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Linear magnetoresistance in metals: Guiding center diffusion in a smooth random potential

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We predict that guiding center (GC) diffusion yields a linear and nonsaturating (transverse) magnetoresistance in 3D metals. Our theory is semiclassical and applies in the regime where the transport time is much greater than the cyclotron period and for weak disorder potentials which are slowly varying on a length scale much greater than the cyclotron radius. Under these conditions, orbits with small momenta along magnetic field \( \mathbf{B} \) are squeezed and dominate the transverse conductivity. When disorder potentials are stronger than the Debye frequency, linear magnetoresistance is predicted to survive up to room temperature and beyond. We argue that magnetoresistance from GC diffusion explains the recently observed giant linear magnetoresistance in 3D Dirac materials.

Magnetoresistance provides a powerful means with which to probe the scattering history of particles in a magnetic field. Departure from the conventional paradigm—quadratic magnetoresistance at low fields, saturating at high fields [1]—signals anomalous particle scattering behavior. One particularly appealing regime is nonsaturating and linear magnetoresistance (LMR), which has a long standing history [2–5] given its potentially disruptive technological impact [6].

Very few theories predict LMR in a closed single component Fermi surface. A well known example is Ref. [7], which showed that Dirac metals in the extreme quantum limit (when only the \( n = 0 \) Landau level is occupied) exhibit LMR in the presence of screened Coulomb impurities. Another mechanism yielding quasilinear MR arises from inhomogeneity [8–10]. However, significant LMR in these requires strong inhomogeneity [10]. Contemporary proposals that extend the above treatments have also found LMR under similar requirements [11–12].

Recently, giant LMR that lie outside the above two paradigms [see (i) and (ii) below] were reported in the newly discovered class of three-dimensional Dirac materials (3DDM) [13–17]. LMR in 3DDM exhibit puzzling features including (i) its occurrence when multiple Landau levels are occupied far from the extreme quantum limit, and (ii) arising in weakly disordered, high mobility samples. Further, LMR manifests consistently over a variety of 3DDM experiments, including in TiBiSSe [13], Cd3As2 [14,15], Na3Bi [16], and TaAs [17], where chemical potential \( \mu \) typically lies 0.1 eV above the Dirac point, hinting at a single underlying explanation.

Here we propose a semiclassical mechanism for LMR in metals, wherein charge transport is dominated by guiding center (GC) motion. Importantly, this mechanism naturally gives giant LMR under (i) and (ii) above, explaining the puzzling behavior [13–17]. The main requirement is that the disorder potential is smoothly varying on a scale \( \xi \) which is large as compared to the cyclotron radius \( r_c \). The main features of GC magnetoresistance are exposed by writing the transverse resistivity as

\[
\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} = \frac{\mathcal{G}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \quad \mathcal{G} = \frac{\tan \theta_H}{1 + [\tan \theta_H]^2},
\]

where \( \sigma_{xx} \) and \( \sigma_{xy} \) are the transverse (\( x-y \) plane) conductivity and Hall conductivities, respectively, and \( \tan \theta_H = \sigma_{xy}/\sigma_{xx} \) is the Hall angle. Using the familiar \( \sigma_{xy} = ne/B \) with \( n \) the density and \( e \) the carrier charge, we have

\[
\rho_{xx} = \frac{B\mathcal{G}}{ne^2}.
\]

As we argue below, in the regime of \( \omega_c \tau \gg 1 \) and \( \xi \gg r_c \), GC diffusion gives a Hall angle, and therefore \( \mathcal{G} \), that is independent of magnetic field magnitude, leading to LMR in Eq. (2). Here \( \omega_c \) is the cyclotron frequency, \( \tau \) is the transport time, and the magnetic field \( \mathbf{B} = B\hat{z} \).

Guiding center magnetoresistance can be understood as follows. In semiclassically large \( B \) fields \( (\omega_c \tau \gg 1) \), electrons exhibit in-plane trajectories \( \mathbf{r}_z(t) \) characterized by slow guiding center motion \( \mathbf{R}(t) \) accompanied by fast cyclotron orbits \( \mathbf{r}_{\text{cycl}}(t) \). The latter, characterized by \( r_c \), depends on intrinsic material properties and \( B \); whereas the former depends on the potential profile sampled by the electron over one cycle which can yield unusual trajectories [18]. A unique situation arises for slowly varying disorder potentials \( V(r) \). In this regime \( \xi \gg r_c \) [see Fig. 1(a)], electron trajectories are dominated by guiding center motion which follows the local disorder landscape at \( \mathbf{R} \), with velocity \( \mathbf{v}_{gc} = [\nabla_V V(\mathbf{R})] \times \hat{\mathbf{z}}/B \).

Guiding center diffusion is characterized by diffusion constant \( D_{\text{gc}} \sim v_{gc}^2 \tau \). The central question is: what is \( \tau \)? First, it is important to note this picture is not valid in strictly 2D, because GCs form closed orbits along equipotential lines. Hence it is crucial to include motion in the \( z \) direction which restores diffusive motion. There are two classes of electron motion depending on their \( k_z \) value with respect to \( k^*_z \) [Fig. 1(b)]. For \( k_z > k^*_z \), electrons possess kinetic energy in the \( z \) direction exceeding the typical potential fluctuation. As a result, the electron moves freely across many potential fluctuations shown in Fig. 1(d). Within time \( \tau_z \approx \xi/v_z \), the GC senses a different local electric field and changes direction. As a result, \( D_{\text{gc}}(k_z > k^*_z) \sim v_{gc}^2 \tau_z \propto 1/B^2 \). Using \( \sigma_{xy} = ne/B \) and Eq. (1), we recover the standard saturated magnetoresistance.

On the other hand, electrons with \( k_z < k^*_z \) are typically squeezed by a local potential barrier. As shown in Fig. 1(c),
Instead we are interested in LMR in 3DDM [13–17] which are observed in the metallic regime with carriers of a single type [14].

We begin by considering the diffusive motion of charged particles in a magnetic field $\mathbf{B} = B\mathbf{z}$ and a slowly varying and weak disorder potential $V(\mathbf{r})$. While formally interested in 3DDM, our analysis below is general; we will only specify 3DDM as needed to compare to recent experiments. Disorder is characterized by $\langle V(\mathbf{r})V(\mathbf{r}')\rangle = V_0^2\mathcal{F}(|\mathbf{r} - \mathbf{r}'|/\xi)$, where $\mathcal{O}$ denotes disorder averaging and $\xi$ the correlation length. $\mathcal{F}$ is a dimensionless function that vanishes for $|\mathbf{r} - \mathbf{r}'| \gg \xi$. Lastly, we will be interested in weak disorder strength $eV_0 < \mu$ seen in 3DDM experiments [13–17] and recent estimates [22].

Equations of motion. The motion of particles on the Fermi surface with chemical potential $\mu$ can be described by the semiclassical equations of motion

\[ m\mathbf{v}_\perp = -e\mathbf{v}_\perp \times \mathbf{B}, \]

\[ m\dot{v}_z = -e\partial_z V(\mathbf{r}), \]

where $m$ is the cyclotron mass, $v_{\perp,kz,\mu} = (v_x, v_y)$, and $v_{z,kz,\mu}$ are velocities transverse to the magnetic field and along the magnetic field, respectively. We note that throughout our analysis below, these quantities depend on momentum along the field, $k_z$, and $\mu$. For, e.g., velocity is captured via group velocity $v_k = h^{-1}\partial \mathbf{r}/\partial \mathbf{k}$ so that the $x$-$y$ plane speed for Dirac particles is $|v_{\perp}| = v_F \sqrt{1 - k_z^2/k_F^2}$, and $m = \mu/v_F^2$ [25], where $v_F$ is Fermi velocity and $k_F$ the Fermi wave vector; $\epsilon_k$ is the particle dispersion. For brevity, we will drop explicit mention of $k_z$ dependence, bringing it up when necessary. We do not expect Berry phase related terms to contribute to the transverse magnetoresistance behavior that we are interested in here [26].

The trajectories of charged particles $\mathbf{r}(t)$ in crossed $\mathbf{B}$ and $V(\mathbf{r})$ can be complex, since they involve transport processes spanning multiple time scales (e.g., cyclotron period, guiding center scattering time, and transport time). However, in semiclassically strong fields ($\omega_c \tau_{tr} \gg 1$), and for a slowly varying potential so that correlation length is larger than cyclotron radius ($\xi \gg r_c$), its motion is conveniently captured via $\mathbf{r}(t) = \mathbf{R}(t) + r_{cycl}(t)$. Here $\mathbf{R}(t)$ is the slow moving 3D guiding center coordinate, whereas $r_{cycl}(t)$ describes fast cyclotron motion lying in the $x$-$y$ plane.

This reasoning yields the following ansatz for velocity in the $\mathbf{r}_\perp = (r_x, r_y)$ plane $\mathbf{v}_\perp$ as [18]

\[ \hat{v}_\perp(t) = v_{\perp0}e^{\omega_c t} + \hat{v}_{gc}(t), \]

\[ \hat{v}_{gc} = \frac{i\tilde{E}(\tilde{r}_\perp)}{B}, \]

where $\omega_c = eB/m$, and we used complex notation $\mathbf{a} = a_x + i a_y$ for vectors in the $x$-$y$ plane. The latter part of Eq. (4) was obtained by substituting the ansatz into Eq. (3a) and setting $mv_{gc} = 0$ for slowly varying $V(\tilde{r})$. Equation (4) is valid for $|mv_{gc}| \ll |e\tilde{E}(\tilde{r}_\perp)|$. Estimating $E \approx V_0/\xi$, we obtain the condition

\[ \xi^2 \gg eV_0/\omega_c^2 m = r_c^2 eV_0/\mu, \]

where $r_c = v_0/\omega_c$. Since we are interested in weak disorder $eV_0 < \mu$, the above condition is satisfied within our regime of validity, $\xi \gg r_c$. 

![FIG. 1. (Color online) (a) Magnetoresistance can be dominated by guiding center (GC) motion when disorder correlation lengths $\xi \gg r_c$. Here $r_c$ is the cyclotron radius. This regime is characterized by slow GC motion, $v_{gc} = v_F V(\mathbf{r})/\hat{z}/B$, accompanied by fast cyclotron orbits, $v_{cycl}$. GC diffusion in this environment gives rise to LMR. (b) Electrons perform closed orbits of the Fermi surface, with GC motion classified into two types, $k_z < k_z^c$ (red) and $k_z > k_z^c$ (blue); critical $k_z^c$ (green). (c) For $k_z < k_z^c$, electrons are squeezed in $z$ yielding mean free paths $\ell \approx \xi$ and in-plane $D_{xx} \sim v_{gc}\xi \propto 1/B$. (d) In contrast, $k_z > k_z^c$ electrons exhibit unconstrained $z$ motion yielding in-plane $D_{xx} \sim v_{gc}^2/\xi v_z \propto 1/B^2$ (see text).](image)
Motion in $z$ can be understood in the following way. First, we note that for $\xi \gg r_c$ and $\omega_c v_{tr} \gg 1$, the potential the electron feels is determined by $(\mathbf{r}(t))_{\text{cycle}} = \mathbf{r}(t)$. Next, for $v_{gc} \ll v_e$ electrons, the GC moves slowly in the $x$-$y$ plane as compared with $z$. As a result, integrating Eq. (3b) yields energy conservation

$$\frac{m}{2} \left[ v_{zGC}^2(R(t)) - v_z^2(R(0)) \right] = -e \left[ V(R(t)) - V(R(0)) \right], \tag{6}$$

where we have set $v_{z}\mathbf{V}(\mathbf{r}) \cdot \partial_{r_c} = 0$. This is valid when $\mathbf{V}(\mathbf{r}) \cdot \partial_{r_c} \ll |v_e \partial_{r_c} V(\mathbf{r})|$. Estimating $|\partial_{r_c} V| \approx v_{gc}$ and using disorder that is isotropic yields the original condition $v_{gc} \ll v_e$.

**Guiding Center Transport.** The separation of time scales between slow GC motion and fast cyclotron motion enables us to write the velocity correlator as

$$\langle v_{z}(t)v_{z}(0) \rangle \approx \langle v_{gc}(t)v_{gc}(0) \rangle + v_{0}^2 e^{i\omega_{c}(t-t)/\tau}, \tag{7}$$

where we have used a relaxation-time approximation in the last term to capture the Drude contribution to magnetotransport [18]. Replacing $\mathbf{r}(t)$ with its average over one cycle as above, and using Eq. (4), we find GC diffusion, $D_{gs}^{GC} = (1/2) \int_0^\infty \langle v_{gc}(t)v_{gc}(0) \rangle dt$, as

$$D_{gs}^{GC} = \int_0^\infty \langle E[R(t)]E[0]|(2B^2) \rangle dt = E_0^2 \tau/(2B^2),$$

$$\tau = \int_0^\infty dt F(\Delta R/\xi), \tag{8}$$

where $\Delta R = |\mathbf{R}(t) - \mathbf{R}(0)|$, $E_0$ is the characteristic electric field strength of the disorder potential, and $\tau$ is the scattering time that is sensitive to the GC trajectory.

We adopt a mean-field approach in estimating $\tau$. Since $F$ rapidly decays for $\Delta R > \xi$, $\tau$ is most sensitive to the way the GC moves in $\Delta R(t) < \xi$. As a result, we write $d\Delta R = v_{zGC} dt$, with speed $v_{zGC} = \langle |v_{gc}(x)| + \langle v_e^2 \rangle \rangle^{1/2}$ averaged over a single domain; here $\langle \rangle_k$ denotes averaging across a single domain. Changing variables $t \to \Delta R$ yields

$$\tau \approx \frac{\xi A}{\langle |v_{gc}(x)| + \langle v_e^2 \rangle \rangle^{1/2}}, \quad A = \int_0^\infty dx F(x), \tag{9}$$

where $A$ is a number of order unity. Using gaussian correlations, $\langle V(x)V(0) \rangle = V_0^2 F(x) = V_0^2 e^{-x^2/\sigma^2}$, we obtain $A = \sqrt{\pi}/2$ and $\sigma^2 \approx 6V_0^2$.

Two distinct classes of GC trajectories can be discerned: (a) squeezed $z$ motion [Fig. 1(c)] and (b) unrestricted $z$ motion [Fig. 1(d)]. Squeezing in class (a) arises from energy conservation in Eq. (6): For particles with $mv_{zGC}^2/2 < \mathbf{V}(\mathbf{r})$, $z$ motion is constrained within a $V(\mathbf{r})$ puddle. It escapes when GC diffuses out of the $V(\mathbf{r})$ puddle [Fig. 1(c)]. Squeezing yields $\langle v_z \rangle \xi$ that vanishes and $v_{zGC} \approx \langle v_{gc} \rangle \xi \approx E_0/B$. As a result, Eq. (9) yields $\tau \approx \xi A/\langle v_{gc} \rangle \xi$ and

$$D_{gs}^{GC} = \frac{E_0 \xi A}{2B}, \quad \text{for } v_z \leq (e2V_0/m)^{1/2} = v_e, \tag{10}$$

corresponding to electrons in Fig. 1(b) with $k_z < k_z^* < k_z^{**}$; $k_z^{**}$ depends on the dispersion relation and $v_e$. For 3DDM, $\hbar k_z^{**} = (e2V_0/\mu)^{1/2}$. We note that Eq. (6) can only be used for electrons with $v_{zGC} \gg v_{gc}$, Eq. (6). However, in the opposite limit $v_z \ll v_{gc}$, $\langle v_z \rangle \xi$ is obviously smaller than $\langle v_{gc} \rangle \xi$ in Eq. (9), allowing us to neglect the former’s contribution, yielding $D_{gs}^{GC}$ as in Eq. (10). As a consistency check, we note that $v_z \gg v_{gc}$ for our regime of validity $\xi \gg r_c$, $eV_0/\mu < 1$. Therefore $v_z$ determines the range of electrons that obey Eq. (10).

In contrast to Eq. (10), electrons with $v_z \gg v_e$ do not have $z$ motion squeezed [case (b), see Fig. 1(d)]. As a result, GC samples many $V(\mathbf{r})$ domains, with its $x$-$y$ plane velocity scrambled over times $\tau_r \sim \xi/v_z$, yielding an $x$-$y$ plane mean free path $\ell \sim v_{gc}/(\xi/v_z)$. This is captured in Eq. (9) where $\langle v_{zGC} \rangle \xi \ll \langle v_e \rangle \xi$, giving $v_{zGC} \approx \langle v_e \rangle \xi \approx v_e$. As a result, Eq. (9) yields $D_{gs}^{GC} \propto 1/B^2$. Importantly, for sufficiently large $B$, $v_z > v_e$ electrons, while mobile in the $z$ direction, exhibit suppressed $x$-$y$ plane mobility as compared with $v_z < v_e$. As a result, class (a) trajectories dominate $x$-$y$ plane transport.

**Linear magnetoresistance in 3DDM.** To illustrate the striking effects of GC diffusion we specialize to 3DDM. Using the Einstein relation, and Eqs. (8)–(10), we obtain

$$\sigma_{xx}^{GC} = e^2 \sum_k D_{gs}^{GC}(k) \delta(\epsilon_k - \mu) = a \left[ \frac{1}{B} + \frac{B}{B_c} \right], \tag{11}$$

where $\epsilon_k$ is the electron energy, $a/(e^2\nu_{2D}) \approx E_0\epsilon x A k_z^*/(4\pi)$, and $B \approx (E_0/v_e) \times \ln(k_F/k^*)$. Here we have used the 2D density of states for a $k_z$ slice in 3DDM as $\nu_{2D}(\mu) = \sum_{k_z, k} \delta(\epsilon_k - \mu) = \mu/2\pi \hbar^2 v_e^2$, and $D_{gs}^{GC}(k_z)$ obtained from the two trajectory classes (a) and (b). We note that the first term dominates over the second when $B > B_c$. It is useful to rewrite this condition as $r_c < \xi K$, where $K = \sqrt[2]{2(\epsilon_x/v_0)} \langle \ln(k_F/k^*) \rangle^{-1} \approx 1$, since we are interested in $\mu > eV_0$. Hence, the first term always dominates in our regime of validity, $\xi \gg r_c$.

In the same way, the second term in Eq. (7) yields the usual expressions

$$\sigma_{xx}^{2D} = \sum_{k_z} \xi \tau_r, \quad \sigma_{yy} = \sum_{k_z} \xi \omega_c \tau_r^2 \approx \frac{ne}{B}, \tag{12}$$

where $\xi = e^2\nu_{2D}(\mu)v_0^2/[2(1 + \omega_c^2 v_0^2)]$; we have taken $\omega_c \tau_r \gg 1$ in the last expression. Since $\sigma_{xx}^{2D} \propto 1/B^2$, for sufficiently large fields it provides a negligible contribution to $\sigma_{xx}$ as compared with Eq. (11).

An important diagnostic of magnetotransport is the Hall angle, tan$\theta_H = \rho_{xy}/\rho_{xx} = \sigma_{xy}/\sigma_{xx}$. Using Eq. (11) and writing $\sigma_{xx} = \sigma_{xx}^{GC}$ (neglecting $\sigma_{xx}^{2D}$ since $\omega_c \tau_r \gg 1$), we obtain a $B$-field magnitude independent

$$\tan\theta_H = \frac{2}{\sqrt{2\pi}} \left( \frac{\mu}{eV_0} \right)^{3/2}, \tag{13}$$

where we have used $n = \mu^2/(\pi^2 e^2 V_0^2)$ for a single fermion flavor in 3DDM and gaussian correlated $\langle V(\mathbf{r})V(\mathbf{r'}) \rangle$. We note that the Hall angle changes sign when $B$ field flips sign. Interestingly, the Hall angle can be tuned by $V_0$ and $\mu$. Estimating $V_0 \approx 20$ mV in 3DDM [22] and $\mu \sim 0.1$ eV [13–17], we obtain tan$\theta_H \approx 2.4$.

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1 Using Eq. (4), Eq. (10), and $E_0 \approx V_0/\xi$ yields $v_z/v_{gc} \approx \sqrt{\langle (\xi/r_c)(\mu/eV_0)^{1/2} \rangle}$. 

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We note that tunable Hall angle [Eq. (13)] controls $G$. Indeed, $G$ is a nonmonotonic function of Hall angle (and hence it depends on $\mu/eV_0$), reaching a peak when Hall angle becomes unity.

To summarize, we find that under the conditions $\omega_c\tau_r \gg 1$, $\xi \gg r_c$, $\mu > eV_0$, $G$ is independent of $B$ field magnitude, yielding LMR according to Eq. (2). Of the first two conditions, $\xi \gg r_c$ can be expressed as $B > B_0 = m v_F/|e\xi|$ which is a more stringent condition than $\omega_c\tau_r \gg 1$. This is seen by estimating $\tau_{tr}$ using the Born approximation, giving $B_r$ that exceeds the field marking the onset of $\omega_c\tau_r > 1$ by a factor $\sim (\mu/eV_0)^2$. Hence, we predict LMR as long as $B > B_0$.

An important figure of merit for magnetoresistance is the ratio $MR = \rho_{xx}(B)/\rho_{xx}(0)$. Using Eq. (2), and noting the mobility $\eta = \sigma_{xx}(0)/ne$, we obtain

$$MR = \frac{\rho_{xx}(B) - \rho_{xx}(0)}{\rho_{xx}(0)} \approx \left(\frac{\eta [\text{cm}^2/\text{Vs}]}{10^4}\right) B |T| G.$$  

(14)

For typical $\eta \approx 1 - 20 \times 10^4 \text{cm}^2/\text{Vs}$ in 3DDM, Eq. (14) yields giant $MR \approx 5-100$ at $B = 10$ T. Here we have used maximal $G = 1/2$. For fixed $G$, Eq. (14) is consistent with Kohler’s rule [27] since it scales with mobility. This mirrors the experiments where $MR$ scaled with temperature dependent mobility over a wide range of $B$ [15].

We note that our treatment above follows through for other dispersions as well, yielding LMR under the same conditions of $\omega_c\tau_r \gg 1$, $\xi \gg r_c$, $\mu > eV_0$. However, features, e.g., $k^2\alpha$, $\alpha$, and Hall angle are altered appropriately.\textsuperscript{2}

\textit{Inelastic scattering.} Energy relaxation through inelastic scattering (e.g., through phonon scattering) in the $z$ direction can drastically affect GC motion by mixing squeezed $z$ with unconstrained $z$ trajectories. Absorption of phonons with $h\omega \gtrsim V_0 - \frac{1}{2}v_{eD}^2$ relaxes the energy constraint [Eq. (6)], allowing $v_z < v_z$ electrons to jump out of $V(r)$ troughs. If $\tau_c \approx \xi/v_{pe} \gg \tau_{tr}(e = V_0 - \frac{1}{2}v_z^2)$, these electrons exhibit $D_{xx}(k_z) \propto 1/B^2$. Here $\tau_{tr}(e)$ is the time for an electron to absorb energy $e$. Suppressed at low $T$, phonon-assisted escape leads to LMR degradation when $k_BT \gtrsim V_0$.

However, when typical $V_0 > h\omega_{pe}$, phonon-assisted escape becomes difficult even at high temperatures since the maximum energy that can be absorbed from phonons is $h\omega_{pe} \ll V_0$; $\omega_{pe}$ is the Debye frequency. As a result, in this regime LMR is stable even at high temperatures and large fields, as recently observed in Cd$_3$As$_2$ [14,15] where LMR persisted at 300 K and high fields.

While detrimental to LMR from GC diffusion in 3D, inelastic scattering can have the opposite effect in 2D. Conventionally in 2D, GCs form closed orbits along equipotential lines of a disorder potential yielding localization behavior [28]. However, for inelastic phonon scattering which is not so strong to entirely disrupt the GC motion, but strong enough ($\xi/v_{pe} \gg \tau_{tr}$) to induce switching between adjacent equipotentials [29], the GC trajectories can become open, moving through multiple $V(r)$ domains. In this regime, we speculate $D_{xx}^{2D} \sim v_{pe}\xi \propto 1/B$ as above. Interestingly, 2D semiclassical regime LMR was reported previously [30].

Semiclassical GC diffusion can conspire to produce LMR in metals. Importantly, the requirements for GC magnetoresistance are modest, arising in the semiclassical regime with multiple occupied Landau levels and for weak and smooth disorder. Giant MR ratios, $B$-field magnitude independent Hall angles, $\mu$ and $V_0$ tunability, and stability at high temperatures make GC diffusion and its magnetoresistance easy to identify in experiment. Indeed, these features bear striking resemblance to LMR measured recently in a variety of 3DDM [13–17]. Additionally, oscillatory motion of the GC trajectories along $B$ could have interesting, polarization-dependent, absorption signatures in the Terahertz regime.

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