SLAC-PUB-13905

Semiclassical Time Evolution of the Holes from Luttinger Hamiltonian

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We study the semi-classical motion of holes by exact numerical solution of the Luttinger model. The trajectories obtained for the heavy and light holes agree well with the higher order corrections to the abelian and the non-abelian adiabatic theories in Ref. [1] [S. Murakami *et al.*, Science **301**, 1378 (2003)], respectively. It is found that the hole trajectories contain rapid oscillations reminiscent of the "Zitterbewegung" of relativistic electrons. We also comment on the non-conservation of helicity of the light holes.

PACS numbers: 72.25.Dc, 85.75.-d, 71.70.Ej, 03.65.Sq

The field of spintronics holds the promise of using the spin degree of freedom for building low-power integrated information processing and storage devices [2, 3]. Spintronics devices also promises to access the intrinsic quantum regime of transport, paving the path towards quantum computing. Recently, it has been predicted theoretically that a dissipationless spin current can be induced by an external DC electric field in a large class of p-doped semi-conductors [1]. The dissipationless spin current arises from the spin-orbit coupling in semiconductors and several other groups have shown that it also applies to a broader class of models [4, 5].

The theory of Ref.[1] is based on the adiabatic solution to the Luttinger model, which describes holes near the top of the fourfold degenerate valence band. It was pointed out that the abelian adiabatic approximation applies for the heavy-hole (HH), while the non-abelian adiabatic approximation is required to obtain the correct result for the light-hole (LH). The adiabatic approximation is generally based on the separation of the light and the heavy hole bands. However, at the top of the valence band, these two bands intersect each other, and it is not clear to which extent the adiabatic approximation is valid. In this paper, we solve the semi-classical trajectory for the Luttinger model exactly by numerical integration of the Heisenberg equation of motion. We find that the full trajectory of the holes consists of two parts, a rapidly oscillating part, reminiscent of the "Zitterbewegung" of a relativistic electron [6], is super-posed on a smooth part, which is accurately described by the adiabatic theory. The separation of the rapid and the smooth parts of the trajectory is also similar to the cyclotron and the guiding center motion of a charged particle in an uniform magnetic field and a spatially varying potential. In this sense, the adiabatic approximation in the spin-orbit coupled systems is similar to the lowest-Landau-level approximation in the quantum Hall effect.

The Luttinger effective Hamiltonian [7] with an d.c. electric field $\mathbf{E} = E_z\hat{z}$ can be written as [1]

$$H = \frac{\hbar^2}{2m}((\gamma_1 + \frac{5}{2}\gamma_2)k^2 - 2\gamma_2(\mathbf{k}\cdot\mathbf{S})^2) + eE_z z. \qquad (1)$$

where γ_1, γ_2 are the valence-band parameters for semiconductor materials. Luttinger [7] pointed out that there are 16 linearly independent spin matrices which can be chosen as E, S_x, S_y, S_z, S_x^2, S_y^2, $\{S_x, S_y\}$, $\{S_y, S_z\}$, $\{S_z, S_x\}$, $\{S_x, S_y^2 - S_z^2\}$, $\{S_y, S_z^2 - S_x^2\}$, $\{S_z, S_x^2 - S_y^2\}$, S_x^3, S_y^3, S_z^3, $S_xS_yS_z + S_zS_yS_x$. The full set of dynamic variables in the theory consists of three position operators x, y and z, three momentum operators k_x, k_y and k_z, and the 16 spin matrices listed above. The Heisenberg equation of motion for the expectation value of any operator A is determined by a differential equation $d\langle A\rangle/dt = (i\hbar)^{-1}\langle[A, H]\rangle$. The equations of motion for the momentum and the position operators are given by

$$\frac{d}{dt}\begin{bmatrix}\langle k_x\rangle\\ \langle k_y\rangle\\ \langle k_z\rangle\end{bmatrix} = \frac{1}{\hbar}\begin{bmatrix}0\\ 0\\ c\end{bmatrix}, \qquad (2)$$

and

$$\frac{d}{dt}\begin{bmatrix}\langle x\rangle\\ \langle y\rangle\\ \langle z\rangle\end{bmatrix} = \frac{2a}{\hbar}\begin{bmatrix}\langle k_x\rangle\\ \langle k_y\rangle\\ \langle k_z\rangle\end{bmatrix} + \frac{b}{\hbar}\begin{bmatrix}2\langle k_xS_x^2\rangle + \langle k_y\{S_x, S_y\}\rangle + \langle k_z\{S_z, S_x\}\rangle\\ \langle k_x\{S_x, S_y\}\rangle + 2\langle k_yS_y^2\rangle + \langle k_z\{S_y, S_z\}\rangle\\ \langle k_x\{S_z, S_x\}\rangle + \langle k_y\{S_y, S_z\}\rangle + 2\langle k_zS_z^2\rangle\end{bmatrix}, \qquad (3)$$

where $a \equiv \hbar^2(\gamma_1 + 5\gamma_2/2)/2m, b \equiv -\hbar^2\gamma_2/m, c \equiv -eE_z$, and $\{\ \}$ represents the anticommutative relation. The equation of motion for the spin operators can be obtained straightforwardly, but they are lengthy and will not be given explicitly here.

Thus the evolution of momentum is simply determined by Eq. (2), and can be solved trivially analytically. Next we numerically solve the equations for the spin operators,

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Work supported in part by US Department of Energy contract DE-AC02-76SF00515.

which depends only on the solution of the momentum, not on the position. Finally, we decompose the mean value of the product of the momentum and the spin into the products of their mean values in Eq. (3), and numerically solve for the position operators. For convenience, we can always choose a coordinate frame which make the hole's initial momentum have no y-component.

Time evolution of the heavy-hole: The initial state of the HH with helicity $\lambda = 3/2$ can expressed as $\psi(0) = U^{\dagger}(\mathbf{k}(0))\begin{pmatrix} 1, & 0, & 0, & 0 \end{pmatrix}^T$, where $U^{\dagger}(\mathbf{k}(0)) = \exp(-i\phi S_z)\exp(-i\theta S_y)$ is defined in Ref. [1], and $\mathbf{k}(0)$ is the initial momentum. The initial mean value of any operator A is $\langle A(0)\rangle \equiv \langle \psi(0)|A|\psi(0)\rangle$. From this definition of the initial state, we obtain $\langle x(0)\rangle$, $\langle k_x(0)\rangle$, $\langle S_x(0)\rangle$, $\langle\{S_x(0), S_y(0)\}\rangle$ *etc.* as the initial conditions for Eqs. (2, 3) and the spin equations.

In Fig. 1, we plot the trajectory of the HH as a function of time. We clearly see that besides the acceleration in the z direction and the uniform velocity motion along the x direction, there is a side-way drift along the y direction, which is responsible for the dissipationless spin current. We can compare the trajectories between our numerical solution and the result from Ref. [1]. The abelian adiabatic equations of Ref. [1] describe the overall trend very well. However, we see that there are rapid oscillations on the exact numerical curve. The frequency of the oscillations increases and the amplitude decreases as the time increases. This "Zitterbewegung" effect can be obtained from the higher orders of the adiabatic approximation theory [8]. The oscillation on $z(t)$ can't be seen clearly because the figure space is limited, but the oscillation on $x(t)$ is really small which is analyzed as below.

In order to study the higher orders of the adiabatic approximation, we transform the Hamiltonian

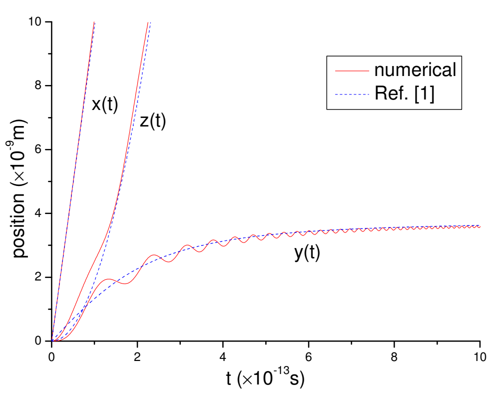

FIG. 1: A heavy-hole ($\lambda = 3/2$) position three-component vs. time. The red solid lines are numerical results, and the blue dash lines are from the formulas of Ref. [1]. The initial momentum is parallel to x-axis, and the electric field is parallel to z-axis. These conditions are same in other figures.

(1). We assume the wavefunction has the form of $|\Psi(\mathbf{x},t)\rangle = \exp(-ieE_z zt/\hbar)\,|u(\mathbf{k},t)\rangle$, then substitute $|\Psi(\mathbf{x},t)\rangle$ into the Schödinger equation, so that we get a new time-dependent Schödinger equation $i\hbar\partial_t\,|u(\mathbf{k},t)\rangle = H_0'(t)\,|u(\mathbf{k},t)\rangle$, where the new time-dependent effective Hamiltonian $H_0'(t) = ak(t)^2 + b(\mathbf{k}(t)\cdot\mathbf{S})^2$,where $\mathbf{k}(t)$ is determined by Eq.(2). In the adiabatic approximation, we assume $|u(\mathbf{k},t)\rangle = \sum_{\lambda} C_{\lambda}(t)\exp(-\frac{i}{\hbar}\int_0^t \epsilon_{\lambda}(t')dt')U^{\dagger}(\mathbf{k})\,|\lambda\rangle$, where $|\lambda\rangle$ represents any eigenstate of S_z, so $U^{\dagger}(\mathbf{k})\,|\lambda\rangle$ is the instant eigenstate of $H_0'(t)$. $H_0'(t)U^{\dagger}(\mathbf{k})\,|\lambda\rangle = \epsilon_{\lambda}(t)U^{\dagger}(\mathbf{k})\,|\lambda\rangle$, where $\epsilon_{\lambda}(t) = \frac{\hbar^2 k(t)^2}{2m_{\lambda}}$. We substitute $|u(\mathbf{k},t)\rangle$ into the time-dependent Schödinger equation, so that we get the equation of $C_{\lambda}(t)$ is

$$\frac{d}{dt}C(t) + B\cdot C(t) = 0, \tag{4}$$

where $C(t) \equiv \begin{pmatrix} C_{\frac{3}{2}} & C_{\frac{1}{2}} & C_{-\frac{1}{2}} & C_{-\frac{3}{2}} \end{pmatrix}^T$, and

$$B \equiv \begin{pmatrix} 0 & -\frac{\sqrt{3}}{2}\dot{\theta}e^{-i\alpha} & 0 & 0 \\ \frac{\sqrt{3}}{2}\dot{\theta}e^{i\alpha} & 0 & -\dot{\theta} & 0 \\ 0 & \dot{\theta} & 0 & -\frac{\sqrt{3}}{2}\dot{\theta}e^{i\alpha} \\ 0 & 0 & \frac{\sqrt{3}}{2}\dot{\theta}e^{-i\alpha} & 0 \end{pmatrix}, \tag{5}$$

where $\alpha \equiv \frac{1}{\hbar}\int_0^t \Delta\epsilon(t')dt'$ is the dynamic phase, and $\Delta\epsilon(t') \equiv \epsilon_L(t') - \epsilon_H(t')$ is the energy difference of HH and LH. If we choose the initial state $C(0) \equiv \begin{pmatrix} 1, & 0, & 0, & 0 \end{pmatrix}^T$, the adiabatic approximation assumes that $0 \approx C_{-\frac{3}{2},\pm\frac{1}{2}}(t) \ll C_{\frac{3}{2}}(t) \approx 1$ is always satisfied. So only one equation remains, $\frac{d}{dt}C_{\frac{1}{2}}(t) = \frac{\sqrt{3}}{2}\dot{\theta}e^{i\alpha}$. We can solve it after the approximation that both $\Delta\epsilon$ and $\dot{\theta}$ are slowly varying functions of t. Then the first-order correction of trajectory is $\mathbf{x}^{(1)} = C^*_{\frac{3}{2}}(t)C_{\frac{1}{2}}(t)\cdot e^{-i\alpha}\cdot \left\langle \frac{3}{2}\right| U(\mathbf{k})i\frac{\partial}{\partial\mathbf{k}}U^{\dagger}(\mathbf{k})\left|\frac{1}{2}\right\rangle + h.c.$. This method is applicable to the other three kinds of holes, too. So we get the unified formulas of the first-order correction on the trajectory of any helicity state,

$$\begin{aligned} x^{(1)} &= \frac{\lambda(2\lambda^2-\frac{7}{2})eE_z\sin 2\theta}{2k^2\Delta\epsilon}(1-\cos(\frac{\Delta\epsilon}{\hbar}t)), \\ y^{(1)} &= -\frac{\lambda(2\lambda^2-\frac{7}{2})eE_z\sin\theta}{k^2\Delta\epsilon}\sin(\frac{\Delta\epsilon}{\hbar}t), \\ z^{(1)} &= \frac{\lambda(2\lambda^2-\frac{7}{2})eE_z\sin^2\theta}{k^2\Delta\epsilon}(1-\cos(\frac{\Delta\epsilon}{\hbar}t)), \end{aligned} \tag{6}$$

From these formulas, we can see that the frequency $\omega = \Delta\epsilon/\hbar$ will increase while the amplitude $(k^2\Delta\epsilon)^{-1}$ will decrease as time increases, as shown in Fig. 1. We can evaluate the quantities of frequency and amplitude in Fig. 1, which agree with Eq. (6) very well. The oscillation on $x(t)$ is small because $\sin 2\theta \approx 0$.

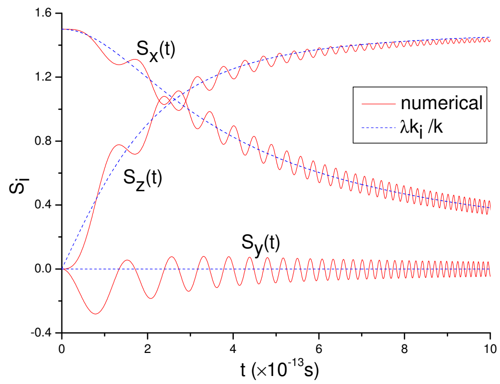

FIG. 2: The mean values of spin three-component of a heavy-hole ($\lambda = 3/2$) vs. time. The red solid lines are numerical results, and the blue dash lines are $\lambda k_i/k$.

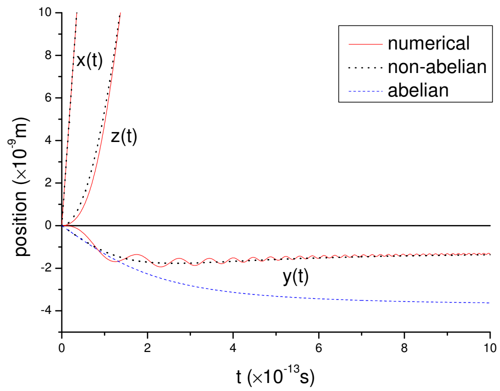

FIG. 3: A light-hole ($\lambda = 1/2$) position three-component vs. time. The red solid lines are numerical results, the blue dash line is from the abelian adiabatic theory, and the black dot lines are from the non-abelian adiabatic theory.

Now let's study the applicability of Eq. (6). We have used the approximation that both $\Delta\epsilon$ and $\dot{\theta}$ are slowly varying functions of t, which is equivalent to $\dot{\Delta\epsilon} dt \ll \Delta\epsilon$ and $\ddot{\theta} dt \ll \dot{\theta}$. They imply the same result, $eE_z\Delta t \ll \hbar k$, which means that the approximation is valid when the electric field has not brought large changes in momentum. If we assume $E_z = 1 \times 10^3 V/m$, and $k = 4 \times 10^8 m^{-1}$, we get $\Delta t \ll 2000T$. So we have enough periods of oscillations in which Eq. (6) is applicable.

Fig. 2 indicates $S_i(t) \approx \lambda k_i(t)/k(t)$, which implies the approximate conservation of HH's helicity. This can be seen clearly in Fig. (5). The oscillations show that the semiclassical spin vector always precesses around the momentum direction as the momentum changes in an electric field. The oscillation can be calculated with the similar method above. The deep reason for the HH's helicity conserving is the matrix element representing transition between $\lambda = \pm 3/2$ is zero. But the LH's helicity isn't conserved as shown in the next section.

Time evolution of the light-hole: When we choose the initial state as $\psi(0) = U(\mathbf{k}(0))^\dagger (\ 0,\ 1,\ 0,\ 0\ )^T$, Eqs. (2, 3) and the spins' equations describe the evolution of a LH with helicity $\lambda = 1/2$. The trajectory is shown in Fig. 3, and the evolution of spin is showed in Fig. 4. The anomalous shift in y-direction is not as large as predicted from the abelian adiabatic theory of Ref. [1], and the helicity is no longer as conserved as that of HH. However, both the trajectory and the evolution of spin can be explained in the non-abelian adiabatic theory [1, 8], which properly takes into account the transition between the two LH states.

If we confine the problem in the light hole's space, Eq. (4) is reduced to

$$\frac{d}{dt}\begin{pmatrix} C_{\frac{1}{2}} \\ C_{-\frac{1}{2}} \end{pmatrix} + \begin{pmatrix} 0 & -\dot{\theta} \\ \dot{\theta} & 0 \end{pmatrix}\begin{pmatrix} C_{\frac{1}{2}} \\ C_{-\frac{1}{2}} \end{pmatrix} = 0. \quad (7)$$

It describes the evolution of two degenerate states. The solution is

$$C(t) = \begin{bmatrix} \cos(\theta_t - \theta_0) & \sin(\theta_t - \theta_0) \\ -\sin(\theta_t - \theta_0) & \cos(\theta_t - \theta_0) \end{bmatrix} C(0), \quad (8)$$

where θ_t is the the polar angle at the time t. So we can get the anomalous shift in y directions

$$\begin{aligned} y_{\pm\frac{1}{2}}(t) &= C^\dagger(t)U(\mathbf{k}) \cdot i\partial_{k_y} U^\dagger(\mathbf{k})C(t) \\ &= \pm\frac{3\cos(\theta_t - 2\theta_0) - \cos(3\theta_t - 2\theta_0) - 2\cos\theta_0}{4k_0 \sin\theta_0}, \end{aligned} \quad (9)$$

and the evolution of spin is $\langle \mathbf{S}(t) \rangle = C^\dagger(t)U(\mathbf{k})\mathbf{S}U^\dagger(\mathbf{k})C(t)$,

$$\begin{aligned} S_{x,\pm\frac{1}{2}}(t) &= \mp[\frac{3}{4}\sin(\theta_t - 2\theta_0) + \frac{1}{4}\sin(3\theta_t - 2\theta_0)], \\ S_{y,\pm\frac{1}{2}}(t) &= 0, \\ S_{z,\pm\frac{1}{2}}(t) &= \pm[\frac{3}{4}\cos(\theta_t - 2\theta_0) - \frac{1}{4}\cos(3\theta_t - 2\theta_0)]. \end{aligned} \quad (10)$$

The results from Eq. (9) and (10) has been plotted in Fig. 3 and Fig. 4, they describe the trends of numerical curves very well except for the rapid oscillation on the numerical curves, which have been explained in the previous sections due to higher order corrections to the adiabatic theory.

At last, we obtain the anomalous velocity in y-direction,

$$v_{y,\pm\frac{1}{2}}(t) = \pm\frac{3eE_z}{4\hbar k^2}[\sin(\theta_t - 2\theta_0) - \sin(3\theta_t - 2\theta_0)]. \quad (11)$$

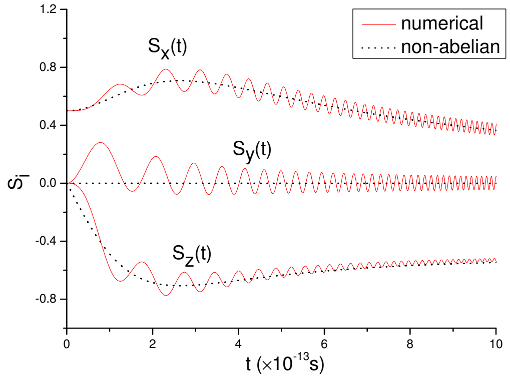

FIG. 4: The mean values of spin three-component of a light-hole ($\lambda = 1/2$) vs. time. The red solid lines are numerical results, and the black dot lines are from the non-abelian adiabatic theory.

When $t = 0$, $v_{y,\pm\frac{1}{2}}(0) = \lambda(2\lambda^2 - \frac{7}{2})eE_z k_{x0}/(\hbar k_0^3)$, which is just the Eq. (7) of Ref. [1] (where F_{ij} is given by Eq. (S5) of SOM). Eq. (11) represent the anomalous velocity at any time.

Unlike the HH, the LH does not always stay as an eigenstate, it will evolute according to Eq. (8). Fig. (5) compares the spins' evolution of HH and LH. Obviously, LH's helicity is not as conserved as HH, so LH's spin can't be always parallel to its momentum like HH. The non-abelian adiabatic theory of Ref. [1] properly takes this effect into account.

The adiabatic condition: Ref. [9] raised a criticism by asking why the anomalous shift in Ref. [1] is independent of λ_2. Actually, if $\lambda_2 = 0$, the anomalous shift vanishes because the Hamiltonian degenerates to an ordinary one without the spin-orbit coupling, and the adiabatic approximation is no longer valid. Below can we see explicitly that the adiabatic approximation fails when λ_2 is less than a certain quantity. The condition of adiabatic approximation [8] is

$$\left| \frac{\langle H, \alpha \left| \frac{d}{dt} \right| L, \beta \rangle}{\frac{E_H - E_L}{\hbar}} \right| = \frac{\frac{\sqrt{3}}{2}\frac{d\theta}{dt}}{2k^2 \frac{b}{\hbar}} = \frac{\sqrt{3} meE_z \sin\theta}{4k^3\hbar^2\gamma_2} \ll 1. \quad (12)$$

The condition is better satisfied if E_z is smaller and γ_2 is larger. The small E_z ensures that the time-dependent Hamiltonian changes slowly, and the large γ_2 ensures that the energy difference between the HH and LH bands is large ($\Delta\epsilon = \frac{2\hbar^2 k^2 \gamma_2}{m}$), so the transition probability between HH and LH is small.

In most semiconductors, Eq. (12) can be satisfied. For example as GaAs, $\gamma_2 = 1.01$, $k_F \approx 8 \times 10^8 m^{-1}$, if we assume $E_z = 10^3 V/m$, $\theta_0 = 90^o$, we get the condition is $k \gg 0.02 k_F$. So only a little part in the middle of Fermi Ball doesn't meet the conditions. We can neglect them when we integrate the whole Fermi ball.

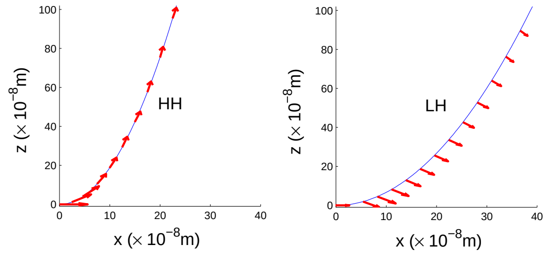

FIG. 5: Comparison of the trajectories and spins between heavy-hole and light-hole.

Conclusion We have studied the motions of the heavy-hole and light-hole in a large class of hole-doped semiconductor based on the Luttinger Hamiltonian. The trajectory of HH has rapid, small amplitude oscillations, which can be explained as the first-order correction on the trend described in Ref. [1]. The trajectory of LH is more complicated and the helicity of the LH is not conserved. The non-conservation of the helicity invalidates the abelian adiabatic approximation. However, the motion of LH can be well explained by the non-abelian adiabatic theory. The excellent agreement between the exact numerical solution of the Heisenberg equation of motion and the adiabatic approximation validates the key assumptions leading to the dissipationless spin current, and addresses the naive criticism raised in Ref. [9]. In the future, we plan to apply the formalisms developed in this paper to study the Luttinger Hamiltonian under more general external conditions.

We thank Andrei Bernevig, D. Culcer and Q. Niu for helpful discussion. This work was supported by the NSF of China under grant number 10174095 and 90103024, the US NSF under grant number DMR-0342832, and the US Department of Energy, Office of Basic Energy Sciences under contract DE-AC03-76SF00515.

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