BERRY'S PHASE AND WEAK LOCALIZATION IN THE PRESENCE OF SPIN-ORBIT INTERACTION

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ABSTRACT

Weak localization due to coherent back-scattering in the presence of spin-orbit coupling is examined for a possible manifestation of Berry's phase. The pairs of counter-propagating wave-amplitudes along the time-reversed Boltzmannian paths are shown to accumulate random relative phase which is purely geometric in the adiabatic limit. The resulting dephasing time τ_{so} has quartic field dependence and scales as c_i^{-1} and $c_i^{-2/3}$, respectively, in two and three dimensions, where c_i is the spin-orbit impurity concentration. Optimal experimental conditions are discussed.

THE existence and the operational meaning of the non-integrable geometric phase shift $\gamma(C)$ associated with the cyclic evolution of a quantum system as its Hamiltonian is modified adiabatically in time T along a closed circuit (C) in its parameter (R) space, has become the subject of intense discussion following the recent work of Berry[1]. This geometric phase was predicted in wave-optics by Pancharatnam[2]. Berry showed that in addition to the familiar dynamical phase factor

$$\exp\left(-\frac{i}{\hbar}\int_o^T E_n(R(t))\,\mathrm{d}t\right)$$

the system acquires a purely geometric phase factor $\exp(i\gamma(C))$, where $\gamma(C)$ depends on the circuit C but not on how C is traversed, providing adiabaticity of course. The sign of $\gamma(C)$ is the sense of the circuital traversal. In the particular case of a two-level system (e.g. a spin-1/2 object in a magnetic field), $\gamma(C)$ is simply half the solid angle subtended by C at the origin of the 3-dimensional parameter space (a purely geometric quantity). The origin is the point of degeneracy. The decomposition of the total phase shift between the dynamical and the geometric components is unambiguous in the adiabatic cyclic limit. The topological nature of this phase has now been well confirmed experimentally by several workers in optical[3-5], NQR[6] and polarized neutron spin rotation[7] experiments designed specifically to detect the phase. In this note we point out a natural manifestation of this geometric phase in the solid state phenomenon of magneto-conductance[8] in the weak localization[9] regime in the presence of spin-orbit coupling. This is an important problem in its own right, in the physics of quantum transport is disordered systems.

For the sake of clarity, let us first consider the following operational viewpoint. In principle a quantum system can be made to acquire the geometric phase shift $\gamma(C)$ by varying a parameter, say, by turning a 'knob' slowly. Operationally, however, this phase cannot be detected inasmuch as the phase is detected only by comparison, i.e. by interference of alternatives. There can be two kinds of interference experiments. In the first kind, exemplified by the Bohm-Aharonov effect in the parameter space, there is interference of the system with itself when the partial amplitudes propagate through the parameter space in a split-beam manner. Thus the system itself turns the 'knob'. Here the adiabatic condition may be effectively satisfied by the nature of the coupling (to vector potential). The second kind is more subtle, and is exemplified by a Stern-Gerlach type experiment. Here the system is factorizable into a fast (spin) subsystem S_1 and a slow (orbital) subsystem S_2. The fast (spin) sub-system S_1 evolves under its own (spin) Hamiltonian involving the parameters (magnetic field), but the latter are function of the slow (translational) degrees of freedom of S_2. The slow evolution of S_2 modifies adiabatically the parameters of S_1 causing it to pick up the geometric phase shift. Thus S_2 turns the 'knob' for S_1. In the following we will see that weak-localization provides an ideal system of the second kind.

Weak localization results from coherent back-scattering: the partial scattering amplitudes counter-propagating along a closed path returning to the origin, add up in phase in the absence of magnetic field, spin-orbit coupling or magnetic impurities, despite potential disorder assumed quenched (elastic scattering only). This doubling of back-scattered amplitudes reduces the diffusion coefficient—the weak localization effect in disordered systems, e.g. a-Mg. Now the dephasing of the partial amplitudes due to magnetic flux enclosed by the translatory motion (Aharonov-Bohm effect) and that due to dynamical spin-orbit coupling in the presence of heavier atoms, e.g. Au in a-Mg can lead to magneto-conductance. This has been studied extensively in recent years, theoretically as well as experimentally[8]. We will now show that under suitable conditions, realizable experimentally, the geometric phase shift due to spin-orbit coupling can become the dominant effect. Here adiabaticity would require strong magnetic field (large Zeeman splitting) and slow electrons (small Fermi speed).

The Hamiltonian describing the electron motion in a random potential (v_R) in the presence of an external field (h_o) and spin-orbit coupling is:

$$H = \frac{1}{2m}\left(\mathbf{P} - \frac{e}{c}\mathbf{A}\right)^2 + 2\mu_B\, h_o\, S_Z + \frac{\hbar}{2m^2c^2}\,(\mathbf{S}\times\nabla V_{\mathrm{imp}})\cdot\mathbf{P}, \tag{1}$$

with $\nabla\times\mathbf{A} = (0, 0\, h_o)$ and $\mathbf{S}$ the electron spin. As usual the translatory motion of the electron is assumed and determined by the random static potential (V_R) giving Boltzmannian diffusion coefficient $D_e = v_F\, l_e$ and a dimensionality (d)-dependent diffusion correction due to coherent backscattering. Here v_F is the Fermi speed and l_e the elastic mean-free path. Vector potential $\mathbf{A}$ leads to negative magneto-resistance by cutting off the diffusion correction through the Bohm–Aharonov type dephasing of the translational motion[8]. We will consider only the last two terms of (1) affecting the spin-wavefunction. The instantaneous magnetic field sensed by the electron spin is

$$\mathbf{h}(\mathbf{r}) = \mathbf{h}_o + \frac{1}{ec}(\nabla V_{\mathrm{imp}}\times\dot{\mathbf{r}}) \equiv \mathbf{h}_o + \mathbf{h}_{\mathrm{so}}(\mathbf{r}). \tag{2}$$

Here V_{imp} is a short-range potential due to the randomly distributed dilute concentration c_i of heavier impurity atoms (e.g. Au) with mean spacing $\gg$ meanfree path l_e due to disordered host (e.g., a-Mg). Thus, while the translatory motion may be taken to be diffusive (velocity not defined) on length scale $\gg l_e$, it is still smooth on the length scale $\sim$ range of V_{imp} with $|\dot{\mathbf{r}}(t)| = v_F$, that is we have constant speed but randomly changing direction at a mean rate $1/\tau_e = v_F/l_e$. In the parameter space of magnetic field the counter-propagating partial amplitudes trace out closed circuits P_i and $\bar{P}_i$ shown in figure 1 as the ith impurity is visited. Since P_i and $\bar{P}_i$ are traversed in the opposite sense, they contribute a relative phase shift $\Delta\phi_i$ given by the solid angle subtended at the origin:

$$|\Delta\phi_i| \sim \eta 4\pi (h_{\mathrm{so}}/h_o)^2, \tag{3}$$

where η is a numerical constant of order unity. Here h_{so} is the typical spin-orbit magnetic field. Now the mean time interval between such encounters is $c_i^{-2/d}/\mathfrak{D}_e$(= time to diffuse through mean impurity spacing). Thus in the circuit time T there will be $T\mathfrak{D}_e c_i^{2/d}$ such events. As $\Delta\phi_i$ are random in sign, we get for the root mean-squared phase shift $\Delta\phi$:

$$\Delta\phi \sim 4r\eta (T\mathfrak{D}_e\, c_i^{2/d})^{1/2}\,(h_{\mathrm{so}}/h_o)^2. \tag{4}$$

Now the dephasing time $T = \tau_{\mathrm{so}}$ can be estimated by requiring $\Delta\phi \sim 1$ giving

$$\tau_{\mathrm{so}} \sim \left(\frac{1}{16r^2\eta^2\mathfrak{D}_e c_i^{2/d}}\right)\left(\frac{h_o}{h_{\mathrm{so}}}\right)^4. \tag{5}$$

The above calculation assumes adiabaticity which must be examined now. The condition for adiabaticity is

$$\left(\frac{\hbar\, h_{\mathrm{so}}\, v_F}{4\mu_B h_o^2 \lambda_{\mathrm{so}}}\right) \ll 1, \tag{6}$$

where λ_{so} is the typical spatial range of the spin orbital field. Thus $\lambda_{\mathrm{so}}/v_F$ is the collision time during

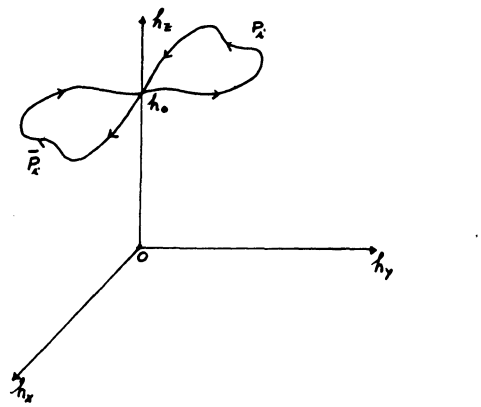

Figure 1. Showing schematically the trajectories P_i and $\bar{P}_i$ in the parameter space of the counter-propagating partial amplitudes as Ω = impurity is visited. Note the opposite sense of traversal due to velocity dependence of the spin-orbit magnetic field.

which the spin Hamiltonian changes by an amount $\sim \mu_B h_{so}$ while $2\mu_B h_0$ is the Zeeman splitting. Thus the larger Berry phase requires larger h_{so}/h_o but adiabaticity demands just the opposite.

We now consider the experimental situation and make order-of-magnitude estimates. First consider the two-dimensional case, 1d = 2. By this we mean sufficiently thin films (thickness $< 1_e$) but the spin orbit field $\mathbf{h}_{so}(\mathbf{r})$ is still three dimensions. We take external field parallel to the film so that the usual Aharonov-Bohm type translational dephasing is eliminated. Also, let the sample be free from magnetic impurities so that we are left just with the spin-orbital dephasing. We consider temperature low enough to eliminate inelastic cut-offs. Indeed, the inversion layer of a MOSFET or a heterostructure with proper doping is ideal for our purpose. For this situation we can have $v_F \sim 5\times 10^6$ cm^{-1}, for carrier concentration $\sim 2\times 10^{12}$ cm^{-2}, $h_o \sim 10$ tesla, $D_e = V_F l_e \sim 1$ cm^2 s^{-1}. Now for $h_{so} = Ev_{F/c}$ we take the Coulombic field E as due to a singly ionized impurity at a distances $\sim$ layer thickness ~ 5 Å. This gives $h_{so} \sim 50G$ for c_i we choose $\frac{1}{10}$-atomic layer coverage giving $c_i \sim 10^{14}$ cm^{-2}. Then we get $\tau_{so} \sim 10^{-9}$ s, and the adiabaticity parameter $\sim 10^{-1} \ll 1$. The diffusion correction to conductance in $d = 2$ is proportional to $\ln \tau_{so}/\tau_e$ and is thus measurable. For $d = 3$ with corresponding choice of parameters, we find τ_{so}^{1} large enough but the adiabaticity condition is badly violated. One needs systems with low carrier concentration (small v_F and, of course, small meanfree path). This should be possible with compensated semiconductors. The characteristic field and concentration dependence is verifiable. We should also remark here that in the adiabatic limit our system suffers no dynamical phase shift as the energy is simply exchanged between the spin and the translational degrees of freedom during the spin-orbital encounters. Also, simple estimates for the 3-dimensional case (where the adiabatic condition is violated) show that the probability of spin-flip (adiabatic leakage) is still quite small for a given encounter. Now a remark about the geometric phase and the dephasing due to magnetic impurities. In the adiabatic limit the cyclic evolution of a spin-1/2 system in a Zeeman field is a unitary transformation, e.g. $\exp(i\gamma\,\sigma_y)\exp(i_\beta\,\sigma_z)\exp(i\alpha\,\sigma_x)$, where α, β and γ evolve successively, slowly from zero to $\pi/4$. The Hamiltonian returns to the original value in this limit. The system, however, suffers a phase shift which is half the solid angle (octant) subtended at the origin in the parameter space of the Hamiltonian as predicted by the Berry-Pancharatnam formula. This is precisely what happens when the conduction electron spin suffers rotation due to coupling with the magnetic impurity spins. It is the non-commutativity of the rotations in the parameter space that gives this effect as the counter-propagating partial amplitudes visit the impurity spins in opposite sequences. Adiabaticity just provides a unique 'connection'.

Finally, we must note that an exact treatment of the scattering problem would of course, automatically include the geometric as well as the dynamical phase shift. It is, however, not clear if the perturbative treatments of Hikami, Larkin and Nagaoka and that of Maekawa and Fukuyama incorporate the geometric phase shift (for references see ref. 9). The point is that a dynamical treatment emphasizes *transition* between states while the geometric phase is associated with the adiabatic *modification* of the initial state. Further work is needed to analyse this point.

It can therefore be concluded that the Berry-Pancharatnam phase has experimental consequences for weak localization in the presence of spin-orbit coupling. Quartic-field and $c_i^{-2/d}$ concentration dependence for the dephasing time τ_{so} is predicted.

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