Diffusive-Ballistic Crossover and the Persistent Spin Helix

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Conventional transport theory focuses on either the diffusive or ballistic regimes and neglects the crossover region between the two. In the presence of spin-orbit coupling, the transport equations are known only in the diffusive regime, where the spin precession angle is small. In this paper, we develop a semiclassical theory of transport valid throughout the diffusive - ballistic crossover of a special $SU(2)$ symmetric spin-orbit coupled system. The theory is also valid in the physically interesting regime where the spin precession angle is large. We obtain exact expressions for the density and spin structure factors in both 2 and 3 dimensional samples with spin-orbit coupling.

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The physics of systems with spin-orbit coupling has generated great interest from both academic and practical perspectives [1]. Spin-orbit coupling allows for purely electric manipulation of the electron spin [2,3,4,5,6], and could be of practical use in areas from spintronics to quantum computing. Theoretically, spin-orbit coupling is essential to the proposal of interesting effects and new phases of matter such as the intrinsic and quantum spin Hall effect [7,8,9,10,11,12[.

While the diffusive transport theory for a system with spin-orbit coupling has recently been derived [13,14], the analysis of diffusive-ballistic transport - where the spin precession angle during a mean free path is comparable to (or larger than) 2π - has so far remained confined to numerical methods [15]. This situation is experimentally relevant since the momentum relaxation time τ in high-mobility GaAs or other semiconductors can be made large enough to render the precession angle $\phi = \alpha k_F \tau > 2\pi$, where α, k_F are the spin-orbit coupling strength and Fermi momentum respectively. The mathematical difficulty in obtaining the crossover transport physics rests in the fact that one has to sum an infinite series of diagrams which, due to the spin-orbit coupling, are not diagonal in spin-space. In this paper we obtain the explicit transport equations for a the series of models with spin-orbit coupling where a special $SU(2)$ symmetry has recently been discovered [16].

We first consider a two-dimensional electron gas without inversion symmetry for which the most general form of linear spin-orbit coupling includes both Rashba and Dresselhaus contributions:

$$\mathcal{H} = \frac{k^2}{2m} + \alpha(k_y\sigma_x - k_x\sigma_y) + \beta(k_x\sigma_x - k_y\sigma_y), \qquad (1)$$

where $k_{x,y}$ is the electron momentum along the [100] and [010] directions respectively, α, and β are the strengths of the Rashba, and Dresselhauss spin-orbit couplings and m is the effective electron mass. At the point $\alpha = \beta$, which may be experimentally accessible through tuning of the Rashba coupling via externally applied electric fields [2], a new $SU(2)$ finite wave-vector symmetry was theoretically discovered [16]. The Dresselhauss [110] model, describing quantum wells grown along the [110] direction, exhibits the above symmetry without tuning to a particular point in the spin-orbit coupling space. At the symmetry point, the spin relaxation time becomes infinite giving rise to a Persistent Spin Helix. The energy bands in Eq.[1] at the $\alpha = \beta$ point have an important *shifting property*: $\epsilon_\downarrow(\vec{k}) = \epsilon_\uparrow(\vec{k} + \vec{Q})$, where $Q_+ = 4m\alpha, Q_- = 0$ for the $\mathcal{H}_{[\mathrm{ReD}]}$ model and $Q_x = 4m\alpha, Q_y = 0$ for the $\mathcal{H}_{[110]}$ model. The exact $SU(2)$ symmetry discovered in [16] is generated by the spin operators (written here in a transformed basis as):

$$S^-_Q = \sum_{\vec{k}} c^\dagger_{\vec{k}\downarrow} c_{\vec{k}+\vec{Q}\uparrow}, \quad S^+_Q = \sum_{\vec{k}} c^\dagger_{\vec{k}+\vec{Q},\uparrow} c_{\vec{k}\downarrow}$$
$$S^z_0 = \sum_{\vec{k}} c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} - c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow}, \qquad (2)$$

with $c_{k\uparrow,\downarrow}$ being the annihilation operators of spin-up and down particles. These operators obey the commutation relations for angular momentum, $[S^z_0, S^\pm_Q] = \pm 2 S^\pm_Q$ and $[S^+_Q, S^-_Q] = S^z_0$. Early spin-grating experiments on GaAs exhibit phenomena consistent with the existence of such a symmetry point [17].

In [16] the spin-charge transport equations for the Hamiltonian Eq.[1] have been obtained in the diffusive limit in which $\alpha k_F \tau << 1$. However the regions $\alpha k_F \tau \sim 1$ and $\alpha k_F \tau >> 1$ are also experimentally accessible, and no theory is yet available to deal with these regimes. We now present the exact spin and charge structure factors at the exact symmetry point for any value of the parameter $\alpha k_F \tau$.

We first obtain the spin and charge structure factors in the absence of spin-orbit coupling, but valid in both the $\tau \to 0$ and in $\tau \to \infty$ regimes. One should think of the structure factor obtained this way as a generalization of the classic Lienhard formulas in the presence of disorder. We then use a non-abelian gauge transformation

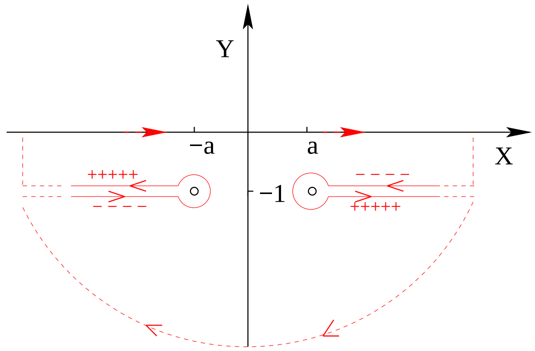

FIG. 1: The sketch of the branch cut and the integral contour in the calculation of $S(t,q)$.

introduced in [16] to obtain the structure factors for the spin-orbit coupling problem described above.

We start by formulating the problem in the language of the Keyldish formalism [14,18]. Assuming isotropic scattering with momentum lifetime τ, the retarded and advanced Green's functions are:

$$G^{R,A}(k,\epsilon) = (\epsilon - \mathcal{H} \pm \frac{i}{2\tau})^{-1}. \tag{3}$$

We introduce a momentum, energy, and position dependent charge-spin density which is a 2×2 matrix $g(k,r,t)$. Summing over momentum:

$$\rho(r,t) \equiv \int \frac{d^2k}{(2\pi)^3\nu} g(k,r,t), \tag{4}$$

gives the real-space spin-charge density $\rho(r,t) = n(r,t) + S^i(r,t)\sigma_i$, where $n(r,t)$ and $S^i(r,t)$ are the charge and spin density and $\nu = m/2\pi$ is the density of states in two-dimensions. $\rho(r,t)$ and $g(k,r,t)$ satisfy a Boltzman-type equation 14,18:

$$\frac{\partial g}{\partial t} + \frac{1}{2}\left\{\frac{\partial \mathcal{H}}{\partial k_i}, \frac{\partial g}{\partial r_i}\right\} + i\left[\mathcal{H}, g\right] = -\frac{g}{\tau} + \frac{i}{\tau}(G^R\rho - \rho G^A). \tag{5}$$

that we now solve for a free electron gas Hamiltonian. To obtain the spin-charge transport equations, we follow the general sequence of technical manipulations: time-Fourier transform the above equation; find a general solution for $g(k,r,t)$ involving $\rho(r,t)$ and the k-dependent spin-orbit coupling; perform a gradient expansion of that solution (assuming $\partial_r << k_F$ where k_F is the Fermi wavevector) to second order; and, finally, integrate over the momentum. The formalism is valid even through the diffusive-ballistic boundary. For the diffusive limit, when τ is small, we need to keep only the second order term in the gradient expansion which gives rise to the usual spin and charge propagator $(i\omega - Dq^2)^{-1}$. As τ increases, we need to keep higher order terms in the gradient expansion to accurately describe the transport physics. The ballistic limit requires infinite summation over the gradient expansion. This can be easiest seen in the regime of zero spin-orbit coupling, in which the sums can be exactly performed. It is then fortuitous that our spin-orbit coupled problem can be mapped into a free electron plus disorder problem where we can obtain the structure factor exactly. By Fourier transforming in time we obtain the following recursive equation:

$$-i\omega\rho(r,t) = -i\int \frac{d\theta k dk}{(2\pi)^2 m}\Omega \sum_{n=1}^{\infty} g_n(k,r,t) \tag{6}$$

were $\Omega = \omega + i/\tau$ and the n-th order term reads:

$$g_n(k,r,t) = \partial_{r_1}...\partial_{r_n}\left((-\frac{k_{i_1}}{m})...(-\frac{k_{i_n}}{m})(\frac{i}{\Omega})^n g_0(k,r,t)\right) \tag{7}$$

where $g_0(k,r,t)$ contains a term which fixes the momentum at the Fermi surface:

$$g_0(k,r,t) = \frac{i}{\Omega}\frac{2\pi}{\tau}\delta(\epsilon_F - \frac{k^2}{2m}) \tag{8}$$

Since the initial Hamiltonian and the transport equations are rotationally invariant we can assume propagation only on [100] and with the use of the identities:

$$\int_0^{2\pi} d\theta(\cos(\theta))^n = \frac{(1+(-1)^n)\sqrt{\pi}\Gamma(\frac{1+n}{2})}{\Gamma(1+\frac{n}{2})} \tag{9}$$

$$\sum_{n=1}^{\infty}\frac{(1+(-1)^n)\sqrt{\pi}\Gamma(\frac{1+n}{2})}{\Gamma(1+\frac{n}{2})}\frac{1}{2\pi}a^n = \frac{1-\sqrt{1-a^2}}{\sqrt{1-a^2}} \tag{10}$$

we can integrate over the Fermi surface angles to obtain the structure factor pole:

$$S(\omega,q) = \frac{1}{i\omega - \frac{1}{\tau} + \frac{1}{\tau}\frac{1}{\sqrt{1-\frac{v_F^2 q^2}{(\omega+\frac{i}{\tau})^2}}}} \tag{11}$$

The correct interpretation of our structure factor requires consistently picking a branch of the square-root function in the denominator. We pick the branch cut along the positive x-axis. The pole in the structure factor represents the characteristic frequencies of the system:

$$\omega_{1,2} = -\frac{i}{\tau} \pm \sqrt{q^2 v_F^2 - \frac{1}{\tau^2}} \tag{12}$$

which in the diffusive and ballistic limits reduces to the well known expressions:

$$\begin{aligned} \tau \to \infty &\Rightarrow \omega_{1,2} \approx \pm v_F q \\ \tau \to 0 &\Rightarrow \omega \approx -iDq^2 \end{aligned} \tag{13}$$

where $D = v_F^2\tau/2$. The presence of only one (exponentially decaying) solution in the diffusive limit follows directly from correctly treating the branch-cut singularity in our structure factor. It can then be seen that the exponentially divergent solution $\omega \approx iDq^2$ is a false pole of Eq[11].

Although not of immediate interest to the present paper, we also present the structure factor for a bulk Fermi gas in the presence of disorder. With the density of states defined as $\nu = \frac{(2m)^{3/2}E_F^{1/2}}{4\pi^2}$ the transport equation becomes:

$$- i\omega\rho = -i\int\int\int \frac{d\phi\sin\theta d\theta k^2 dk}{(2\pi)^4\nu\tau}\Omega\sum_{n=1}^{\infty} g_n \qquad (14)$$

where g_n and Ω are as before and $\Omega = \omega + i/\tau$. Rotational invariance allows us to take $k_i = k_z$ and we obtain:

$$- i\Omega\rho = \frac{mk_F}{(2\pi)^2\nu\tau}\sum_{n=0}^{\infty}\left(\frac{v_F q}{\Omega}\right)\int_{-1}^{1} x^n dx = \frac{mk_F}{(2\pi)^2\nu\tau}\frac{\Omega}{v_F q}\ln\left(\frac{1+\frac{q}{v_F\Omega}}{1-\frac{q}{v_F\Omega}}\right)\rho \qquad (15)$$

Introducing the three-dimensional density of states at the Fermi surface, as well as a δ-function source term, the structure factor reads:

$$\rho = \frac{1}{i\Omega + \frac{\Omega}{2\tau v_F q}\ln\left(\frac{1+\frac{q}{v_F\Omega}}{1-\frac{q}{v_F\Omega}}\right)} \qquad (16)$$

To see the diffusive pole we need to carefully expand the logarithm:

$$\tau \to 0: \quad \rho = \frac{1}{i\omega - \frac{v_F^2\tau}{3}q^2} \qquad (17)$$

Which is the right diffusive pole in $3D$. For the ballistic pole we solve the equation (the one below is valid for any τ):

$$\omega = v_F q\frac{e^{-iv_F q\tau} + e^{iv_F q\tau}}{e^{-iv_F q\tau} - e^{iv_F q\tau}} - \frac{i}{\tau} \qquad (18)$$

In the ballistic limit $\tau \to \infty$ the exponentials in the fraction are oscillating wildly and must be regularized. Depending on on the regularization $q \to q + 0^{\pm}$ the characteristic frequencies are:

$$\omega = \pm v_F q \qquad (19)$$

which are the ballistic poles.

Having solved the free-Fermi gas case, we now add spin-orbit coupling at the special $SU(2)$ symmetric point of the Persistent Spin Helix. Following [16], we express the spin-orbit coupling Hamiltonian Eq.[1] in the form of a background non-abelian gauge potential $\mathcal{H}_{\rm ReD} = \frac{k_-^2}{2m} + \frac{1}{2m}(k_+ - 2m\alpha\sigma_z)^2 + const.$ where the field strength vanishes identically for $\alpha = \beta$. Therefore, we can eliminate the vector potential by a non-abelian gauge transformation: $\Psi_\uparrow(x_+, x_-) \to \exp(i2m\alpha x_+)\Psi_\uparrow(x_+, x_-)$, $\Psi_\downarrow(x_+, x_-) \to \exp(-i2m\alpha x_+)\Psi_\downarrow(x_+, x_-)$. Under this transformation, the spin-orbit coupled Hamiltonian is mapped to that of the free Fermi gas, but, while diagonal operators such as the charge n and S_z remain unchanged, off-diagonal operators, such as $S^-(\vec{x}) = \psi_\downarrow^\dagger(\vec{x})\psi_\uparrow(\vec{x})$ and $S^+(\vec{x}) = \psi_\uparrow^\dagger(\vec{x})\psi_\downarrow(\vec{x})$ are transformed: $S^-(\vec{x}) \to \exp(-i\vec{Q}\cdot\vec{r})S^-(\vec{x})$, $S^+(\vec{x}) \to \exp(i\vec{Q}\cdot\vec{r})S^+(\vec{x})$. Here $\vec{Q}$ is the shifting wavevector of the spin-orbit coupled Hamiltonian. Since in the gauge transformed basis, all three components of the spin and charge have the structure factor derived above, in the original (experimentally measurable) basis, the S_x and S_y have the following form:

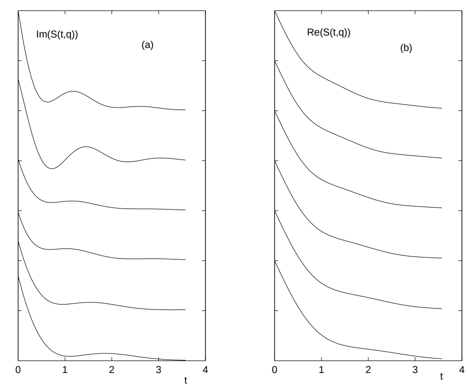

FIG. 2: (a) The imaginary part and (b) the real part of $S(t, q)$. We set $\tau = 1$. For both figures, from bottom to top, the curves are corresponding to $a = 2.2, 2.6, 3, 3.4, 3.8, 4.2$.

$$S^{\pm}(\omega, \vec{q}) = \frac{1}{i\omega - \frac{1}{\tau} + \frac{1}{\tau}\frac{1}{\sqrt{1-\frac{v_F^2(\vec{q}\pm\vec{Q})^2}{(\omega+\frac{i}{\tau})^2}}}} \qquad (20)$$

The above result represents the exact form factor for a spin-orbit coupled system valid everywhere from the diffusive to ballistic regimes. The Persistent Spin Helix is clearly maintained for any values of τ, α, v_f since $S(\omega, \vec{Q}) = 1/i\omega$ which renders the spin life-time infinite.

The transient grating experiments [17,19] measure the ω Fourrier transform of $S(\omega, q)$, i.e. $S(t, q) = \frac{1}{2\pi}\int dt e^{-i\omega t}S(\omega, q)$. $S(\omega, q)$ is analytic in the upper half complex plane. Thus, $S(t, q)$ is zero for $t < 0$. For $t > 0$,

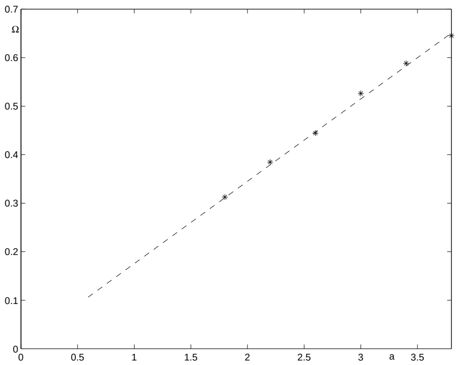

FIG. 3: The oscillation frequency Ω in the imaginary part of $S(t,q)$ as a function of $a = \nu_F|\vec{q} \pm \vec{Q}|\tau$.

by selecting the integral contour as shown in fig.(1), we obtain its real part and imaginary part as follows:

$$\frac{Im(S(t,q))}{e^{-\frac{t}{\tau}}} = \frac{a}{1+a^2} + P\int_a^\infty \frac{2}{\pi}\frac{\sqrt{x^2-a^2}cos(\frac{xt}{\tau})}{x(x^2-1-a^2)}$$
$$\frac{Re(S(t,q))}{e^{-\frac{t}{\tau}}} = -\frac{a^2+cos(\sqrt{1+a^2}\frac{t}{\tau})}{1+a^2} \qquad (21)$$

where $a = v_F|\vec{q} \pm \vec{Q}|\tau$ and P indicates the principal value of the integral.

In Fig.(2), we plot the real and imaginary part of $S(t,q)$ for different values of a. In the figure, we set $\tau = 1$ and from bottom to top, the curves are corresponding to $a = 2.2, 2.6, 3, 3.4, 3.8, 4.2$. Although the real part is clearly an oscillating function of t with an oscillation frequency, $\frac{\sqrt{1+a^2}}{\tau}$, the oscillation is not easily seen in the figure. However, the imaginary part has a much larger oscillation amplitude than the real part and the oscillation becomes clear as increasing a, reflecting the ballistic nature of the sample. The oscillation frequency Ω in the imaginary part is linearly dependent on a as shown in Fig.(3).

In this paper we have obtained the exact transport equations valid in the diffusive, ballistic, and crossover regimes of a special type of spin-orbit coupled system which enjoys an $SU(2)$ gauge symmetry. We obtained the exact form of the structure factors, and found the dependence of the spin-density as would be observed in a transient-grating experiment. It would be interesting to work out the transport equations in the diffusive-ballistic regime in perturbation theory away from the Persistent Spin Helix.

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[1] S. A. Wolf *et. al.*, Science **294**, 1488 (2001).
[2] J. Nitta *et. al.*, Phys. Rev. Lett. **78**, 1335 (1997).
[3] D. Grundler, Phys. Rev. Lett. **84**, 6074 (2000).
[4] Y. Kato *et. al.*, Phys. Rev. Lett. **93**, 176601 (2004).
[5] Y. Kato *et. al.*, Nature **427**, 50 (2004).
[6] C.P. Weber *et. al*, Nature **437**, 1330 (2005).
[7] S. Murakami, N. Nagaosa, and S. Zhang, Science **301**, 1348 (2003).
[8] J. Sinova *et. al.*, Phys. Rev. Lett. **92**, 126603 (2004).
[9] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
[10] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
[11] B.A. Bernevig and S.C. Zhang, Phys. Rev. Lett. **96**, 106802 (2006).
[12] B.A. Bernevig, T.L.Hughes, and S.C. Zhang, Science **314**, 1757 (2006).
[13] A. Burkov, A. Nunez, and A. MacDonald, Phys. Rev. B **70**, 155308 (2004).
[14] E.G. Mishchenko, A.V.Shytov, and B.I. Halperin, Phys. Rev. Lett. **93**, 226602 (2004).
[15] K. Nomura and *et. al.*, Phys. Rev. B **72**, 245330 (2005).
[16] B.A. Bernevig, J. Orenstein, and S.C. Zhang, Phys. Rev. Lett. **97**, 236601 (2006).
[17] C.P. Weber and J. Orenstein *et. al*, Phys. Rev. Lett. **98**, 076604 (2007).
[18] J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).
[19] N. Gedik *et. al.*, Science **300**, 1410 (2003).