Theory of orbital magnetization in disordered systems

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We present a general formula of the orbital magnetization of disordered systems based on the Keldysh Green's function theory in the gauge-covariant Wigner space. In our approach, the gauge invariance of physical quantities is ensured from the very beginning, and the vertex corrections are easily included. Our formula applies not only for insulators but also for metallic systems where the quasiparticle behavior is usually strongly modified by the disorder scattering. In the absence of disorders, our formula recovers the previous results obtained from the semiclassical theory and the perturbation theory. As an application, we calculate the orbital magnetization of a weakly disordered two-dimensional electron gas with Rashba spin-orbit coupling. We find that for the short-range disorder scattering, its major effect is to the shifting of the distribution of orbital magnetization corresponding to the quasiparticle energy renormalization.

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I. INTRODUCTION

Magnetization is one of the most important and intriguing material properties. An adequate account of magnetization should not only include the contribution from the spin polarization of electrons, but also the contribution from the orbital motion of electrons. In crystals, due to the reduced spatial symmetry, the orbital contribution to the magnetization is usually quenched. For example, it is only of the order of a few percent of the total magnetization in Fe, Co, and Ni.[1] However, that is not to say that the orbital magnetization is small in all materials. In certain materials with topologically nontrivial band structures, large contributions can arise from the effective reciprocal space monopoles near the band anticrossings. The orbital magnetization can have a more important effect, cancel, and even is larger than the spin magnetization, which has been confirmed in recent experiments.[2,3] Furthermore, the orbital magnetization is directly connected to many important applications and it also determines several important material properties. Some examples include the NMR,[4–6] the EPR[7] shielding tensors, the magnetic susceptibility,[8,9] the orbital magnetoelectric coupling and response,[10–13] and the Hall conductivity.[14] All these highlight the need to develop a complete description of the orbital magnetism in solids.

Several different methods have been employed to study the orbital magnetization (OM) in crystals.[15–32] One major difficulty in the calculation is posed by the evaluation of the operator[15,16] $\hat{r} \times \hat{j}$, because the the position $\hat{r}$ is ill defined in the Bloch representation. This difficulty can be avoided in a semiclassical approach or be circumvented by a transformation to the Wannier representation. Xiao *et al.*[18,19] presented a general formula for OM for metal and insulator, derived from a semiclassical formalism with the Berry-phase corrections. Thonhauser *et al.*[20,21] derived an expression of the OM for periodic insulators using the Wannier representation. From the elementary thermodynamics, Shi *et al.*[24] obtained a formula for the OM in a periodic system using the standard perturbation theory, and their result can in principle take into account the electron-electron interaction effects. The OM for periodic systems with first principles were studied by Lopez *et al.*[23] and Ceresoli *et al.*[26]

Previous studies are mainly concerned with clean crystal systems. However, real crystals are never perfect; disorders such as defects, impurities, phonons, etc. constantly break the translational symmetry and lead to scattering events. The effect of disorder scattering on the OM has not been carefully studied so far. On one hand, the OM is a thermodynamic quantity, hence it is expected to be less susceptible to disorder scattering. On the other hand, the appearance of current operator $\hat{j}$ in the definition suggests behaviors similar to transport quantities, which might be strongly affected by the disorder scattering. Therefore, it is important and desirable to have a good understanding of the role played by the disorder scattering in the OM.

In this paper, we present a general formula of the OM in disordered systems based on the Keldysh-Green's function formalism in the gauge-covariant Wigner space.[33–38] This approach was developed as a systematic approach to the nonequilibrium electron dynamics under external fields. Our formula derived from this approach shares the advantage of being able to capture the disorder effects in a systematic way and ensure the gauge invariance property from the very beginning. We show that in the clean limit, our formula reduces to the previous results obtained from other approaches. As an application, we study the OM in a disordered two-dimensional (2D) electron gas with the Rashba spin-orbit coupling. We find that the OM is robust against short-range disorders. The main effect of the scattering by short-range disorders is a rigid shift of the distribution of OM in energy.

The structure of this paper is organized as follows. In Sec. II A, we outline the Keldysh-Green's function formalism, which is employed for our derivation. Our general formula of OM is presented in Sec. II B. In Sec. III, we apply the formula to study the OM of a two-dimensional disordered electron gas with the Rashba spin-orbit coupling. Summary and conclusion are given in Sec. IV. Some details of the calculation are provided in the Appendices.

II. ORBITAL MAGNETIZATION OF DISORDERED SYSTEMS

A. Keldysh-Green's function formalism

We employ the Keldysh-Green's function formalism in the Wigner representation,[33] which has recently been used to study the current response of multiband systems under an electric field.[34,35] In the Wigner representation, Green's functions and the self-energies are expressed as functions of the center-of-mass coordinates (T,X), the energy ε and the mechanical momentum $\mathbf{p}$. The energy and the mechanical momentum are the Fourier transforms of the relative time and space coordinates respectively.

The Dyson equations in the presence of external electromagnetic fields can be written as

$$[\varepsilon\underline{\hat{I}} - \underline{\hat{H}}_0(\mathbf{p}) - \underline{\hat{\Sigma}}(\varepsilon)] \star \underline{\hat{G}}(\varepsilon,\mathbf{p}) = \underline{\hat{I}}, \tag{1a}$$

$$\underline{\hat{G}}(\varepsilon,\mathbf{p}) \star [\varepsilon\underline{\hat{I}} - \underline{\hat{H}}_0(\mathbf{p}) - \underline{\hat{\Sigma}}(\varepsilon)] = \underline{\hat{I}}. \tag{1b}$$

Each quantity with an underline in the above equations is a matrix in Keldysh space. Specifically, we have

$$\underline{\hat{G}} \equiv \begin{pmatrix} \hat{G}^R & 2\hat{G}^< \\ 0 & \hat{G}^A \end{pmatrix}, \quad \underline{\hat{\Sigma}} \equiv \begin{pmatrix} \hat{\Sigma}^R & 2\hat{\Sigma}^< \\ 0 & \hat{\Sigma}^A \end{pmatrix}, \tag{2}$$

$$\underline{\hat{H}}_0 \equiv \begin{pmatrix} \hat{H}_0 & 0 \\ 0 & \hat{H}_0 \end{pmatrix}, \quad \underline{\hat{I}} = \begin{pmatrix} \hat{\sigma}^0 & 0 \\ 0 & \hat{\sigma}^0 \end{pmatrix}, \tag{3}$$

where $\hat{G}^{(R,A,<)}$ are the (retarded, advanced, lesser) Green's functions, and $\hat{\Sigma}^{(R,A,<)}$ are the corresponding self-energies, $\hat{H}_0$ is the Hamiltonian in the absence of external electromagnetic fields, $\hat{\sigma}^0$ is the identity matrix. The $\star$ operator in Eq. (1) is defined as

$$\star \equiv \exp\left[\frac{iq\hbar}{2}F^{\mu\nu}\left(\overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{p^\nu} - \overleftarrow{\partial}_{p^\nu}\overrightarrow{\partial}_{p^\mu}\right)\right], \tag{4}$$

with the differential operators $\overleftarrow{\partial}$ and $\overrightarrow{\partial}$ operating on the left-hand and the right-hand sides respectively, $q = -|e|$ is the electron charge, and $F^{\mu\nu} = \partial_{X_\mu}A^\nu(X) - \partial_{X_\nu}A^\mu(X)$ is the electromagnetic field tensor, μ and ν label the four-dimensional space-time components and the Einstein summation convention is assumed. It should be noted that the energy ε and the mechanical momentum $\mathbf{p}$ include the electromagnetic potentials $A^\mu(X)$, both are gauge invariant quantities. The $\star$ operator in Eq. (1) only involves the physical fields, so it is also gauge invariant. In this formalism the gauge invariance is respected from the very beginning and easily maintained during the perturbative expansion, which is an important advantage.[33]

Here we consider the situation with a uniform weak magnetic field along the z direction, [i.e., $\mathbf{B} = (0,0,B)$]. Then the various quantities can be expanded in terms of B. In particular, Green's functions and the self-energies can be expressed as

$$\hat{G}^\alpha(\varepsilon,\mathbf{p}) = \hat{G}_0^\alpha(\varepsilon,\mathbf{p}) + e\hbar B\hat{G}_B^\alpha(\varepsilon,\mathbf{p}) + O(B^2), \tag{5}$$

$$\hat{\Sigma}^\alpha(\varepsilon) = \hat{\Sigma}_0^\alpha(\varepsilon) + e\hbar B\hat{\Sigma}_B^\alpha(\varepsilon) + O(B^2), \tag{6}$$

with $\alpha = R, A, <$ for the retarded, advanced, and lesser components respectively. Here functions with the subscript 0 are of zeroth order in the external magnetic field strength (note that they include scattering effects). We have

$$\hat{G}_0^{R(A)}(\varepsilon,\mathbf{p}) = \left[\varepsilon - \hat{H}_0(\mathbf{p}) - \hat{\Sigma}_0^{R(A)}(\varepsilon)\right]^{-1}, \tag{7}$$

$$\hat{G}_0^<(\varepsilon,\mathbf{p}) = \left[\hat{G}_0^A(\varepsilon,\mathbf{p}) - \hat{G}_0^R(\varepsilon,\mathbf{p})\right]f(\varepsilon), \tag{8}$$

where $f(\varepsilon)$ is the Fermi distribution. The functions with subscript B are the linear response coefficient to the external field. They can be solved from the Dyson equation. It is usually convenient to decompose the lesser component $\hat{G}_B^<$ and $\hat{\Sigma}_B^<$ (which are related to particle distribution) into two parts, with one part from the Fermi surface and the other part from the Fermi sea,[39]

$$\hat{G}_B^<(\varepsilon,\mathbf{p}) = \hat{G}_{B,I}^<(\varepsilon,\mathbf{p})\partial_\varepsilon f(\varepsilon) + \hat{G}_{B,II}^<(\varepsilon,\mathbf{p})f(\varepsilon) \tag{9}$$

$$\hat{\Sigma}_B^<(\varepsilon) = \hat{\Sigma}_{B,I}^<(\varepsilon)\partial_\varepsilon f(\varepsilon) + \hat{\Sigma}_{B,II}^<(\varepsilon)f(\varepsilon). \tag{10}$$

From the Dyson equation (kept to the linear order in B), it is straightforward to show that

$$\hat{G}_{B,I}^< = \hat{\Sigma}_{B,I}^< = 0, \tag{11}$$

(i.e., there is no Fermi surface term in the linear order lesser component) and for the Fermi sea term we have

$$\hat{G}_{B,II}^<(\varepsilon,\mathbf{p}) = \hat{G}_B^A(\varepsilon,\mathbf{p}) - \hat{G}_B^R(\varepsilon,\mathbf{p}), \tag{12}$$

$$\hat{\Sigma}_{B,II}^<(\varepsilon) = \hat{\Sigma}_B^A(\varepsilon) - \hat{\Sigma}_B^R(\varepsilon). \tag{13}$$

The retarded and advanced Green's function $\hat{G}_B^{R(A)}$ and self-energy $\hat{\Sigma}_B^{R(A)}$ are determined from the following self-consistent equations:

$$\begin{aligned}\hat{G}_B^{R(A)} = {} & \frac{i}{2}\left[\hat{G}_0^{R(A)}\hat{v}_x\left(\partial_{p_y}\hat{G}_0^{R(A)}\right) - \left(\partial_{p_y}\hat{G}_0^{R(A)}\right)\hat{v}_x\hat{G}_0^{R(A)}\right] \\ & + \hat{G}_0^{R(A)}\hat{\Sigma}_B^{R(A)}\hat{G}_0^{R(A)},\end{aligned} \tag{14}$$

where the velocity operator is defined as $\hat{v}_i \equiv \frac{1}{i\hbar}[\hat{x}_i, \hat{H}]$.

In this approach, the disorder effects are captured by the self-energies $\hat{\Sigma}_0^{R(A)}$ and $\hat{\Sigma}_B^{R(A)}$, which allows a systematic perturbative treatment. In the weak disorder regime, the self-consistent T-matrix approximation provides a good approximation scheme. In this approximation, we have

$$\hat{\Sigma}_0^{R(A)}(\varepsilon) = n_{\text{imp}}\hat{T}_0^{R(A)}(\varepsilon), \tag{15}$$

and

$$\hat{\Sigma}_B^{R(A)}(\varepsilon) = n_{\text{imp}}\hat{T}_0^{R(A)}(\varepsilon)\int\frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\hat{G}_B^{R(A)}(\varepsilon,\mathbf{p})\hat{T}_0^{R(A)}(\varepsilon), \tag{16}$$

where n_{imp} is the impurity concentration and the T-matrix is expressed as

$$\hat{T}_0^{R(A)}(\varepsilon) = \hat{V}_{\text{imp}}\left(1 - \int\frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\hat{G}_0^{R(A)}(\varepsilon,\mathbf{p})\hat{V}_{\text{imp}}\right)^{-1}, \tag{17}$$

with $\hat{V}_{\text{imp}}$ being the impurity potential.

The equilibrium Green's functions $\hat{G}_0^{R(A)}$ and the self-energies $\hat{\Sigma}_0^{R(A)}$ can be obtained by solving Eqs. (7), (15) and (17) self-consistently. Then the linear order coefficients $\hat{G}_B^{R(A)}$ and $\hat{\Sigma}_B^{R(A)}$ can be solved from Eqs. (14) and (16). Finally, we can obtain $\hat{G}_{B,II}^<$ through Eq. (12) and the linear response of

the system in the external magnetic field can be completely determined.

The lesser Green's function contains the information of particle distribution. In our case, both the external magnetic field and the disorder scattering affect the quasiparticle distribution. Before we proceed, it is interesting to observe how the nontrivial band geometry (described by the Berry curvature) can be captured by the present Wigner space Green's function formalism. For a homogeneous system, the electron density can be written as

$$n_e = \frac{1}{i}\int \frac{d\varepsilon}{2\pi}\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\mathrm{tr}[\hat{G}^<(\varepsilon,\mathbf{p})]. \tag{18}$$

In the absence of the disorder scattering, the eigenstates are well-defined Bloch states grouped into energy bands. Using the theorem of residues, we can express the ground-state electron density in the presence of a constant magnetic field as (see Appendix C)

$$n_e = \sum_{n,occ}\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\left[1+\frac{e}{\hbar}\mathbf{B}\cdot\Omega_n(\mathbf{p})\right]. \tag{19}$$

The summation is over all the occupied states, and $\Omega_n(\mathbf{p}) = i\langle\nabla_{\mathbf{p}}u_{n\mathbf{p}}|\times|\nabla_{\mathbf{p}}u_{n\mathbf{p}}\rangle$ is the Berry curvature of the Bloch state $|n,\mathbf{p}\rangle = e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}|u_{n\mathbf{p}}\rangle$. It can be seen that the Fermi-sea volume is changed linearly by a magnetic field when the Berry curvature is nonzero. This effect was previously interpreted as the modification of the phase space density of states.[18]

B. Formula of orbital magnetization

We start from the standard thermodynamic definition of the OM density at zero temperature,[24]

$$M = -\left(\frac{\partial K}{\partial B}\right)_{\mu}, \tag{20}$$

where $K = E-\mu N$ is the grand thermodynamic potential, B is a weak magnetic field. Since we are concerned with the orbital contribution, the small Zeeman coupling between the electron spin and external field will be dropped. The potential K can be expressed through the lesser Green's function,

$$K = \frac{1}{i}\int \frac{d\varepsilon}{2\pi}\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\mathrm{tr}[(\hat{H}-\mu)\hat{G}^<(\varepsilon,\mathbf{p})]. \tag{21}$$

Using Eqs. (20), (21), and (9), we find that the OM can be written as

$$M = -ie\hbar\int \frac{d\varepsilon}{2\pi}\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2}\mathrm{tr}\big[(\hat{H}-\mu) \times\left(\hat{G}_B^A(\varepsilon,\mathbf{p})-\hat{G}_B^R(\varepsilon,\mathbf{p})\right)\big]f(\varepsilon). \tag{22}$$

From this expression, we can see that the OM has contributions from the whole Fermi sea, with no separate Fermi surface contribution such as that for the transport quantities.

In this formula, the impurity scattering effect comes in through two terms: the self-energy $\hat{\Sigma}_0^{R,A}$, which modifies the ground-state electronic structure and the vertex corrections associated with $\hat{\Sigma}_B^{R,A,<}$, which represent an interplay between the magnetic field and the impurity scattering. We may separate out the terms containing $\hat{\Sigma}_B^{R,A,<}$ and write the OM explicitly as

$$M = M^I + M^{II}, \tag{23}$$

where

$$M^I = \frac{e\hbar}{2}\int \frac{d\varepsilon}{2\pi}f(\varepsilon)\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \times\sum_{ij}\mathrm{Tr}\big[\epsilon_{ij}(\hat{H}-\mu)\hat{G}_0^A(\varepsilon,\mathbf{p})\hat{v}_i\hat{G}_0^A(\varepsilon,\mathbf{p})\hat{v}_j\hat{G}_0^A(\varepsilon,\mathbf{p}) -\left(\hat{G}_0^A\to\hat{G}_0^R\right)\big], \tag{24}$$

and

$$M^{II} = -ie\hbar\int \frac{d\varepsilon}{2\pi}f(\varepsilon)\int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \times\mathrm{Tr}\big[(\hat{H}-\mu)\hat{G}_0^A\hat{\Sigma}_B^A\hat{G}_0^A-(\hat{H}-\mu)\hat{G}_0^R\hat{\Sigma}_B^R\hat{G}_0^R\big], \tag{25}$$

where ϵ_{ij} with $i,j\in\{x,y\}$ is the 2D antisymmetric tensor, and the second term in the bracket in Eq. (24) means that the second term is the same as the first term except that all the $\hat{G}_0^A$ are replaced by $\hat{G}_0^R$. Such a decomposition scheme was also adopted in the study of anomalous Hall conductivity,[35] and in that context, the two parts are referred to as the intrinsic part and extrinsic part respectively. It should be noted that the intrinsic part M^I also has impurity scattering effects in it [see Eq. (7) and Eq. (15)], it is intrinsic in the sense that it only contains quantities that are of zeroth order in the external field. As for the extrinsic part M^{II}, it is easy to see that it is already linear order in n_{imp} [see Eq. (16)]. Therefore in the weak scattering regime, the extrinsic part is expected to be much smaller than the intrinsic part.

The above formula is our main result. From this formula, we see that there is no separate Fermi surface contributions like those in the transport quantities, which is consistent with OM being a thermodynamic equilibrium property. This formula applies for both insulators and metals. The quantities in this formula can be calculated from the Dyson equation according to our prescription described in the previous section. It can also be straightforwardly implemented in the numerical calculation, either from effective models or from first principles.

In the clean limit, we only have the intrinsic part. The general result reduces to (see Appendix D for the derivation)

$$M = \sum_{n\mathbf{p}} f_{n\mathbf{p}}\left[m_n(\mathbf{p})-\frac{e}{\hbar}(\epsilon_{n\mathbf{p}}-\mu)\Omega_n(\mathbf{p})\right], \tag{26}$$

where $m_n(\mathbf{p}) = (e/2\hbar)i\langle\nabla_{\mathbf{p}}u_{n\mathbf{p}}|[\epsilon_n(\mathbf{p})-\hat{H}_0(\mathbf{p})]\times|\nabla_{\mathbf{p}}u_{n\mathbf{p}}\rangle$ is the orbital moment of the Bloch state $|n,\mathbf{p}\rangle$ and $\Omega_n(\mathbf{p}) = i\langle\nabla_{\mathbf{p}}u_{n\mathbf{p}}|\times|\nabla_{\mathbf{p}}u_{n\mathbf{p}}\rangle$ is the Berry curvature. The first term in Eq. (26) is a sum of the orbital magnetic moments associated with each Bloch state,[40,41] and the second term is a Berry-phase correction to the OM. Therefore, the OM can be written as

$$M = \mathcal{M}_{\mathrm{m}} + \mathcal{M}_{\Omega}. \tag{27}$$

This clean limit result was previously derived from the standard perturbation theory of quantum mechanics by Shi *et al.*[24] and also from the semiclassical theory by Xiao *et al.*[18] Now it is also reproduced as a special limiting case of our general formula.

III. APPLICATION TO A TWO-DIMENSIONAL ELECTRON GAS WITH RASHBA SPIN-ORBIT COUPLING

A. Model

In this section, we apply our theory to study the orbital magnetization of a two-dimensional electron gas with Rashba spin-orbiting coupling. The Rashba model was proposed in 1960.[42] It has a great success in describing the two-dimensional electron gas confined at the semiconductor heterostructures, which was a primary playground of the spintronics research in the past two decades, such as spin Hall effect,[43] anomalous Hall effect,[35,36] and topological phase of Rashba superconductor.[44,45] The Rashba spin-orbit interaction is realized in an InGaAs/GaAs heterostructure. The Hamiltonian for the model reads

$$\hat{H} = \hat{H}_0 + \hat{H}_{\rm imp}, \tag{28a}$$

$$\hat{H}_0 = \frac{p^2}{2m}\hat{\sigma}^0 + \alpha(p_x\hat{\sigma}^y - p_y\hat{\sigma}^x) - \Delta_0\hat{\sigma}^z, \tag{28b}$$

$$\hat{H}_{\rm imp} = u_{\rm imp}\hat{\sigma}^0 \sum_{\vec{r}_{\rm imp}} \delta(\vec{r} - \vec{r}_{\rm imp}), \tag{28c}$$

where $(\hat{\sigma}^x,\hat{\sigma}^y,\hat{\sigma}^z)$ are the three Pauli matrices and $\hat{\sigma}^0$ is the identity matrix, α is the strength of the spin-orbit coupling, and term $-\Delta_0\hat{\sigma}^z$ is the Zeeman splitting, which can be introduced by the exchange coupling with a nearby ferromagnet or magnetic dopants. These two terms both lift the spin degeneracy, but have different time-reversal symmetry properties. The spin-orbit coupling term is even under time reversal while the Zeeman term is odd. $\hat{H}_{\rm imp}$ is the disorder potential from the randomly distributed short-range impurities with strength $u_{\rm imp}$. The energy dispersion of the Hamiltonian $\hat{H}_0$ is given by

$$\boldsymbol{E}_\lambda(p) = \frac{p^2}{2m} - (-1)^\lambda\sqrt{\Delta_0^2 + \alpha^2 p^2}, \tag{29}$$

where $\lambda = 1,2$ labels the upper and lower band respectively.

The interplay between spin-orbit interaction and Zeeman splitting can influence the transport property of two-dimensional electron gas.[46] Experimentally, the strength of Rashba coupling can be tuned by controlling the gate voltage,[47,48] as successfully demonstrated in the system of InGaAs/GaAs or $LaAlO_3/SrTiO_3$ heterostructures.[49] For our model, the minima of the lower band occur at a finite wave vector and the dispersion assumes a Mexican hat shape [see Fig. 1(a)] when the Rashba coupling energy scale[50] $m\alpha^2$ is larger than the Zeeman coupling strength. When the Zeeman coupling dominates over the Rashba energy, the minimum of the lower band E_2 occurs at the origin [see Fig. 2(a)] .

Let us first consider the clean limit, in which case the orbital magnetic moment and the Berry curvature of each Bloch state can be calculated straightforwardly,

$$m_1(p) = m_2(p) = \frac{e}{2\hbar}\frac{\Delta_0\alpha^2}{\Delta_0^2 + \alpha^2 p^2}, \tag{30}$$

$$\Omega_1(p) = -\Omega_2(p) = -\frac{1}{2}\frac{\Delta_0\alpha^2}{\left(\Delta_0^2 + \alpha^2 p^2\right)^{\frac{3}{2}}}. \tag{31}$$

It is interesting to observe that for the same wave vector the orbital moments of the two bands have the same magnitude and the same sign, while the Berry curvatures have the same magnitude but opposite signs. It should also be noted that both the orbital moment and the Berry curvature would vanish if either α or Δ_0 vanishes. From Eq. (26), we further see that the OM is *nonzero* only when both the spin-orbit coupling and the exchange coupling are present.

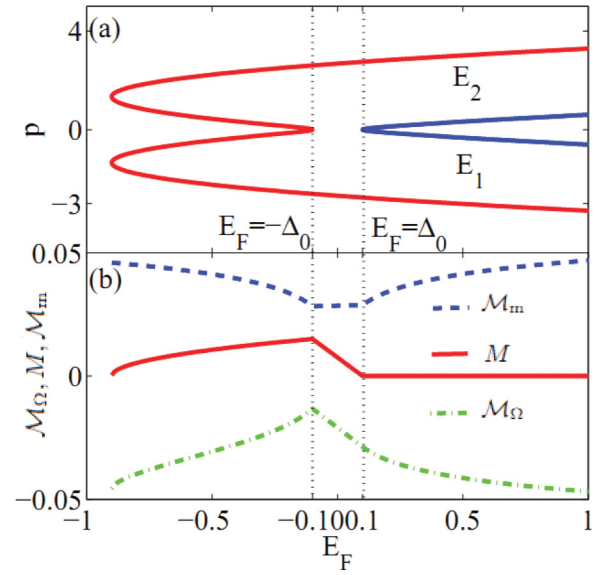

FIG. 1. (Color online) (a) Electronic band dispersions of our model given by Eq. (29). (b) Orbital magnetization (M, solid red curve) of disordered free system and its two components $\mathcal{M}_{\rm m}$ (dashed blue curve) and $\mathcal{M}_\Omega$ (dash-dotted green curve) as functions of Fermi energy E_F. They are plotted in units of $e/\hbar$. The parameters are chosen as $2m\alpha^2 = 3.59$ and $\Delta_0 = 0.1$.

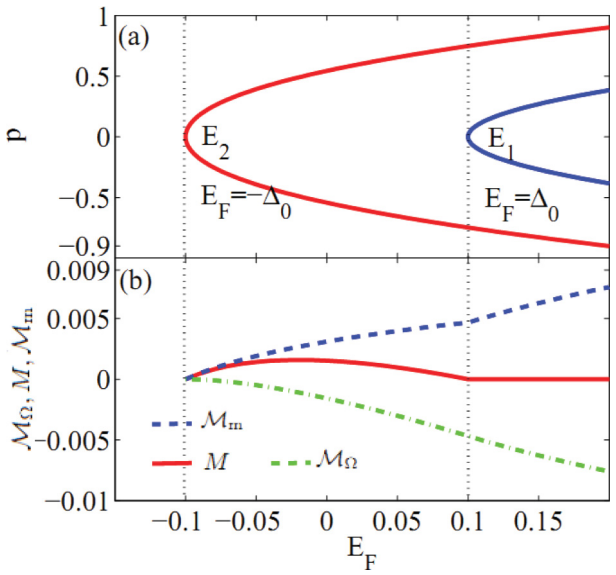

FIG. 2. (Color online) (a) Electronic band dispersions of our model given by Eq. (29). (b) Orbital magnetization ($\mathcal{M}$, solid red curve) of disorder free system and its two components $\mathcal{M}_{\rm m}$ (dashed blue curve) and $\mathcal{M}_\Omega$ (dash-dotted green curve) as functions of Fermi energy E_F. They are plotted in units of $e/\hbar$. The parameters are chosen as $2m\alpha^2 = 0.08$ and $\Delta_0 = 0.1$.

Analytical expressions of the OM can be easily obtained for the clean limit using Eq. (26). For example, for the case with $E_F > \Delta_0$, we have

$$M = \frac{e\Delta_0}{4\pi\hbar}\left(E_F + \frac{\Delta_0^2}{2m\alpha^2}\right) \times \left[\frac{1}{\left(\Delta_0^2 + \alpha^2 p_{F_1}^2\right)^{\frac{1}{2}}} - \frac{1}{\left(\Delta_0^2 + \alpha^2 p_{F_2}^2\right)^{\frac{1}{2}}}\right] + \frac{e\Delta_0}{8\pi m\hbar\alpha^2}\left[\left(\Delta_0^2 + \alpha^2 p_{F_1}^2\right)^{\frac{1}{2}} - \left(\Delta_0^2 + \alpha^2 p_{F_2}^2\right)^{\frac{1}{2}}\right], \quad (32)$$

where $p_{F_{1,2}}$ is the Fermi momenta of the two bands.

B. Results

Now we analyze the OM of the disordered 2D Rashba model in detail. The calculation procedure follows our discussion in Secs. II A and II B. Since we have seen that both the spin-orbit coupling and the exchange coupling are essential ingredients for the OM, in the following we shall consider two different regimes of the model determined by the competition between the Rashba spin-orbit coupling and the exchange coupling. For each regime, we first analyze the clean limit where the physical picture is more transparent, and then study the influence of disorder scattering, which is the focus in this paper.

We first consider the regime where the Rashba coupling dominates over the exchange coupling (i.e. $2m\alpha^2 \gg \Delta_0$). The typical band dispersion in this regime is shown in Fig. 1(a) (with $2m\alpha^2 = 3.59$ and $\Delta_0 = 0.1$). In this regime, the bottom of the lower band occurs at a finite wave vector. The energy spectrum around the origin has an effective Dirac cone structure with a local gap $2\Delta_0$ at $p = 0$. Both the orbital moment and the Berry curvature are concentrated near this band anticrossing point, as is evident from Eqs. (30) and (31). Figure 1(b) shows the OM for the clean limit. The orbital moment contribution $\mathcal{M}_{\rm m}$ and the Berry curvature contribution $\mathcal{M}_\Omega$ are also plotted in Fig. 1(b). We can see that as the Fermi energy E_F increases from the lower band bottom, $\mathcal{M}_\Omega$ increases while $\mathcal{M}_{\rm m}$ decreases. The increasing rate of $\mathcal{M}_\Omega$ is higher than the decreasing rate of $\mathcal{M}_{\rm m}$, so the overall OM is increasing. The OM reaches its maximum when $E_F = -\Delta_0$, which corresponds to the local band top around the origin in momentum space. As the Fermi energy sweeps across the local energy gap between $-\Delta_0$ and $+\Delta_0$, the OM decreases approximately linearly with E_F. The linearity can be understood by noticing that from Eq. (26) the derivative of the OM with respect to E_F is just the momentum space integral of the Berry curvature. The Berry curvature distribution is concentrated near the band anticrossing point, corresponding to the small region around the origin in the present model. When the Fermi energy is within the gap, the Berry curvature integral only has contribution from the lower band and is almost constant, therefore leading to the linear energy dependence of OM. This linear decrease of OM stops when the Fermi energy touches the bottom of the upper band at $+\Delta_0$. Above the upper band bottom, $\mathcal{M}_\Omega$ and $\mathcal{M}_{\rm m}$ almost cancel each other and the OM is vanishingly small. Throughout the spectrum,

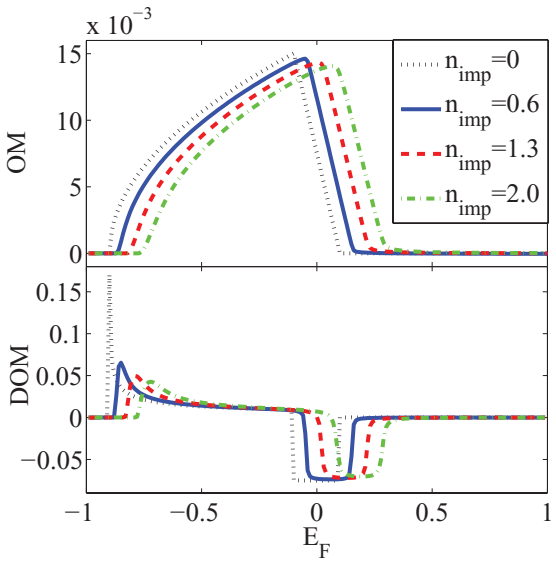

FIG. 3. (Color online) (a) Orbital magnetization (OM) as a function of Fermi energy E_F with different impurity concentration $n_{\rm imp}$. (b) Density of OM with different impurity concentration $n_{\rm imp}$. These quantities are plotted in units of $e/\hbar$. The parameters are chosen as $2m\alpha^2 = 3.59$, $\Delta_0 = 0.1$, and $u_{\rm imp} = 0.1$.

$\mathcal{M}_{\rm m}$ is positive while $\mathcal{M}_\Omega$ is negative, corresponding to the paramagnetic and diamagnetic responses respectively. This has a clear explanation in the semiclassical picture: $\mathcal{M}_{\rm m}$ is due to the self-rotation of the wave packet, which is paramagnetic, while $\mathcal{M}_\Omega$ is from the center-of-mass motion of the wave packet, hence is diamagnetic.[16]

When the exchange coupling dominates over the Rashba energy, The minimum of the lower band occurs at the origin. Compared with the previous case, there is no local gap at $p = 0$. The typical band dispersion is shown in Fig. 2(a) (with $\Delta_0 = 0.1$ and taking $2m\alpha^2 = 0.08$). The overall shape of the OM is similar to that for the first case. Its distribution over spectrum is mainly below the upper band bottom. However, due to the absence of the local gap, the kink point at $-\Delta_0$ in Fig. 1(a) merges with the lower band bottom. Moreover, the two contributions $\mathcal{M}_\Omega$ and $\mathcal{M}_{\rm m}$ strongly cancel each other and the resulting OM is much smaller.

Now let us consider the effects of disorder scattering on the OM in our model. When the disorder scattering is turned on, the translational invariance is broken. We can no longer define quantities such as $\mathcal{M}_\Omega$ and $\mathcal{M}_{\rm m}$. Their effects are merged into the sophisticated expression in Eq. (23). Figures 3(a) and 4(a) show the OM versus E_F for the two regimes we discussed above. The different curves in each figure correspond to different impurity concentrations $n_{\rm imp}$. Compared with the clean limit where $n_{\rm imp} = 0$, we see that the shape of the OM curve is almost unchanged but mainly its position is shifted by the scattering. This behavior is more obvious when we look at the density of OM shown in Figs. 3(b) and 4(b). For the clean limit, we see that the major contribution to the OM is from the states at the band bottom and at the local band edge. The effect of disorder scattering here is to shift the the density of OM distribution in energy. Such a shift can be understood by noticing that the OM only has the Fermi-sea contribution. The

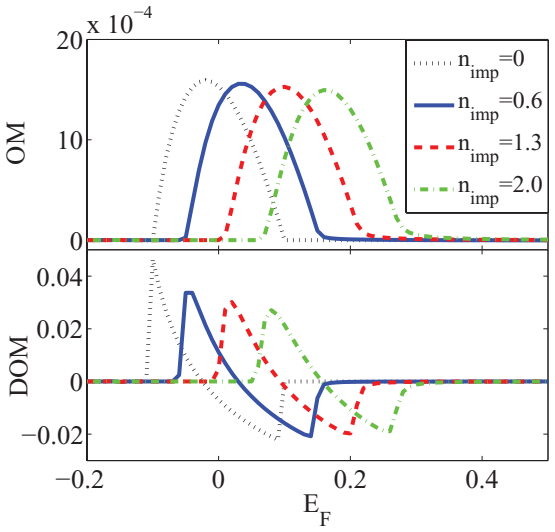

FIG. 4. (Color online) (a) Orbital magnetization (OM) as a function of Fermi energy E_F with different impurity concentration $n_{\rm imp}$. (b) Density of OM with different impurity concentration $n_{\rm imp}$. These quantities are plotted in units of $e/\hbar$. The parameters are chosen as $2m\alpha^2 = 0.08$, $\Delta_0 = 0.1$, and $u_{\rm imp} = 0.1$.

main effect of scattering in Eq. (23) is the shift of energy arising from the real part of the self-energy correction.[51] For the short-range disorder model, the disorder potential is a constant in momentum space, hence the self-energy is independent of the state, which results in a rigid energy shift for all the states. For a general disorder potential, the energy shift would be generally different for different states therefore the distribution of OM would be distorted. The effects of finite-range disorders are currently under investigation.

To leading order, the shift should be linear in the disorder density $n_{\rm imp}$. In Fig. 5 we plot the OM as a function of E_F and $n_{\rm imp}$. The linear dependence of the energy shift in $n_{\rm imp}$ is clearly observed. Apart from the energy shift, the scattering-induced state broadening is manifested as the smoothing of the peaks of the density of OM, which can be clearly observed in Figs. 3(b) and 4(b). The peaks of OM are only slightly decreased by the scattering. This means that the OM carried by the electronic states are quite robust against scattering.

Moreover, Figs. 3(b) and 4(b) show us a sign change of density of OM when the OM sweeps across its maximum. The change indicates the transition from the paramagnetic

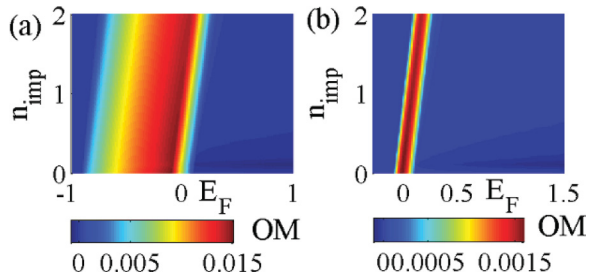

FIG. 5. (Color online) Orbital magnetization (OM) as functions of Fermi energy E_F and the impurity concentration $n_{\rm imp}$ in units of $e/\hbar$. The parameters are chosen as $\Delta_0 = 0.1$, and $u_{\rm imp} = 0.1$, except the Rashba energy: (a) $2m\alpha^2 = 3.59$, (b) $2m\alpha^2 = 0.08$.

to diamagnetic susceptibility.[52,53] When the impurities are present, the position of transition point is moving along E_F axis with increasing $n_{\rm imp}$.

IV. CONCLUSION AND OUTLOOK

In summary, we have derived a formula of the OM of disordered electron systems based on the Keldysh-Green's function theory. This approach was developed as a systematic approach to the nonequilibrium electron dynamics under external fields. In the formula, OM is expressed in terms of the Green's functions and self-energies, which can be solved from the Dyson equations, and systematic approximation schemes to the disorder effects can be employed. We find that there is no Fermi surface contribution as in the case of the current response. Our formula applies not only for insulators but also for metallic systems, where the quasiparticle behavior is usually strongly modified by the disorder scattering. It can also be straightforwardly implemented in the numerical calculation. In the clean limit, our formula reduces to the previous result obtained from other approaches. As an application, we calculate the OM of a weakly disordered two-dimensional electron gas with Rashba spin-orbit coupling. The result shows that in the simplest white noise short-range disorder model, the OM is robust against weak scattering and the main effect of scattering is a rigid shift of the distribution of OM in energy, which can be attributed to the real part of the self-energy.

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APPENDIX A: SELF-CONSISTENT EQUATION FOR $\hat{\Sigma}_0^R$ AND EXPLICIT FORMS OF $\hat{G}_0^R$

The Green's functions and self-energies in the absence of the external fields are obtained from the coupled self-consistent equations (7), (15), and (17). In our model, a direct analytical integration in ε shows that

$$\Sigma_0^{R0}(\varepsilon) = \frac{n_{\rm imp} u_{\rm imp}\left[1 - u_{\rm imp} g_0^{R0}(\varepsilon)\right]}{\left[1 - u_{\rm imp} g_0^{R0}(\varepsilon)\right]^2 - u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2}, \quad \text{(A1)}$$

$$\Sigma_0^{Rz}(\varepsilon) = \frac{n_{\rm imp} u_{\rm imp}^2 g_0^{Rz}(\varepsilon)}{\left[1 - u_{\rm imp} g_0^{R0}(\varepsilon)\right]^2 - u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2}, \quad \text{(A2)}$$

$$\Sigma_0^{Rx}(\varepsilon) = \Sigma_0^{Ry}(\varepsilon) = 0, \quad \text{(A3)}$$

where

$$g_0^{R0}(\varepsilon) = \frac{m}{4\pi\hbar^2} \sum_\sigma \ln \frac{G_0^R(\varepsilon,\Lambda,\sigma)}{G_0^R(\varepsilon,0,\sigma)} - m\alpha^2 \tilde{g}_0^R(\varepsilon), \quad \text{(A4)}$$

$$g_0^{Rz}(\varepsilon) = \left[-\Delta_0 + \Sigma_0^{Rz}(\varepsilon)\right] \tilde{g}_0^R(\varepsilon), \quad \text{(A5)}$$

and

$$\tilde{g}_0^R(\varepsilon) = \frac{m}{4\pi\hbar^2 R^R(\varepsilon)}\Big\{\sum_\sigma \sigma \ln\big[\varepsilon - p^2/2m + \mu - \Sigma_0^{R0}(\varepsilon) + m\alpha^2 + \sigma R^R(\varepsilon)\big]\Big\}_{p=0}^{p=\Lambda}, \quad \text{(A6)}$$

$$G_0^R(\varepsilon,p,\pm) = \Big\{\varepsilon - p^2/2m + \mu - \Sigma_0^{R0}(\varepsilon) \mp \sqrt{\alpha^2 p^2 + \big[-\Delta_0 + \Sigma_0^{Rz}(\varepsilon)\big]^2}\Big\}^{-1}, \quad \text{(A7)}$$

$$R^R(\varepsilon) = \big\{(m\alpha^2)^2 + 2m\alpha^2\big[\varepsilon + \mu - \Sigma_0^{R0}(\varepsilon)\big] + \big[-\Delta + \Sigma_0^{Rz}(\varepsilon)\big]^2\big\}^{\frac{1}{2}}, \quad \text{(A8)}$$

where Λ is the cut-off in momentum integration, and

$$\hat{G}_0^R(\varepsilon) = G_0^{R0}(\varepsilon)\hat{\sigma}^0 + \sum_{l=x,y,z} G_0^{Rl}(\varepsilon)\hat{\sigma}^l, \quad \text{(A9)}$$

with

$$G_0^{R0}(\varepsilon,\mathbf{p}) = \big[\varepsilon - p^2/2m + \mu - \Sigma_0^{R0}(\varepsilon)\big]\tilde{G}_0^R(\varepsilon,p), \quad \text{(A10)}$$

$$G_0^{Ri}(\varepsilon,\mathbf{p}) = \big\{-\alpha\epsilon_{ijz}p_j + \delta_{iz}[-\Delta_0 + \Sigma_0^{Rz}(\varepsilon)]\big\}\tilde{G}_0^R(\varepsilon,p), \quad \text{(A11)}$$

$$\tilde{G}_0^R(\varepsilon,p) = \big[\varepsilon - p^2/2m + \mu - \Sigma_0^{R0}(\varepsilon)\big]^2 + \alpha^2 p^2 + \big[-\Delta_0 + \Sigma_0^{Rz}(\varepsilon)\big]^2, \quad \text{(A12)}$$

and ϵ_{ijl} is the antisymmetric tensor, $(i, j, l, \ldots)$ label the Cartesian components. The same results have been obtained in Ref. 35.

For each ε, the self-energy can be calculated by iterations, which can be performed until the the prescribed accuracy is reached.

APPENDIX B: SELF-CONSISTENT EQUATION FOR $\hat{G}_B^R$ AND $\hat{\Sigma}_B^R$ AND THEIR EXPLICIT FORMS

The equations for solving the first-order corrections $\hat{G}_B^R$ and $\hat{\Sigma}_B^R$ are presented here. Using Eqs. (14) and (16), the retarded Green's function $\hat{G}_B^R$ can be rewritten as

$$\hat{G}_B^R(\varepsilon) = G_B^{R0}(\varepsilon)\hat{\sigma}^0 + \vec{G}_B^R(\varepsilon)\cdot\hat{\sigma}, \quad \text{(B1)}$$

with

$$G_B^{R0}(\varepsilon,\mathbf{p}) = \big[G_0^{R0}(\varepsilon,\mathbf{p})^2 + \vec{G}_0^R(\varepsilon,\mathbf{p})^2\big]\Sigma_B^{R0}(\varepsilon) + 2G_0^{R0}(\varepsilon)\vec{G}_0^R(\varepsilon,\mathbf{p})\cdot\vec{\Sigma}_B^R(\varepsilon) + \tilde{G}_0^R(\varepsilon,\mathbf{p})\big[\partial_{p_x}\hat{H}_0(\mathbf{p})\times\vec{G}_0^R(\varepsilon,\mathbf{p})\big]\cdot[\partial_{p_y}\hat{H}_0(\mathbf{p})], \quad \text{(B2a)}$$

$$\vec{G}_B^R(\varepsilon,\mathbf{p}) = \tilde{G}_0^R(\varepsilon,\mathbf{p})\vec{\Sigma}_B^R(\varepsilon) - \tilde{G}_0^R(\varepsilon,\mathbf{p})G_0^{R0}(\varepsilon,\mathbf{p})[\partial_{p_x}\hat{H}_0(\mathbf{p})]\times[\partial_{p_y}\hat{H}_0(\mathbf{p})] - \tilde{G}_0^R\big[\partial_{p_x}H_0^0(\mathbf{p})\big]\vec{G}_0^R(\varepsilon,\mathbf{p})\times[\partial_{p_y}\hat{H}_0(\mathbf{p})] + \tilde{G}_0^R\big[\partial_{p_y}H_0^0(\mathbf{p})\big]\vec{G}_0^R(\varepsilon,\mathbf{p})\times[\partial_{p_x}\hat{H}_0(\mathbf{p})] + 2\vec{G}_0^R(\varepsilon,\mathbf{p})\big(G_0^{R0}(\varepsilon,\mathbf{p})\Sigma_B^{R0}(\varepsilon) + \vec{G}_0^R(\varepsilon,\mathbf{p})\cdot\vec{\Sigma}_B^R(\varepsilon)\big), \quad \text{(B2b)}$$

and the inner product of two vectors are defined as

$$\vec{A}\cdot\vec{B} = \sum_{l=x,y,z} A^l B^l. \quad \text{(B3)}$$

From Eqs. (16) and (17), we write the self-energy $\hat{\Sigma}_B^R(\varepsilon)$ as

$$\hat{\Sigma}_B^R(\varepsilon) = \Sigma_B^{R0}(\varepsilon)\hat{\sigma}^0 + \sum_{l=x,y,z}\Sigma_B^{Rl}(\varepsilon)\hat{\sigma}^l, \quad \text{(B4)}$$

with

$$\Sigma_B^{R0}(\varepsilon) = n_{\rm imp}u_{\rm imp}^2\big\{\big[1 - u_{\rm imp}g_0^{R0}(\varepsilon)\big]^2 - u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2\big\}^{-2}\big(\big\{[1 - u_{\rm imp}g_0^{R0}(\varepsilon)]^2 + u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2\big\}g_B^{R0}(\varepsilon) + 2\big[1 - u_{\rm imp}g_0^{R0}(\varepsilon)\big]u_{\rm imp}g_0^{Rz}(\varepsilon)g_B^{Rz}(\varepsilon)\big), \quad \text{(B5a)}$$

$$\Sigma_B^{Rz}(\varepsilon) = n_{\rm imp}u_{\rm imp}^2\big\{\big[1 - u_{\rm imp}g_0^{R0}(\varepsilon)\big]^2 - u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2\big\}^{-2}\big(\big\{[1 - u_{\rm imp}g_0^{R0}(\varepsilon)]^2 + u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2\big\}g_B^{Rz}(\varepsilon) + 2[1 - u_{\rm imp}g_0^{R0}(\varepsilon)\big]u_{\rm imp}g_0^{Rz}(\varepsilon)g_B^{R0}(\varepsilon)\big), \quad \text{(B5b)}$$

$$\Sigma_B^{Ri}(\varepsilon) = n_{\rm imp}u_{\rm imp}^2\big\{[1 - u_{\rm imp}g_0^{R0}(\varepsilon)]^2 - u_{\rm imp}^2 g_0^{Rz}(\varepsilon)^2\big\}^{-1}g_B^{Ri}(\varepsilon), \quad \text{(B5c)}$$

and we have

$$g_{0,B}^{R\alpha}(\varepsilon) = \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} G_{0,B}^{R\alpha}, \tag{B6}$$

where $\alpha \in \{0,x,y,z\}$. The zeroth-order components $G_0^{R\alpha}$ are computed as in Appendix A and are used as input for the above equations.

APPENDIX C: PARTICLE DENSITY

Here, we present the derivation of Eq. (19). In the absence of disorder scattering,

$$\hat{G}_0^{R,A}(\varepsilon,\mathbf{p}) = [\varepsilon - \hat{H}_0(\mathbf{p}) \pm i0^+]^{-1}. \tag{C1}$$

At zero temperature, plugging Eq. (C1) into Eqs. (12) and (18), we can obtain

$$n_e = -\int \frac{d\varepsilon}{\pi} \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \left\{ \sum_n \frac{1}{\epsilon - \epsilon_{n\mathbf{p}} + i0^+} + e\hbar B \sum_{nm} \frac{1}{(\epsilon - \epsilon_{n\mathbf{p}} + i0^+)^2} \frac{1}{\epsilon - \epsilon_{m\mathbf{p}} + i0^+} \Im[\langle u_{n\mathbf{p}}|\hat{v}_x(\mathbf{p})|u_{m\mathbf{p}}\rangle\langle u_{m\mathbf{p}}|\hat{v}_y(\mathbf{p})|u_{n\mathbf{p}}\rangle] \right\}. \tag{C2}$$

$u_{n\mathbf{p}}$ are the eigenfunctions of the unperturbed Hamiltonian and $\epsilon_{n\mathbf{p}}$ the eigenvalues. The integral over ϵ contains simple and double poles. Using the residue theorem,[54] we obtain

$$n_e = \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \sum_{n,occ} \{1 + 2ie\hbar B \sum_m \Im[\langle u_{n\mathbf{p}}|\hat{v}_x(\mathbf{p})|u_{m\mathbf{p}}\rangle\langle u_{m\mathbf{p}}|\hat{v}_y(\mathbf{p})|u_{n\mathbf{p}}\rangle]\}, \tag{C3}$$

where *occ* denotes summing over occupied states. Further simplification can be made by using the Sternheimer equation

$$\hat{v}_j(\mathbf{p})|u_{n\mathbf{p}}\rangle = (\epsilon_{n\mathbf{p}} - \epsilon_{n'\mathbf{p}}) \left| \frac{\partial u_{n\mathbf{p}}}{\partial p_j} \right\rangle + \frac{\partial \epsilon_{n\mathbf{p}}}{\partial p_j} |u_{n\mathbf{p}}\rangle, \tag{C4}$$

and we finally arrive at the equation

$$n_e = \sum_{n,occ} \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \left[1 + \frac{e}{\hbar} \mathbf{B} \cdot \Omega_n(\mathbf{p}) \right]. \tag{C5}$$

APPENDIX D: ORBITAL MAGNETIZATION IN THE CLEAN LIMIT

The derivations of Eq. (27) for the OM in the clean limit are present below. When the relaxation rate vanishes, substituting Eq. (C1) into Eq. (24), we can write Eq. (24) as

$$\begin{aligned} M = e\hbar \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \sum_{nm} (\epsilon_{n\mathbf{p}} - \mu) \Im[\langle u_{n\mathbf{p}}|\hat{v}_x(\mathbf{p})|u_{m\mathbf{p}}\rangle\langle u_{m\mathbf{p}}|\hat{v}_y(\mathbf{p})|u_{n\mathbf{p}}\rangle] \\ \times \left[\frac{1}{(\epsilon - \epsilon_{n\mathbf{p}} + i0^+)^2} \frac{1}{\epsilon - \epsilon_{m\mathbf{p}} + i0^+} - \frac{1}{(\epsilon - \epsilon_{n\mathbf{p}} + i0^+)^2} \frac{1}{\epsilon - \epsilon_{m\mathbf{p}} + i0^+} \right] \end{aligned} \tag{D1}$$

Using the residue theorem, we find that

$$M = -e\hbar \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \times \left[\frac{f(\epsilon_{m\mathbf{p}}) - f(\epsilon_{n\mathbf{p}})}{(\epsilon_{m\mathbf{p}} - \epsilon_{n\mathbf{p}})^2} + \frac{f'(\epsilon_{n\mathbf{p}})}{\epsilon_{n\mathbf{p}} - \epsilon_{m\mathbf{p}}} \right] \times \Im \sum_{nm} (\epsilon_{n\mathbf{p}} - \mu)[\langle u_{n\mathbf{p}}|\hat{v}_x(\mathbf{p})|u_{m\mathbf{p}}\rangle\langle u_{m\mathbf{p}}|\hat{v}_y(\mathbf{p})|u_{n\mathbf{p}}\rangle] \tag{D2}$$

where $f'_{n\mathbf{p}} \equiv \partial f(\epsilon_{n\mathbf{p}})/\partial \epsilon_{n\mathbf{p}}$. With the help of the Sternheimer equation Eq. (C4), we obtain

$$M = \frac{i}{2} e\hbar \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \sum_n \left[(\epsilon_{n\mathbf{p}} - \mu) \left\langle \frac{\partial u_{n\mathbf{p}}}{\partial \mathbf{p}} \right| [\epsilon_{n\mathbf{p}} - \hat{H}_0(\mathbf{p})] \times \left| \frac{\partial u_{n\mathbf{p}}}{\mathbf{p}} \right\rangle f'_{np} - \left\langle \frac{\partial u_{n\mathbf{p}}}{\partial \mathbf{p}} \right| [\epsilon_{n\mathbf{p}} + \hat{H}_0(\mathbf{p}) - 2\mu] \times \left| \frac{\partial u_{n\mathbf{p}}}{\partial \mathbf{p}} \right\rangle f_{n\mathbf{p}} \right]_z. \tag{D3}$$

The above result can be written as

$$M = \sum_{n\mathbf{p}} \left\{ m_n(\mathbf{p}) f_{n\mathbf{p}} + (\epsilon_{n\mathbf{p}} - \mu) m_n(\mathbf{p}) f'_{n\mathbf{p}} - \frac{e}{\hbar} (\epsilon_{n\mathbf{p}} - \mu) \Omega_{n\mathbf{p}}(\mathbf{p}) \right\}, \tag{D4}$$

where $m_n(\mathbf{p}) = (e/2\hbar) i \langle \nabla_{\mathbf{p}} u_{n\mathbf{p}}| [\epsilon_n(\mathbf{p}) - \hat{H}_0(\mathbf{p})] \times |\nabla_{\mathbf{p}} u_{n\mathbf{p}}\rangle$ is the orbital moment of state $n,\mathbf{p}$ and $\Omega_n(\mathbf{p}) = i\langle \nabla_{\mathbf{p}} u_{n\mathbf{p}}| \times |\nabla_{\mathbf{p}} u_{n\mathbf{p}}\rangle$ is the Berry curvature. At zero temperature, f' becomes a δ function of $(\epsilon_{n\mathbf{p}} - \mu)$, therefore we have in this case

$$M = \sum_{n\mathbf{p}} \left[m_n(\mathbf{p}) f_{n\mathbf{p}} - \frac{e}{\hbar} (\epsilon_{n\mathbf{p}} - \mu) \Omega_n(\mathbf{p}) \right]. \tag{D5}$$

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[1] A. J. P. Meyer and G. Asch, J. Appl. Phys. **32**, S330 (1961).
[2] S. Qiao, A. Kimura, H. Adachi, K. Iori, K. Miyamoto, T. Xie, H. Namatame, M. Taniguchi, A. Tanaka, T. Muro, S. Imada, and S. Suga, Phys. Rev. B **70**, 134418 (2004).
[3] J. W. Taylor, J. A. Duffy, A. M. Bebb, M. R. Lees, L. Bouchenoire, S. D. Brown, and M. J. Cooper, Phys. Rev. B **66**, 161319(R) (2002).
[4] D. Ceresoli, N. Marzari, M. G. Lopez, and T. Thonhauser, Phys. Rev. B **81**, 184424 (2010).
[5] T. Thonhauser, D. Ceresoli, A. A. Mostofi, N. Marzari, R. Resta, and D. Vanderbilt, J. Chem. Phys. **131**, 101101 (2009).
[6] T. Thonhauser, D. Ceresoli, and N. Marzari, Int. J. Quantum Chem. **109**, 3336 (2009).
[7] D. Ceresoli, U. Gerstmann, A. P. Seitsonen, and F. Mauri, Phys. Rev. B **81**, 060409(R) (2010).
[8] M. Koshino and T. Ando, Phys. Rev. B **81**, 195431 (2010).
[9] Y. Ominato and M. Koshino, Phys. Rev. B **85**, 165454) (2012).
[10] A. M. Essin, J. E. Moore, and D. Vanderbilt, Phys. Rev. Lett. **102**, 146805 (2009).
[11] A. M. Essin, A. M. Turner, J. E. Moore, and D. Vanderbilt, Phys. Rev. B **81**, 205104 (2010).
[12] A. Malashevich, I. Souza, S. Coh, and D. Vanderbilt, New J. Phys. **83**, 053032 (2010).
[13] Sinisa Coh, David Vanderbilt, Andrei Malashevich, and Ivo Souza, Phys. Rev. B **83**, 085108 (2011).
[14] S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).
[15] L. L. Hirst, Rev. Mod. Phys. **69**, 607 (1997).
[16] D. Xiao, M. Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959 (2010).
[17] T. Thonhauser, Int. J. Mod. Phys. B **25**, 1429 (2011).
[18] D. Xiao, J. Shi, and Q. Niu, Phys. Rev. Lett. **95**, 137204 (2005).
[19] D. Xiao, Y. Yao, Z. Fang, and Q. Niu, Phys. Rev. Lett. **97**, 026603 (2006).
[20] T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. **95**, 137205 (2005).
[21] D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B **74**, 024408 (2006).
[22] I. Souza and D. Vanderbilt, Phys. Rev. B **77**, 054438 (2008).
[23] M. G. Lopez, David Vanderbilt, T. Thonhauser, and Ivo Souza, Phys. Rev. B **85**, 014435 (2012).
[24] J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett. **99**, 197202 (2007).
[25] D. Ceresoli and R. Resta, Phys. Rev. B **76**, 012405 (2007).
[26] D. Ceresoli, U. Gerstmann, A. P. Seitsonen, and F. Mauri, Phys. Rev. B **81**, 060409 (2010).
[27] R. Resta, D. Ceresoli, T. Thonhauser, and D. Vanderbilt, Chem. Phys. Chem. **6**, 1815 (2005).
[28] R. Resta, J. Phys.: Condens. Matter **22**, 123201 (2005).
[29] O. Gat and J. E. Avron, Phys. Rev. Lett. **91**, 186801 (2003).
[30] O. Gat and J. E. Avron, New J. Phys. **5**, 44 (2003).
[31] Z. Wang and P. Zhang, Phys. Rev. B **76**, 064406 (2007).
[32] Z. Wang, P. Zhang, and J. Shi, Phys. Rev. B **76**, 094406 (2007).
[33] S. Onoda, N. Sugimoto, and N. Nagaosa, Prog. Theor. Phys. **116**, 61 (2006).
[34] S. Onoda, N. Sugimoto, and N. Nagaosa, Phys. Rev. Lett. **97**, 126602 (2006).
[35] S. Onoda, N. Sugimoto, and N. Nagaosa, Phys. Rev. B **77**, 165103 (2008).
[36] A. A. Kovalev, Y. Tserkovnyak, K. Vyborny, and J. Sinova, Phys. Rev. B **79**, 195129 (2009).
[37] A. A. Kovalev, J. Sinova, and Y. Tserkovnyak, Phys. Rev. Lett. **105**, 036601 (2010).
[38] H. Haug and A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, New York, 1996).
[39] P. Streda, J. Phys. C **15**, L717 (1982).
[40] M.-C. Chang and Q. Niu, Phys. Rev. B **53**, 7010 (1996).
[41] G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).
[42] E. I. Rashba, Fiz. Tverd. Tela (Leningrad) **2**, 1224 (1960) [Sov. Phys. Solid State **2**, 1109 (1960)].
[43] C. Gorini, P. Schwab, M. Dzierzawa, and R. Raimondi, Phys. Rev. B **78**, 125327 (2008).
[44] A. Yamakage, Y. Tanaka, and N. Nagaosa, Phys. Rev. Lett. **108**, 087003 (2012).
[45] S. Nakosai, Y. Tanaka, and N. Nagaosa, Phys. Rev. Lett. **108**, 147003 (2012).
[46] W. Yang and K. Chang, Phys. Rev. B **73**, 045303 (2006).
[47] J. Nitta, T. Akazaki, H. Takayanagi, and T. Enoki, Phys. Rev. Lett. **78**, 1335 (1997).
[48] G. Engels, J. Lange, Th. Schäpers, and H. Lüth, Phys. Rev. B **55**, R1958 (1997).
[49] A. D. Caviglia, M. Gabay, S. Gariglio, N. Reyren, C. Cancellieri, and J.-M. Triscone, Phys. Rev. Lett. **104**, 126803 (2010).
[50] M. S. Garelli and J. Schliemann, Phys. Rev. B **80**, 155321 (2009).
[51] C. W. Groth, M. Wimmer, A. R. Akhmerov, J. Tworzydło, and C. W. J. Beenakker, Phys. Rev. Lett. **103**, 196805 (2009).
[52] Y. A. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984).
[53] I. I. Boiko and E. I. Rashba, Fiz. Tverd. Tela (Leningrad) **2**, 1874 (1960) [Sov. Phys. Solid State **2**, 1692 (1960)].
[54] T. S. Nunner, N. A. Sinitsyn, M. F. Borunda, V. K. Dugaev, A. A. Kovalev, Ar. Abanov, C. Timm, T. Jungwirth, J. I. Inoue, A. H. MacDonald, and J. Sinova, Phys. Rev. B **76**, 235312 (2007).