Dissipationless Circulating Currents and Fringe Magnetic Fields Near a Single Spin Embedded in a Two-Dimensional Electron Gas

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Theoretical calculations predict the dissipationless circulating current induced by a spin defect in a two-dimensional electron gas with spin-orbit coupling. The shape and spatial extent of these dissipationless circulating currents depends dramatically on the relative strengths of spin-orbit fields with differing spatial symmetry, offering the potential to use an electric gate to manipulate nanoscale magnetic fields and couple magnetic defects. The spatial structure of the magnetic field produced by this current is calculated and provides a direct way to measure the spin-orbit fields of the host, as well as the defect spin orientation, e.g. through scanning nanoscale magnetometry.

Single spins associated with point defects in solid-state materials are promising candidates for qubits and novel quantum spintronic devices for communication, sensing, and information processing\textsuperscript{[15]}. Isolated magnetic dopants embedded in two-dimensional electron gases (2DEG) with spin-orbit coupling (SOC) can be electrically and optically addressed\textsuperscript{[9]–[12]} and coherently manipulated. Control of the relative phases of defect spin wave functions through manipulation of the spin-spin coupling enables spin-based quantum computation\textsuperscript{[13]}. To date most spin-spin couplings are achieved either through dipolar magnetic fields arising from the spin\textsuperscript{[9]–[10]}, which are difficult to tune, or through photonic coupling\textsuperscript{[11]}, which is effective for much longer distances. The magnetic moment of a bare spin is modified by the spin-orbit interaction of the host, leading to proposals for single-spin control via \( g \)-tensor manipulation\textsuperscript{[12]–[14]}, however the effects on nanoscale dipolar fields and the consequences for coupling spins remain unexplored.

Here we derive the dissipationless circulating current surrounding a spin embedded in a 2DEG with spin-orbit coupling, and show that these effects are significant and their spatial structure is detectable by current nanoscale magnetometry\textsuperscript{[20]–[23]}. The spin-orbit interaction in a 2DEG can be modified with a perpendicular electric field (without dissipative current flow) thus we further propose that modifying these magnetic fields provides a method of electrically tuning spin-spin interactions to produce quantum entangling gates. Our results rely on a method of electrically tuning spin-spin interactions to propose that modifying these magnetic fields provides the critical role of effective spin-orbit vector potentials\textsuperscript{[11]}, which is effective for much longer distances.

The derived effective spin-orbit interaction\textsuperscript{[14]} is evaluated using the Green’s function (GF) scattering formalism, which is effective for many-body interactions\textsuperscript{[41]}. Another option relies on recent advances in electron ptychography for direct sensing\textsuperscript{[38]}.

Central to our results is the derivation of the current operator associated with the effective Hamiltonian describing a 2DEG with SOC,

\[
H = \frac{\hbar^2 k^2}{2m^*} + \alpha (\sigma_x k_y - \sigma_y k_x) + \beta (\sigma_x k_x - \sigma_y k_y). \quad (1)
\]

The spin orbit fields linear in crystal momentum \( \mathbf{k} \) emerge from both the crystal’s bulk inversion asymmetry (BIA, with coefficient \( \beta \))\textsuperscript{[39]} and the inversion asymmetry of the heterostructure (SIA, with coefficient \( \alpha \), which can be tuned by applied electric fields perpendicular to the 2DEG plane)\textsuperscript{[40]}. We derive the current operator (see Supplementary Material \textsuperscript{[41]}) from the steady-state continuity equation \( \partial_t n + \nabla \cdot \mathbf{j} = 0 \) and group the spin-orbit terms together in an effective spin-dependent vector potential \( \mathbf{A}_{so} \).

The expected value of the charge current is evaluated using the Green’s function (GF) scattering formalism,

\[
\mathbf{j}(\mathbf{r}) = -\frac{e\hbar}{2\pi m^*} \text{Im} \int_{E_{so}}^{E_f} (t_\uparrow - t_\downarrow) \left\{ i \left[ (\nabla G_{\uparrow\downarrow}^0) C_{\downarrow\uparrow}^0 - (\nabla G_{\downarrow\uparrow}^0) C_{\uparrow\downarrow}^0 \right] - \frac{2e}{\hbar} (A_{so\uparrow}^\dagger C_{\downarrow\uparrow}^0 - A_{so\downarrow}^\dagger G_{\downarrow\uparrow}^0) G_{\uparrow\downarrow}^0 \right\} dE. \quad (2)
\]
where \( G^0(\mathbf{r}, \mathbf{r}') \) are the 2DEG retarded GFs, \( t_\sigma \) are the defect T-matrix elements with spin projection \( \sigma \), \( E_{so} \) is the energy minimum of the 2DEG, \( E_f \) is the Fermi energy (determined by the electron density \( n \)) and the effective vector potential

\[
A_{so} = \frac{\hbar E_{so}}{e} \left\{ \left[ \sigma_x \cos(\theta - \tau) - \sigma_y \sin(\theta + \tau) \right] \hat{r} + \left[ \sigma_x \sin(\theta - \tau) - \sigma_y \cos(\theta + \tau) \right] \hat{\theta} \right\},
\]

with \( \tau = \tan(\alpha/\beta) \) and \( k_{so} = (m^* / \hbar^2) \sqrt{\alpha^2 + \beta^2} \).

The retarded Green’s function from Eq. (1) is

\[
g^0(\mathbf{k}; E) = \left( \frac{2m^*}{\hbar^2} \right) \frac{(k_E^2 - k^2)\sigma_0 - 2k_{so}k[U_x\sigma_x - U_y\sigma_y]}{k_E^2 - 2k^2[k_E^2 + 2k_{so}f_\tau(\theta_k)] + k^4}
\]

where \( k_E^2 = 2m^*E/\hbar^2 \) and \( f_\tau(\theta_k) = 1 + \sin(2\tau) \sin(2\theta_k) \). The poles of the Green’s function correspond to Fermi contours of the two spin-split subbands at energy \( E \) and is obtained from the roots of the denominator,

\[
k_\pm = Q \pm k_{so} \sqrt{f_\tau(\theta_k)}, \quad Q = \sqrt{k_E^2 + 2k_{so}f_\tau(\theta_k)}.
\]

The representation of the GF in real space is obtained by Fourier transform of Eq. (4).

Landé \( g \) factor makes this a promising system in which to detect these orbital features since the current magnitude is proportional to \( (\alpha^2 + \beta^2)^{1/2} / m^* \) [Eq. (2)]. Conversion factors for different materials are provided in Table I for the spatial dimensions \( (d_{fac}) \) and for the magnetic field strengths \( (B_{fac}) \) in the figures below.

Figure 1 shows the current density induced by a magnetic defect at the origin \( (\mathbf{r}_0 = 0) \) with spin projection along the [001] out-of-plane direction, calculated from Eq. (2). For \( \alpha \gg \beta \), corresponding to \( \tau = \pi/2 \) [Fig. 1(a)], the isotropic dispersion relation implied by a \( \theta_k \)-independent \( f_\tau \) allows for an analytical solution to Eq. (6) in terms of Hankel functions of the first kind \( H_0 \). The current then has only an angular component and oscillates with two characteristic lengths, reminiscent of Friedel oscillations, given by \( \lambda_f = \pi / k_f \) and \( \lambda_{so} = \pi / k_{so} \).

The emergence of the anisotropy in the dispersion relation when both \( \alpha \) and \( \beta \) are relevant [Fig. 1(bc)] drastically changes the spatial structure of the circulating current compared to Fig. 1(a), stretching the features along the symmetry axes. For \( \alpha / \beta > 0 \) a stronger current density focuses along the \( \theta = 3\pi/4 \) direction [Fig. 1(b)] and rotates by 90° focusing along \( \theta = \pi/4 \) when \( \alpha / \beta < 0 \) [Fig. 1(c)], a consequence of an interfering contribution of stationary points \( \delta \). The currents are equal but rotate in opposite directions for values of \( \tau = \pi/4 \pm \delta \) (\( \tau = \pi/4 \) corresponds to \( \alpha = \beta \), as shown in Fig. 1(bc)). This change in rotation would invert the orbital magnetization around the spin (see Supplementary Material). We note that when \( \alpha = \beta \), the extra SU(2) symmetry implies a fixed spin quantization axis independent of \( \mathbf{k} \), making the 2DEG GF of Eq. (6) spin-diagonal upon a global spin rotation \( \mathbf{g} \) and thus both contributions to
FIG. 1. Current density induced by a magnetic point defect with spin pointing perpendicular to an InAs 2DEG. (a) SIA dominated regime ($\beta = 0, \tau = \pi/2$) showing angular symmetry. (b-d) $\beta \neq 0$: the angularly anisotropic circulating current stretches along the symmetry axis $\theta = 3\pi/4$ for $\alpha/\beta > 0$ (bc) or along $\theta = \pi/4$ for $\alpha/\beta < 0$ (d). Opposite circulation direction of $\tau = \pi/4 + 0.1$ (b) from $\tau = \pi/4 - 0.1$ (c); current vanishes for $\tau = \pi/4$ ($\alpha = \beta$).

The spatial structure of the orbital magnetization density associated with these circulating currents can be calculated in analogy with classical electrodynamics using \[ \mathbf{m}_{\text{orb}}(\mathbf{r}) = \frac{1}{2} \mathbf{r} \times \mathbf{j}(\mathbf{r}) \]; the current density is obtained from Eq. (2). To compare both the orbital and spin contributions to the defect-induced magnetization we calculate the latter by

\[ \mathbf{m}_{\text{spin}}(\mathbf{r}) = -\frac{\mu_B}{\pi} \text{Im} \int_{E_{so}}^{E_f} \mathbf{\sigma G}(\mathbf{r}, E) \, dE, \tag{8} \]

where $\mu_B$ is the Bohr magneton and $\mathbf{\sigma}$ are the Pauli matrices. We note that orbital momentum quenching is reduced for systems with strong spin-orbit coupling, allowing a comparable orbital magnetization to the spin magnetization. As shown in Fig. 2 although the spin-orbit fields alter both orbital and spin magnetization densities around a magnetic defect, the orbital magnetization has distinct spatial oscillations and is highly sensitive to the SOC ratio $\tau$.

The magnetic fringe field above the 2DEG is obtained from the orbital magnetization density of a quantum-well with width $d$ confined along the z-axis under hard-wall boundary conditions. By using the ground-state electron envelope function, $\phi(z) = (1/\sqrt{d}) \cos(\pi z/d)$, the previously calculated two-dimensional current density acquires a $z$-dependence of $\cos^2(\pi z/d)$, and a volumetric orbital magnetization density can be defined inside the quantum well.

In the region outside the magnetized volume, the magnetic fringe field is evaluated by $\mathbf{B} = -\mu_0 \nabla \Phi_{\text{orb}}(\mathbf{r})$, where $\mu_0 = 4\pi \times 10^{-7}$ N/A² is the vacuum permeability and the scalar magnetic potential is

\[ \Phi_{\text{orb}}(\mathbf{r}) = \frac{1}{4\pi} \int d\mathbf{r}' \frac{\mathbf{m}_{\text{orb}}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \tag{9} \]

Figure 2 shows the spatial distribution for each orbital fringe field component is calculated at 20 nm above a 10 nm InAs QW for this magnetic defect, and the largest values are tenths of $\mu T$, within the range of single NV diamond scanning magnetometry. In the left column of Fig. 3 the fringe field structure in the SIA dominated regime ($\tau = \pi/2$) reflects the radial symmetry of the circulating current in this regime, and the fields are generated by concentric current loops with current flowing in opposite directions. The BIA term induces angular anistropy in the field distribution [Fig. 3(bdf)] providing a direct signature of the SOC ratio.

The magnitude of the orbital fringe field depends on the distance measured from the QW, e.g. decreasing fourfold at a distance of 20 nm from the InAs QW with respect to the field magnitude at the surface (Fig. 4), thus the close proximity achievable by nanoscale scanning probes can obtain even stronger responses within

\[ \boxed{\text{FIG. 2. Orbital } (\mathbf{m}_{\text{orb}}) \text{ and spin } (\mathbf{m}_{\text{spin}}) \text{ contributions to the 2DEG magnetization density showing the effects of the current circulation inversion between } \tau = \pi/4 - 0.1 \text{ (a) and } \tau = \pi/4 + 0.1 \text{ (b) along the [110] direction from a magnetic defect pointing perpendicular to the 2DEG.}}\]
FIG. 3. Orbital fringe field components (ab) $B_x$, (cd) $B_y$ and (ef) $B_z$ 20 nm above the surface of an InAs quantum well with width 10 nm for a magnetic defect pointing perpendicular to the 2DEG. (ace) the SIA dominated regime, $\tau = \pi/2$. (bdf) for $\tau = \pi/8$. Its sensitivity range. The higher magnitude shown for currents with both SIA and BIA terms (crosses and blue lines in Fig. 4) occurs from higher currents due to the SOC-induced focusing effects. Furthermore, choices of different materials may lead to more detectable effects. Table I lists a variety of materials with either stronger magnetic fields or larger-scale spatial features, along with some more challenging materials that would have both (i.e. BiSb). In Table I we keep the two-dimensional electron density fixed to be $4 \times 10^{11}$ cm$^{-2}$, and note that the features can also become larger (or smaller) for different electron densities.

The circulating dissipationless current associated with a single spin in a 2DEG formed in non-centrosymmetric materials with SOC creates spatial features highly sensitive to the underlying tunable spin-orbit field and the defect-spin direction, a reminiscent of the anisotropic dispersion relation and Friedel oscillations. Nanoscale scanning probe magnetometry, or potentially electron ptychography, is sufficiently sensitive to measure the spatially-resolved orbital contribution to the magnetic moment of a single spin. The spatial structure of the defect magnetic moment affects its coupling to nearby rapidly oscillating fields from e.g., nuclear-spins, with implications for spin-dynamics and coherent control of single spin states [51].

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TABLE I. Parameters and conversion factors for the spatial dimension ($d_{\text{fac}}$) and magnetic field strength ($B_{\text{fac}}$) for different materials. We assume the QW width is 10 nm.

| Material | $m^*(m_0)$ | $\alpha$ (meV.nm) | $d_{\text{fac}}$ | $B_{\text{fac}}$ |
|----------|-------------|-------------------|----------------|----------------|
| InAs[17] | 0.023       | 50                | 1.0            | 1.0            |
| GaAs/AlGaAs[48] | 0.067       | 4.8               | 3.58           | 0.096          |
| LAO/STO[27] | 2.2         | 3.4               | 0.15           | 0.068          |
| InGaAs/InAlAs[19] | 0.05       | 40.0              | 0.57           | 0.8            |
| BiSb[28]  | 0.002       | 230               | 2.5            | 4.6            |
| LaOBiS$_2$[30] | 0.07        | 478               | 0.034          | 9.56           |
| WSeTe[29, 50] | 0.81       | 92                | 0.015          | 1.84           |

[1] B. E. Kane, Nature (London) **393**, 133 (1998).
[2] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[3] D. D. Awschalom, N. Samarth, and D. Loss, eds., Semiconductor Spintronics and Quantum Computation (Springer Verlag, Heidelberg, 2002).
[4] K. Ichimura, Opt. Commun. **196**, 119 (2001).
[5] G. Woloficz, F. J. Heremans, C. P. Anderson, S. Kanai, H. Seo, A. Gali, G. Galli, and D. D. Awschalom, Nat. Rev. Mater. **6**, 906 (2021).
[6] T. Matsui, C. Meyer, L. Sacharov, J. Wiebe, and
