rashba coupling, due to an external potential introducing structure-inversion asymmetry.^{14,19} For the case of Dresselhaus coupling, it stems from the bulk Dresselhaus coupling term which results from bulk-inversion asymmetry²⁰ and is not included in the 8×8 Kane model. In this sense, Zawadzki’s result appears to be an effect of higher order in the inverse gap energy which can be of importance in materials with particularly small gap such as InSb.³⁹ Moreover, the *zitterbewegung* as discussed in Ref. 4 always occurs in the direction of the group velocity of the particle wave packet, i.e., in the z direction. This feature is clearly different from the *zitterbewegung* investigated here and might pose an obstacle against experimentally observing this effect.

B. Quantum wires

The *zitterbewegung* of an electron in a quantum well as described above is naturally accompanied by a broadening of the wave packet, where the dominant contribution stems from the dispersive effective-mass term in the Hamiltonian. Such a broadening might pose an obstacle for experimentally detecting the *zitterbewegung*. However, the broadening can be efficiently suppressed and limited if the electron moves along a quantum wire. In fact, the motion of electrons in quantum wells is generally under better control if additional lateral confinement is present. We therefore consider a harmonic quantum wire along the y direction described by

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + \frac{1}{2}m\omega^2x^2 + \mathcal{H}_R, \quad (20)$$

where the frequency ω parametrizes the confining potential perpendicular to the wire.^{40,41} It is instructive to write the Hamiltonian in the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \quad (21)$$

with

$$\mathcal{H}_0 = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + \frac{\hbar^2 k_{0y}^2}{2m} + \alpha k_{0y} \sigma^x, \quad (22)$$

$$\mathcal{H}_1 = -i \sqrt{\frac{\hbar m \omega \alpha}{2}} \frac{\alpha}{\hbar} (a - a^\dagger) \sigma^y. \quad (23)$$

Here a , a^\dagger are the usual harmonic climbing operators, and k_{0y} is the component of the electron wave vector along the quantum wire. Due to the properties of the “mixing operator” \mathcal{H}_1 , analytical progress as before without employing further approximations does not seem to be possible. We therefore project the Hamiltonian \mathcal{H} onto the lowest two orbital subbands. This approximation is known to give very reasonable results for not too wide quantum wells,⁴¹ and we will also compare its results with a full numerical simulation of the above multi-band Hamiltonian.

For a given k_{0y} the truncated Hilbert space is spanned by the states $|0, \uparrow\rangle$, $|0, \downarrow\rangle$, $|1, \uparrow\rangle$, $|1, \downarrow\rangle$, where the arrows denote the spin state with respect to the z direction, and 0 and 1 stand for the ground state and the first excited state of the harmonic potential, respectively. In the above basis, the truncated Hamiltonian reads

$$\mathcal{H} = \begin{pmatrix} \varepsilon_0 & -\alpha k_{0y} & 0 & -\sqrt{\frac{\hbar\omega\varepsilon_R}{2}} \\ -\alpha k_{0y} & \varepsilon_0 & \sqrt{\frac{\hbar\omega\varepsilon_R}{2}} & 0 \\ 0 & \sqrt{\frac{\hbar\omega\varepsilon_R}{2}} & \varepsilon_1 & -\alpha k_{0y} \\ -\sqrt{\frac{\hbar\omega\varepsilon_R}{2}} & 0 & -\alpha k_{0y} & \varepsilon_1 \end{pmatrix}, \quad (24)$$

with

$$\varepsilon_0 = \frac{1}{2}\hbar\omega + \frac{\hbar^2 k_{0y}^2}{2m}, \quad (25)$$

$$\varepsilon_1 = \frac{3}{2}\hbar\omega + \frac{\hbar^2 k_{0y}^2}{2m} \quad (26)$$

being the subband energies in the absence of spin-orbit coupling, and $\varepsilon_R = m\alpha^2/\hbar^2$ is the energy scale of the Rashba coupling. When applying the transformation

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad (27)$$

the projected Hamiltonian and in turn the time evolution operator become block diagonal,

$$Ue^{-(i/\hbar)Ht}U^\dagger = \begin{pmatrix} h_+(t) & 0 \\ 0 & h_-(t) \end{pmatrix}, \quad (28)$$

where

$$h_\pm(t) = \left[1 \cos\left(\frac{1}{\hbar}\mu_\pm t\right) - i \frac{\vec{\mu}_\pm}{\mu_\pm} \cdot \vec{\sigma} \sin\left(\frac{1}{\hbar}\mu_\pm t\right) \right] \times \exp\left[-\frac{i}{\hbar}\left(\hbar\omega + \frac{\hbar^2 k_{0y}^2}{2m}\right)t\right] \quad (29)$$

and

$$\vec{\mu}_\pm = \left(\pm\alpha\sqrt{\frac{m\omega}{2\hbar}}, 0, -\frac{\hbar\omega}{2} \mp \alpha k_{0y} \right). \quad (30)$$

Let us first consider an electron with a given momentum k_{0y} along the wire and injected initially into the lowest subband of the confining potential with the spin pointing upwards along the z direction, i.e., the initial wave function $|\psi_z\rangle = |0, \uparrow\rangle$ for the x direction is a Gaussian whose width is determined by the characteristic length $\lambda = \sqrt{\hbar/m\omega}$ of the harmonic confinement. Using

$$UxU^\dagger = \frac{\lambda}{\sqrt{2}} \begin{pmatrix} 0 & \sigma^x \\ \sigma^x & 0 \end{pmatrix}, \quad (31)$$

one obtains for the above initial state the following time-dependent expectation value

$$\langle \psi_z | x_H(t) | \psi_z \rangle = \frac{\lambda}{\sqrt{2}} \frac{\mu_+^x \mu_-^z + \mu_-^x \mu_+^z}{\mu_+ \mu_-} \sin\left(\frac{1}{\hbar}\mu_+ t\right) \sin\left(\frac{1}{\hbar}\mu_- t\right). \quad (32)$$

The amplitude of this oscillatory dynamics perpendicular to the wire direction becomes maximal when the resonance condition $\hbar\omega = \pm 2\alpha k_{0y}$ is fulfilled. At that point we have $\mu_\mp^z = 0$, and if μ_\pm^x can be neglected compared to μ_\pm^z (which is the case for large enough k_{0y}), and the amplitude of the *zitterbewegung* is approximately $\lambda/\sqrt{2}$. This result from the truncated Hamiltonian is in excellent agreement with numerical simulations of the full multiband system. In Fig. 1 we have plotted simulation results for $\langle \psi_z | x_H(t) | \psi_z \rangle$ where the

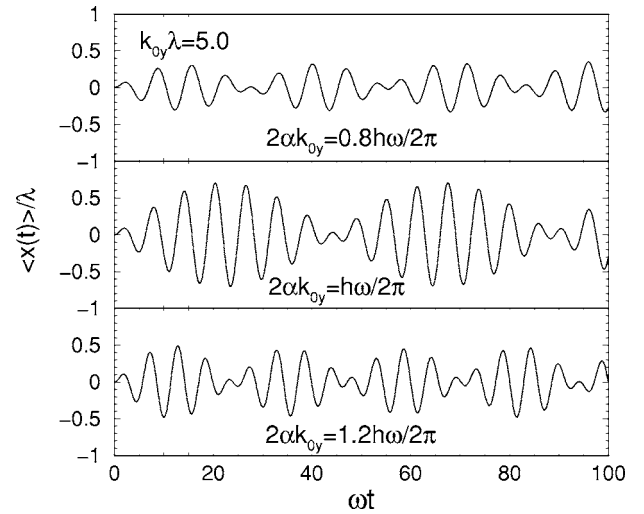


FIG. 1. *Zitterbewegung* of an electron in a harmonic quantum wire perpendicular to the wire direction. The electron is initially injected into the lowest subband with its spin pointing along the z direction. The wave number k_{0y} for the motion along the wire is $k_{0y}\lambda = 5$. The amplitude of the *zitterbewegung* is maximal at the resonance $2\alpha k_{0y} = \hbar\omega$ (middle panel).

wave number along the wire is fixed to be $k_{0y}\lambda = 5$ and the Rashba parameter α is varied around the resonance condition. Clearly, the amplitude is maximum at resonance. Equivalent observations are made if the Rashba coupling is fixed while the wave number k_{0y} is varied. In Fig. 2 we have plotted the amplitude of the *zitterbewegung* as a function of $\Omega/\omega = 2\alpha k_{0y}/\hbar\omega$ for different values of the wave number k_{0y} along the wire. In this range of parameters, the resonance becomes narrower with increasing k_{0y} , while its maximum value is rather independent of this quantity and remarkably well described by $\lambda/\sqrt{2}$.

A qualitative explanation for this resonance can be given in terms of the decomposition $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ of the Hamil-

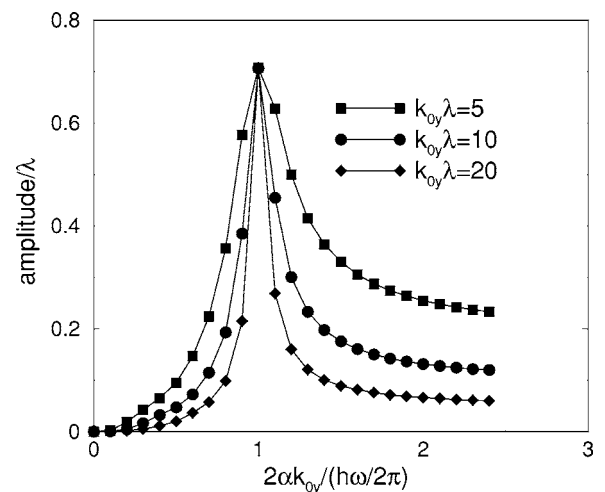


FIG. 2. Amplitude of the *zitterbewegung* perpendicular to the wire direction as a function of $\Omega/\omega = 2\alpha k_{0y}/\hbar\omega$ for different values of the wave number k_{0y} along the wire. Again the electron spin points initially in the z direction.

tonian. The *zitterbewegung* is induced by the perturbation \mathcal{H}_1 which can act most efficiently if the unperturbed energy levels of \mathcal{H}_0 are degenerate having opposite spins. This is the case at $|2\alpha k_{0y}| = \hbar\omega$.

We propose that electron *zitterbewegung* in semiconductor nanostructures as described above can be experimentally observed using high-resolution scanning-probe microscopy imaging techniques as developed and discussed in Refs. 37 and 38. As a possible setup, a tip can be moved along the wire and centered in its middle. For an appropriate biasing of the tip, the electron density at its location is partially depleted leading to a reduced conductance of the wire. Since the amplitude of the *zitterbewegung* reflects the electron density in the center of the wire, the *zitterbewegung* will induce beatings in the wire conductance as a function of the tip position. These beatings are most pronounced at the resonance (see Fig. 1). Note that the oscillations shown there as a function of time can be easily converted to the real-space y coordinate by multiplying the abscissa by $\hbar k_{0y}/m$. Moreover, for tuning the system to the resonance condition $|2\alpha k_{0y}| = \hbar\omega$, at least two parameters can be varied experimentally: the group velocity of the injected electron along the wire given by k_{0y} , and the Rashba parameter α which is tunable by a gate voltage across the quantum well. Thus, quantum wires defined in InAs quantum wells are favorable systems for experiments of the above kind, since this material can exhibit a quite large Rashba coupling but has a comparatively small Dresselhaus term. The group velocity can be varied by changing the gate to the two-dimensional electron gas. This alters the global electron density and therefore also the wave vector for motion along the wire. Generally we expect spin-orbit effects in scanning tunneling microscope (STM) experiments to be more pronounced in the presence of additional confinement such as in a quantum wire.

The present considerations concentrate on the case of pure Rashba coupling neglecting a possible Dresselhaus contribution. Very analogous observations as above can be made for pure Dresselhaus coupling, while in the case of both couplings being present the analytical theory becomes technically more involved. We note that the Dresselhaus coupling, different from the Rashba term, cannot be tuned by an external gate. Therefore, materials with pronounced Rashba coupling are favorable for tuning the system to the above resonance condition.

Let us now analyze the situation when the electron is injected into the lowest subband of the wire, but its spin is not aligned with the z direction. If the spin points along the x direction, no *zitterbewegung* occurs,

$$\langle \psi_x | x_H(t) | \psi_x \rangle = 0. \quad (33)$$

This is a property of both the full multiband model and the truncated Hamiltonian and follows from symmetry considerations: Under a reflection in the yz plane x , p_x and the y and z components of the spin change sign while the other components of spin and momentum remain unchanged. Thus, the Hamiltonian is invariant under this operation, a property which is also shared by the initial state $|\psi_x\rangle$. Therefore, the expectation value of $x_H(t)$ has to be equal to its negative and is consequently zero. Finally, if the spin points initially along

the y direction one finds from the truncated Hamiltonian

$$\begin{aligned} \langle \psi_y | x_H(t) | \psi_y \rangle = & \frac{\lambda}{\sqrt{2}} \frac{1}{2} \left[\frac{\mu_+^x \mu_-^z + \mu_-^x \mu_+^z}{\mu_+ \mu_-} \sin\left(\frac{1}{\hbar} \mu_+ t\right) \sin\left(\frac{1}{\hbar} \mu_- t\right) \right. \\ & + \frac{\mu_+^x}{\mu_+} \cos\left(\frac{1}{\hbar} \mu_+ t\right) \sin\left(\frac{1}{\hbar} \mu_- t\right) \\ & \left. - \frac{\mu_-^x}{\mu_-} \sin\left(\frac{1}{\hbar} \mu_+ t\right) \cos\left(\frac{1}{\hbar} \mu_- t\right) \right]. \quad (34) \end{aligned}$$

Thus, the *zitterbewegung* also occurs if the electron spin is initially aligned along the wire direction.

It is instructive to also investigate the dynamics of the spin degree of freedom as the electron passes along the wire. For a situation where the spin is pointing again initially in the z -direction, the truncated Hamiltonian leads to the following expressions:

$$\begin{aligned} \langle \psi_z | \sigma_H^x(t) | \psi_z \rangle = & \frac{1}{2} \left[\cos^2\left(\frac{1}{\hbar} \mu_+ t\right) \right. \\ & + \frac{-(\mu_+^x)^2 + (\mu_+^z)^2}{\mu_+^2} \sin^2\left(\frac{1}{\hbar} \mu_+ t\right) - \cos^2\left(\frac{1}{\hbar} \mu_- t\right) \\ & \left. - \frac{-(\mu_-^x)^2 + (\mu_-^z)^2}{\mu_-^2} \sin^2\left(\frac{1}{\hbar} \mu_- t\right) \right], \quad (35) \end{aligned}$$

$$\begin{aligned} \langle \psi_z | \sigma_H^y(t) | \psi_z \rangle = & \frac{\mu_-^z}{\mu_-} \cos\left(\frac{1}{\hbar} \mu_+ t\right) \sin\left(\frac{1}{\hbar} \mu_- t\right) \\ & + \frac{\mu_+^z}{\mu_+} \cos\left(\frac{1}{\hbar} \mu_- t\right) \sin\left(\frac{1}{\hbar} \mu_+ t\right), \quad (36) \end{aligned}$$

$$\begin{aligned} \langle \psi_z | \sigma_H^z(t) | \psi_z \rangle = & \cos\left(\frac{1}{\hbar} \mu_+ t\right) \cos\left(\frac{1}{\hbar} \mu_- t\right) \\ & + \frac{\mu_+^x \mu_-^x + \mu_+^z \mu_-^z}{\mu_+ \mu_-} \sin\left(\frac{1}{\hbar} \mu_+ t\right) \sin\left(\frac{1}{\hbar} \mu_- t\right). \quad (37) \end{aligned}$$

Interestingly the expectation value $\langle \psi_z | \sigma_H^x(t) | \psi_z \rangle$ shows a particular behavior at the resonance $\hbar\omega = \pm 2\alpha k_{0y}$. Here we have $\mu_{\mp}^z = 0$, and if μ_{\pm}^x can again be neglected compared to μ_{\pm}^z (as it is the case for the choice of parameters used in Figs. 1 and 2), this expectation value is approximately given by

$$\langle \psi_z | \sigma_H^x(t) | \psi_z \rangle \approx \pm \left[1 - \cos\left(\frac{2}{\hbar} \mu_{\mp}^x t\right) \right]. \quad (38)$$

Thus, the time dependence is, to a very good degree of approximation, governed by a single frequency. This remarkable result is also confirmed by numerical simulations of the full multiband model shown in Fig. 3.

Finally, if the electron spin points initially in the x direction, we have

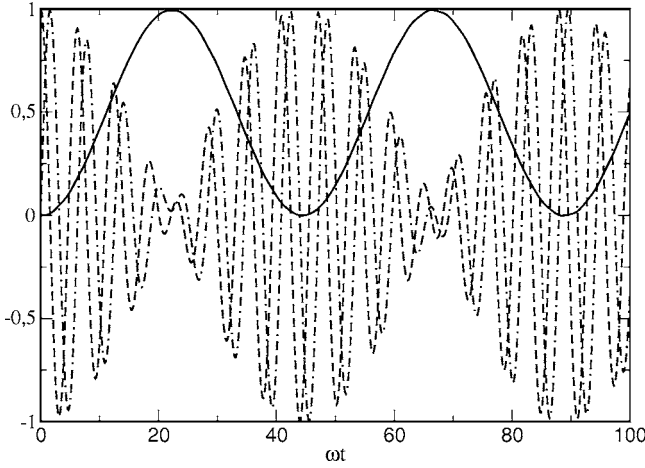


FIG. 3. The spin expectation values $\langle \psi_z | \vec{\sigma}_H(t) | \psi_z \rangle$ as a function of time at the resonance condition $2ak_{0y} = \hbar\omega$ with $k_{0y}\lambda = 5$ (cf. mid panel of Fig. 1). The time evolution of $\langle \psi_z | \sigma_H^x(t) | \psi_z \rangle$ (solid line) is governed by a single frequency as shown in Eq. (38), while the other components $\langle \psi_z | \sigma_H^y(t) | \psi_z \rangle$ and $\langle \psi_z | \sigma_H^z(t) | \psi_z \rangle$ (dashed lines) show beatings between two frequencies given by μ_{\pm} .

$$\langle \psi_x | \sigma_H^x(t) | \psi_x \rangle = \cos^2\left(\frac{1}{\hbar}\mu_+ t\right) + \frac{-(\mu_+^x)^2 + (\mu_+^z)^2}{\mu_+^2} \sin^2\left(\frac{1}{\hbar}\mu_+ t\right), \quad (39)$$

while the expectation values of the other two spin components strictly vanish. The latter result is also true for the full multiband model and follows from the same symmetry considerations as above.

Let us finally summarize other recent theoretical developments pertaining to the issue of *zitterbewegung* in quantum wires. The electron dynamics in ballistic quantum wires in the presence of spin-orbit coupling were also recently analyzed by Nikolic *et al.* concentrating on transverse forces on the electron induced by spin-orbit coupling.⁶ A study similar in spirit was carried out by Shen, who also made a connection between transverse forces due to spin-orbit interaction and the occurrence of *zitterbewegung*.⁷ Lee and Bruder recently studied quantum wires with spin-orbit coupling of both the Rashba and Dresselhaus types.⁵ Their approach is mainly numerical and concentrates on mapping out charge- and spin-density modulations in ferromagnet-semiconductor single-junction quantum wires. The shape of these modulations is explained in terms of the symmetry properties of the eigenstates of the wire. Finally, Zawadzki has most recently analyzed the band structure of narrow-gap single-wall carbon nanotubes, making a connection to relativistic effects in the free Dirac equation.⁸ Similar to Ref. 4, the kind of *zitterbewegung* predicted from these investigations is along the group velocity of the electron wave packet, i.e., along the wire, which is considered there as a strictly one-dimensional system. This is in contrast to the present study where we consider a quantum wire of finite width and obtain a *zitterbewegung* of electronic wave packets perpendicular to the wire direction.

III. HOLES IN A TWO-DIMENSIONAL QUANTUM WELL

We now turn to the case of holes in the *p*-type valence band of III-V semiconductors as opposed to *s*-type conduction band electrons studied so far. We note that Jiang *et al.* have very recently performed a semiclassical study of the time evolution of holes in three-dimensional bulk systems under the influence of a homogeneous electric field.³ This investigation was motivated by the recent prediction of the intrinsic spin-Hall effect.⁹⁻¹¹ Here we shall analyze the full quantum time evolution of heavy-hole states in quantum wells, a scenario for which spin-Hall transport was most recently predicted¹¹ and experimentally reported.⁴²

At low temperatures and for not too wide wells, only heavy-hole states are occupied with their angular momentum pointing predominantly along the growth direction,⁴³ corresponding to the total angular momentum states $\pm\frac{3}{2}$. Due to this constraint, the effects of structure-inversion asymmetry on the hole spins are trilinear in the momentum, and the Hamiltonian incorporating this type of spin-orbit coupling reads for appropriate growth directions of the quantum well,^{43,44}

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + i\frac{\tilde{\alpha}}{2\hbar^3}(p_x^3\sigma_+ - p_y^3\sigma_-), \quad (40)$$

using the notations $p_{\pm} = p_x \pm ip_y$, $\sigma_{\pm} = \sigma_x \pm i\sigma_y$, where \vec{p} , $\vec{\sigma}$ denote the hole momentum operator and Pauli matrices, respectively. These Pauli matrices operate on the total angular momentum states with spin projection $\pm\frac{3}{2}$ along the growth direction; in this sense they represent a pseudospin degree of freedom rather than a genuine spin $\frac{1}{2}$. In the above equation, m is the heavy-hole mass, and $\tilde{\alpha}$ is Rashba spin-orbit coupling coefficient due to structure inversion asymmetry. The components of the time-dependent position operator read

$$\begin{aligned} x_H(t) = & x(0) + \frac{p_x}{m}t + \frac{p_y}{p^2}\frac{3\hbar}{2}\sigma^z \left[1 - \cos\left(\frac{2\tilde{\alpha}p^3}{\hbar^4}t\right) \right] \\ & + \frac{p_x}{p^5}\frac{3\hbar}{2}[(3p_x p_y^2 - p_x^3)\sigma^x - (3p_x^2 p_y - p_y^3)\sigma^y] \\ & \times \left[\sin\left(\frac{2\tilde{\alpha}p^3}{\hbar^4}t\right) - \frac{2\tilde{\alpha}p^3}{\hbar^4}t \right] \\ & + \frac{\tilde{\alpha}}{\hbar^3}t(6p_x p_y \sigma^x + 3(p_y^2 - p_x^2)\sigma^y), \end{aligned} \quad (41)$$

$$\begin{aligned} y_H(t) = & y(0) + \frac{p_y}{m}t - \frac{p_x}{p^2}\frac{3\hbar}{2}\sigma^z \left[1 - \cos\left(\frac{2\tilde{\alpha}p^3}{\hbar^4}t\right) \right] \\ & - \frac{p_y}{p^5}\frac{3\hbar}{2}[(3p_x p_y^2 - p_x^3)\sigma^x - (3p_x^2 p_y - p_y^3)\sigma^y] \\ & \times \left[\sin\left(\frac{2\tilde{\alpha}p^3}{\hbar^4}t\right) - \frac{2\tilde{\alpha}p^3}{\hbar^4}t \right] \\ & + \frac{\tilde{\alpha}}{\hbar^3}t[3(p_x^2 - p_y^2)\sigma^x + 6p_x p_y \sigma^y]. \end{aligned} \quad (42)$$

Again, the *zitterbewegung* of a wave packet with its spin pointing initially in the z direction is perpendicular to the group velocity. Specifically, for an initial state of the form (14) moving along the y direction ($k_{0x}=0$), one finds in the limit $dk_{0y} \gg 1$

$$\langle \psi | x_H(t) | \psi \rangle = \frac{3}{2k_{0y}} \left[1 - \cos\left(\frac{2\tilde{\alpha}k_{0y}^3}{\hbar} t\right) \right]. \quad (43)$$

Thus, the amplitude of the *zitterbewegung* is again proportional to the wavelength $\lambda_{0y}=2\pi/k_{0y}$ of the particle motion perpendicular to it. The frequency of the *zitterbewegung* is given by $\tilde{\Omega}=2\tilde{\alpha}k_{0y}^3/\hbar$. Winkler *et al.*⁴⁵ have studied both theoretically and experimentally the magnitude of the Rashba spin-orbit coupling in GaAs-based quantum well samples with heavy-hole densities of a few 10^{14} m^{-2} and have found typical values for the characteristic length scale $m\tilde{\alpha}/\hbar^2$ of a few nanometers. Assuming a value of 2 nm this corresponds to a coupling parameter of $\tilde{\alpha}=0.3 \text{ eV nm}^3$, where we have used the heavy-hole mass $m \approx 0.5m_0$ for GaAs.³⁹ For a typical wave vector with $k_{0y} \approx 0.1 \text{ nm}^{-1}$ this leads to frequencies $\tilde{\Omega}$ of order 10^{11} Hz , an estimate which is of a similar order of magnitude as for the case of an n -doped quantum well.

IV. CONCLUSIONS

We have investigated the notion of *zitterbewegung* in both n - and p -doped III–V zinc-blende semiconductor quantum wells, extending previous work on the two-dimensional electron gas.² *Zitterbewegung* in the two-dimensional electron gas has been studied for the case of spin-orbit coupling of

both the Rashba and Dresselhaus type. In the context of these investigations we have also discussed recent work by Zawadzki.⁴ The crucial difference between *zitterbewegung* of free electrons and electrons bound in the above semiconductor nanostructures is the fact that in the latter systems the frequency of the oscillations is by orders of magnitude smaller while the amplitude is grossly larger. This circumstance make such systems favorable candidates for the experimental detection of *zitterbewegung*.

The case of electron dynamics in a quantum wire is studied in great detail for various initial conditions. For this type of system we propose possible experiments for detecting the *zitterbewegung* of electronic wave packets. For a harmonic quantum well in the presence of Rashba spin-orbit coupling, the dynamical parameters can be tuned to a resonance condition where the amplitude of the *zitterbewegung* becomes maximal.² This property should facilitate the experimental observation of this effect. In addition to the orbital dynamics, we have also analyzed in detail the electron spin dynamics, which also show peculiarities at the resonance.

Finally we have also discussed in detail the *zitterbewegung* in the two-dimensional hole gas. Here we have considered spin-orbit coupling of heavy holes due to structure-inversion asymmetry. Concerning the frequency and amplitude of the *zitterbewegung*, similar results are obtained as for the two-dimensional electron gas.

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