Reactive Hall and Edelstein effects in a tight-binding model with spin-orbit coupling

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The reactive Hall constant R_H, described by reactive (nondissipative) conductivities, is analyzed within linear response theory in the presence of spin-orbit interaction. Within a two-dimensional tight-binding model the effect of Van Hove singularities is studied. Along the same line a formulation of the Edelstein constant is proposed and studied as a function of coupling parameters and fermion filling.

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I. INTRODUCTION

The spin-orbit interaction [1,2] plays a prominent role in the field of spintronics. It has been extensively studied as a key mechanism in the anomalous Hall effect [3], the spin Hall effect [4–7], induced magnetoelectric torque and edge currents [8,9], and the Edelstein effect [10,11] to name just a very few.

From a different perspective, in a seminal work [12] Kohn brought attention to the reactive response of an electronic system, as a criterion of the Mott metal-insulator transition, given by the imaginary part of the conductivity, $\sigma''(\omega \to 0) = 2D/\omega$. The prefactor D, referred to as "Drude" weight in numerous recent theoretical studies and also equal to the weight of the zero-frequency δ function in the regular part of the conductivity, is finite in a noninteracting gapless system without disorder at all temperatures or a gapless strongly correlated integrable one [13]. In the presence of scattering (e.g., phonons, disorder) the δ function broadens to a peak of width $1/\tau$ (where τ is a characteristic scattering time) and integrated weight D which is experimentally studied.

Along the same line, a formulation of the reactive Hall response was proposed [14] in order to address the problem of Hall constant sign change as a function of doping observed in experiments in high T_c superconductors. In this formulation the Hall constant is given by the logarithmic derivative of the Drude weight with respect to the particle density. This reactive Hall constant approach has recently been extensively used in theoretical [15] and experimental [16] studies of interacting (and synthetic) quantum systems.

In more generality, both Hall and Edelstein constants display signatures of Fermi surface (FS) topological transitions which are abundant in two-dimensional quantum materials. Lifshitz transitions with their associated logarithmically divergent Van Hove singularities occur in many systems including cuprates, iron based superconductors, cobaltates, Sr_2RuO_4, and heavy fermions [17–25]. There is an even more recent surge of interest in higher order Van Hove singularities [26–30]. Some of the materials where they have been discovered include $Sr_3Ru_2O_7$ where a higher order (X_9 with $n = 4$) Van Hove singularity was shown to exist in the presence of an external magnetic field [26], while different types of higher order Van Hove saddles have been reported in highly overdoped graphene [31], the surface of Sr_2RuO_4 [32], kagome metals [33–36], and high-T_c superconductors [37].

In this paper, we will first study the effect of the spin-orbit interaction on the reactive Hall effect of a two-dimensional tight binding model of noninteracting fermions, showing ballistic transport, as a function of spin-orbit coupling. We study its behavior as the Fermi surface evolves as a function of filling. We obtain the signatures on R_H of Fermi surface topological transitions, with the associated Van Hove singularities in a quantum mechanical description. Earlier work using the Boltzmann equation studied these effects at a semiclassical level [38], and a recent work studied the spin and orbital Edelstein effect in a bilayer system with Rashba interaction [39]. Next, we develop a formula, in analogy to the reactive Hall constant, for the Edelstein effect which describes the appearance of a transverse magnetization due to a charge current in a two-dimensional system with spin-orbit interaction. It would be fascinating to experimentally study the reactive Edelstein effect, for instance in synthetic systems [16], as the reactive Hall effect.

II. MODEL

We consider a generic Hamiltonian for fermions on a lattice, where for simplicity we describe the kinetic energy term by a one-band tight-binding model; it is straightforward to extend this formulation to a many-band or continuum system. The sites are labeled $l(m)$ along the $\hat{x}(\hat{y})$ direction with

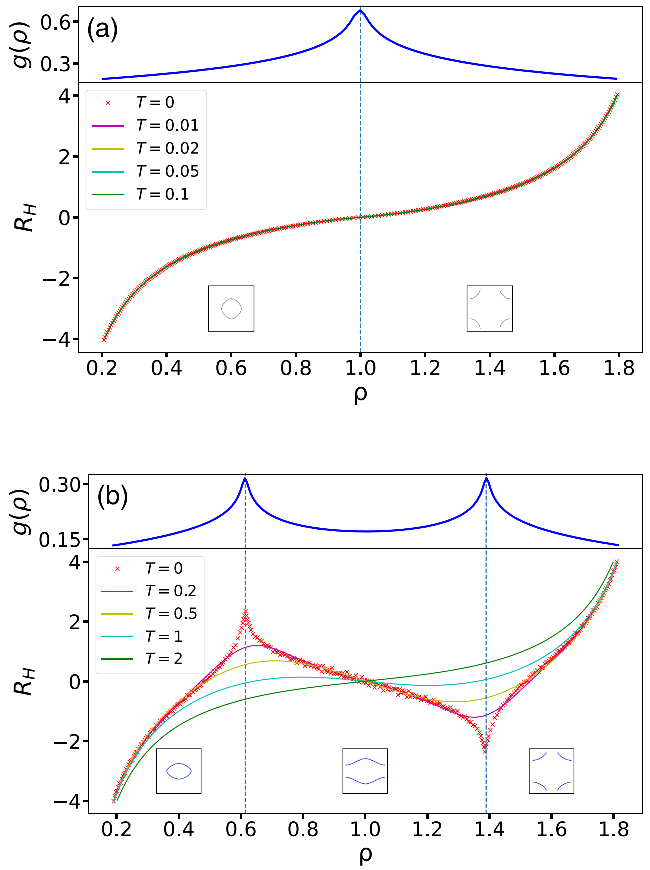

FIG. 1. The density of states $g(\rho)$ and Hall coefficient R_H for cases without SOC: (a) $t_x = t_y = 1$ and (b) $t_x = 1$ and $t_y = 2$.

periodic boundary conditions in both directions:

$$\begin{aligned}
H &= H_0 + H_{\mathrm{SO}}, \\
H_0 &= \sum_{l,m} -t_x e^{i\phi^x(t)} e^{iA_m} c^\dagger_{l+1,m} \cdot c_{l,m} \\
&\quad - t_y e^{i\phi^y_{m+1/2}(t)} c^\dagger_{l,m+1} \cdot c_{l,m} + \text{H.c.}, \\
H_{\mathrm{SO}} &= \sum_{l,m} +\lambda_x e^{i\phi^x(t)} e^{iA_m} c^\dagger_{l+1,m}(-i\sigma^y) c_{l,m} \\
&\quad + \lambda_y e^{i\phi^y_{m+1/2}(t)} c^\dagger_{l,m+1}(i\sigma^x) c_{l,m} + \text{H.c.}, \qquad (1) \\
l &= 1, \ldots, L_x, \\
m &= 1, \ldots, L_y, \\
N &= L_x \cdot L_y.
\end{aligned}$$

where $t_{x,y}$ are the hopping parameters; $\lambda_{x,y}$ are the Rashba spin-orbit couplings; σ^α, $\alpha = x, y, z$ are the spin-1/2 Pauli matrices; and the fermion creation (annihilation) operators are denoted as $c^\dagger_{l,m} = (c^\dagger_{\uparrow l,m}\ c^\dagger_{\downarrow l,m})$.

We take a unit lattice constant, electric charge $e = 1$, and $\hbar = 1$. We add a magnetic field along the $\hat{z}$ direction, modulated by a one component wave vector q along the $\hat{y}$ direction,

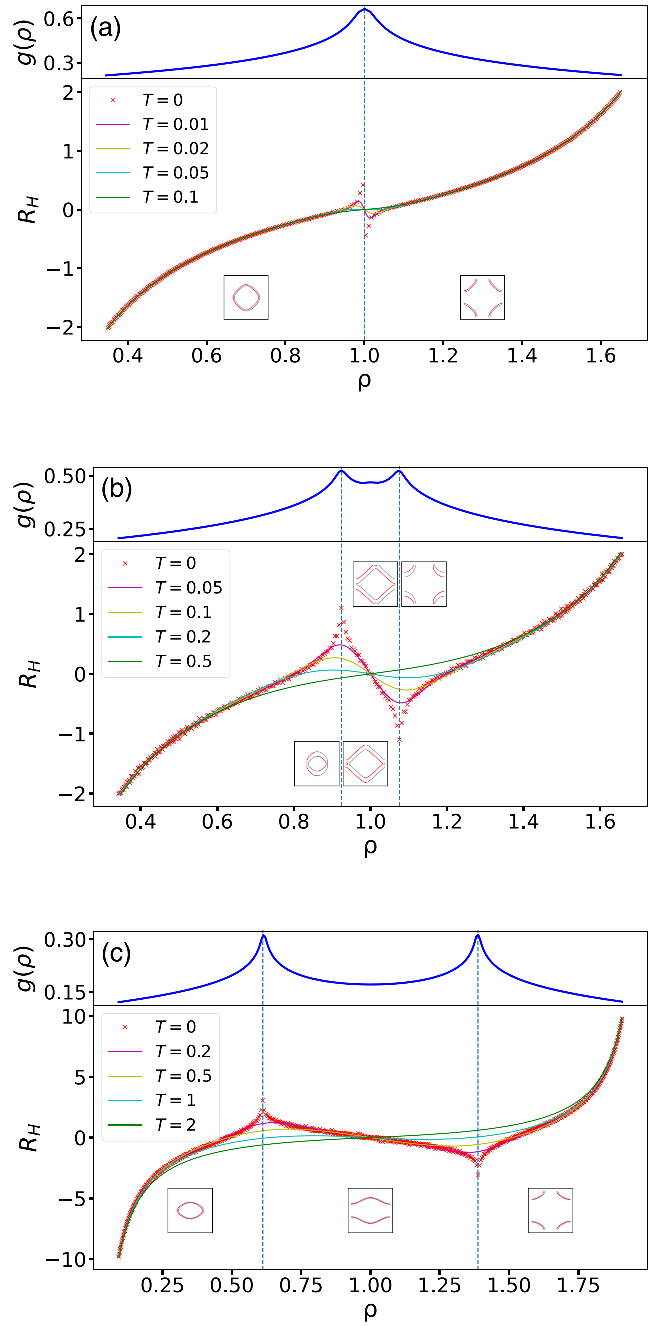

FIG. 2. The density of states $g(\rho)$ and Hall coefficient R_H for cases with SOC: (a) $t_x = t_y = 1$ and $\lambda_x = \lambda_y = 0.1$; (b) $t_x = 1$, $t_y = 1$, $\lambda_x = 0.1$, and $\lambda_y = 0.4$; and (c) $t_x = 1$, $t_y = 2$, and $\lambda_x = \lambda_y = 0.1$.

generated by the vector potential A_m; this allows us to take the zero magnetic field limit smoothly:

$$A_m = e^{iqm} \frac{iB}{2\sin(q/2)} \simeq e^{iqm} \frac{iB}{q},$$

$$B_{m+1/2} = -(A_{m+1} - A_m) = B e^{iq(m+1/2)}$$

[for convenience, we will present the long wavelength limit, substituting $2\sin(q/2) \to q$]. Electric fields along the $\hat{x}$ and $\hat{y}$

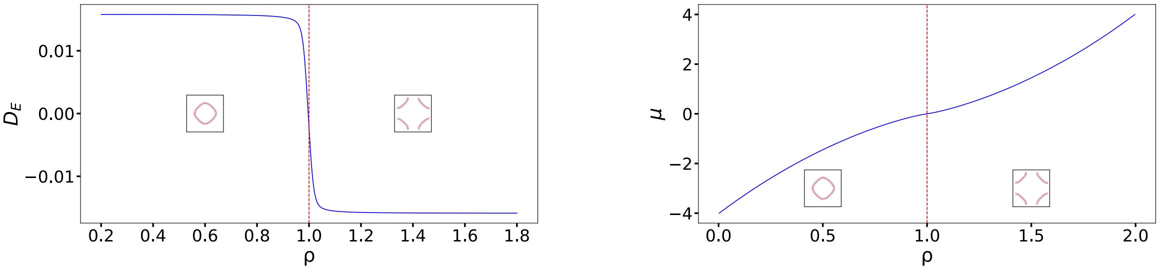

FIG. 3. Left: Edelstein constant D_E as a function of fermion density, for $t_x = t_y = 1$ and $\lambda_x = \lambda_y = 0.1$. Right: Chemical potential as a function of fermion density for the same parameters.

directions are generated by time dependent vector potentials:

$$\phi^{x,y}(t) = \frac{E^{x,y}(t)}{iz},\ \phi^y_{m+1/2}(t) = e^{iq(m+1/2)}\phi^y(t),$$
$$E^{x,y}(t) = E^{x,y}e^{-izt},\quad z = \omega + i\eta.$$

Currents are defined through derivatives of the Hamiltonian in $\phi^{x,y}$:

$$j^x = -\frac{\partial H}{\partial \phi^x},\qquad j^y_q = -\frac{\partial H}{\partial \phi^y},$$

with the paramagnetic parts

$$j^x = \sum_{l,m} t_x e^{iA_m} i c^\dagger_{l+1,m}\cdot c_{l,m} - \lambda_x e^{iA_m} c^\dagger_{l+1,m}\sigma^y c_{l,m} + \text{H.c.},$$
$$j^y_q = \sum_{l,m} e^{iq(m+1/2)}(t_y i c^\dagger_{l,m+1}\cdot c_{l,m} - \lambda_y c^\dagger_{l,m+1}\sigma^y c_{l,m} + \text{H.c.}).$$

III. REACTIVE HALL RESPONSE

We will analyze the reactive Hall response within standard linear response theory:

$$\langle j^x\rangle = \sigma_{j^x j^x}E^x(t) + \sigma_{j^x j^y_q}E^y(t),$$
$$\langle j^y_q\rangle = \sigma_{j^y_q j^x}E^x(t) + \sigma_{j^y_q j^y_q}E^y(t),$$

closely following the development in [14].

Reactive—nondissipative—response occurs in a generic uniform (without disorder) interacting system at zero temperature, in which case the brackets $\langle\dots\rangle$ denote ground state average [14], or at finite temperatures in a uniform noninteracting system, in which case the brackets $\langle\dots\rangle$ denote thermal average. Here we study the reactive Hall constant for the Hamiltonian (1) at finite temperatures in the presence of a magnetic field, with the conductivities given by

$$\sigma_{j^\alpha j^\beta} = \frac{i}{z}\left(\left\langle\frac{\partial^2 H}{\partial\phi^\alpha\partial\phi^\beta}\right\rangle - \chi_{j^\alpha j^\beta}\right),$$
$$\chi_{AB} = i\int_0^\infty dt\, e^{izt}\langle[A(t), B]\rangle.$$

In contrast to the usual derivation of the Hall constant expression, we keep the q dependence explicit by converting the current-current to current-density correlations using the continuity equation

$$\langle j^x\rangle = \sigma_{j^x j^x}E^x(t) + \frac{1}{q}\chi_{j^x n_q}E^y(t),$$
$$\langle j^y_q\rangle = -\frac{1}{q}\chi_{n_q j^x}E^x(t) + \left(\frac{z}{q}\right)^2\chi_{n_q n_q}\frac{i}{z}E^y(t),$$

with $n_q = \sum_{l,m}(-ie^{iqm})c^\dagger_{l,m}\cdot c_{l,m}$.

At this point we consider the "screening" (or slow) response in the $\hat{y}$ direction, by taking the (q,ω) limits in the order $\omega\to 0$ first and $q\to 0$ last. For $H(\lambda,\mu)$, using the following identity,

$$\frac{\partial^2 E_n}{\partial\mu\partial\lambda} = \langle n|\frac{\partial^2 H}{\partial\mu\partial\lambda}|n\rangle - \sum_{m\neq n}\frac{\langle n|\frac{\partial H}{\partial\mu}|m\rangle\langle m|\frac{\partial H}{\partial\lambda}|n\rangle + \text{H.c.}}{E_m - E_n}, \tag{2}$$

we arrive at

$$R_H = -\frac{1}{D}\frac{\partial D}{\partial\rho}, \tag{3}$$

with ρ the electron density. The Drude weight D can be evaluated by Kohn's expression [12] and its finite temperature extension [40] as the second derivative of energy eigenvalues

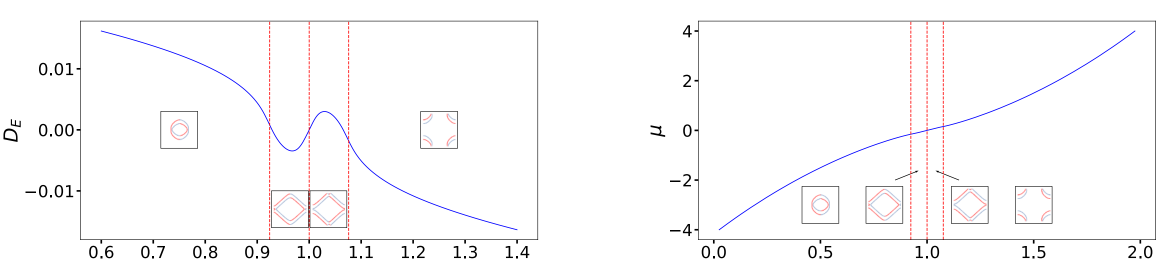

FIG. 4. Left: Edelstein constant D_E as a function of fermion density for $t_x = 1$, $t_y = 1$, $\lambda_x = 0.1$, and $\lambda_y = 0.4$. Right: Chemical potential as a function of fermion density.

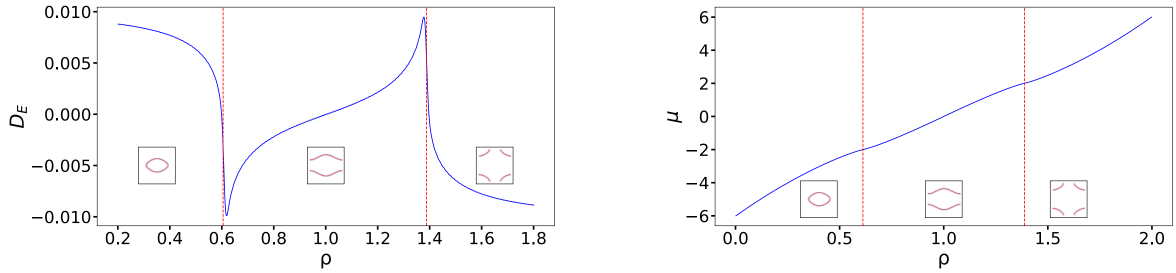

FIG. 5. Left: Edelstein constant D_E as a function of fermion density now for $t_x = 1$, $t_y= 2$, and $\lambda_x = \lambda_y = 0.1$ with the corresponding chemical potential as a function of density.

E_n with respect to a uniform fictitious flux ϕ_x:

$$D = \frac{1}{2N} \sum_n p_n \frac{\partial^2 E_n}{\partial \phi_x^2}\bigg|_{\phi_x \to 0} \tag{4}$$

where $p_n = e^{-\beta E_n}/\sum_n e^{-\beta E_n}$ with $\beta = 1/k_B T$ is the inverse temperature, $k_B = 1$ is the Boltzmann constant, and ρ is the fermion density.

To evaluate the eigenvalues/eigenstates we diagonalize the Hamiltonian (1) in the presence of the fictitious flux ϕ_x by transforming to momentum $\mathbf{k} = (k_x, k_y)$ space:

$$\begin{vmatrix} \epsilon_{\mathbf{k}}^{(0)} - \epsilon & \Delta_{\mathbf{k}} e^{+i\theta_{\mathbf{k}}} \\ \Delta_{\mathbf{k}} e^{-i\theta_{\mathbf{k}}} \epsilon_{\mathbf{k}}^{(0)} - \epsilon & \end{vmatrix} = 0,$$

$$\epsilon_{\mathbf{k}}^{(0)}(\phi_x) = -2t_x \cos(k_x + \phi_x) - 2t_y \cos k_y,$$

$$\Delta_{\mathbf{k}} = 2\sqrt{\lambda_x^2 \sin^2(k_x + \phi_x) + \lambda_y^2 \sin^2 k_y},$$

$$\theta_{\mathbf{k}} = \tan^{-1} \frac{\lambda_x \sin k_x}{\lambda_y \sin k_y}.$$

We obtain $H = \sum_{\mathbf{k}\pm} \epsilon_{\mathbf{k}\pm} c_{\mathbf{k}\pm}^\dagger c_{\mathbf{k}\pm}$ with the two spin states turning by the spin-orbit interaction to two chirality eigenstates $c_{\mathbf{k}\pm} = \frac{1}{\sqrt{2}}(c_{\mathbf{k}\uparrow} \pm e^{-i\phi_{\mathbf{k}}} c_{\mathbf{k}\downarrow})$ and eigenvalues:

$$\epsilon_{\mathbf{k}\pm}(\phi_x) = \epsilon_k(\phi_x) \pm \Delta_{\mathbf{k}}.$$

Finally the reactive Hall constant is given by

$$D = \sum_{\pm} \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} f_{\mathbf{k}\pm} \frac{\partial^2 \epsilon_{\mathbf{k}\pm}}{\partial \phi_x^2},$$

$$f_{\mathbf{k}\pm} = \frac{1}{1 + e^{\beta(\epsilon_{\mathbf{k}\pm} - \mu)}}.$$

Using this equation, we show in Figs. 1 and 2 the Hall constant for different values of the hopping and spin-orbit parameters as a function of fermion density ρ in parallel to the density of states:

$$g(\rho) = \sum_{\pm} \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} \delta(\mu(\rho) - \epsilon_{\mathbf{k}\pm}).$$

In Fig. 1, without any spin-orbit coupling, we observe a clear indication in the Hall constant of the Van Hove singularities. When there is a Fermi surface topological transition, there is a discontinuity in the derivative of R_H with respect to ρ. In addition, there is a change of sign when there is a transition from an electronlike to a holelike dispersion. At finite temperature the behavior is continuous and the signature of the transition from an electronlike to a holelike dispersion is reflected in the monotonic behavior of R_H. This goes away at very high temperature where R_H has a monotonic behavior independent of the parameters.

IV. EDELSTEIN COEFFICIENT

Along the same line, we can also study the Edelstein effect in a two-dimensional system with spin-orbit coupling where a charge current in the $\hat{x}$ direction induces a bulk magnetization density $\langle s^y \rangle = \langle \frac{1}{N} \sum_{l,m} c_{l,m}^\dagger \sigma^y c_{l,m} \rangle$ pointing in the $\hat{y}$ direction. The corresponding response is given by

$$\alpha_{yx}(\omega) = \frac{1}{i\omega} i \int_0^\infty e^{izt} \langle [s^y(t), j^x] \rangle dt, \quad z = \omega + i\eta.$$

Here we consider the system (1) in zero magnetic field $A_m = 0$ and zero electric field $\phi_{m+1/2}^y(t) = 0$ along the $\hat{y}$ direction. Now we can define a "reactive Edelstein constant" as the prefactor of the $1/\omega$ imaginary part of α_{yx},

$$\frac{D_E}{\omega} = \lim_{\omega \to 0} \mathrm{Im}\alpha_{yx}(\omega),$$

$$D_E = -\sum_n p_n \sum_m \frac{\langle n|s^y|m\rangle\langle m|j^x|n\rangle + \mathrm{H.c.}}{\epsilon_m - \epsilon_n},$$

which using the identity (2) can be written similarly to the Kohn formula:

$$D_E = \frac{1}{N} \sum_n p_n \frac{\partial^2 E_n}{\partial h^y \partial \phi_x}\bigg|_{h^y, \phi_x \to 0}.$$

Here the energy derivatives are over a uniform fictitious flux ϕ_x in the $\hat{x}$ direction and a Zeeman field h^y along the $\hat{y}$ direction.

For the noninteracting fermion Hamiltonian (1), the imaginary part of the response function becomes

$$D_E = \lim_{\omega \to 0} \sum_k (2\lambda_x \cos k_x \cos^2 \phi_{\mathbf{k}})(f_{\mathbf{k}+} - f_{\mathbf{k}-}) \cdot$$

$$\times \left[\frac{\omega - \delta_{\mathbf{k}}}{(\omega - \delta_{\mathbf{k}})^2 + \eta^2} - \frac{\omega + \delta_{\mathbf{k}}}{(\omega + \delta_{\mathbf{k}})^2 + \eta^2} \right],$$

$$\delta_{\mathbf{k}} = \epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}-}.$$

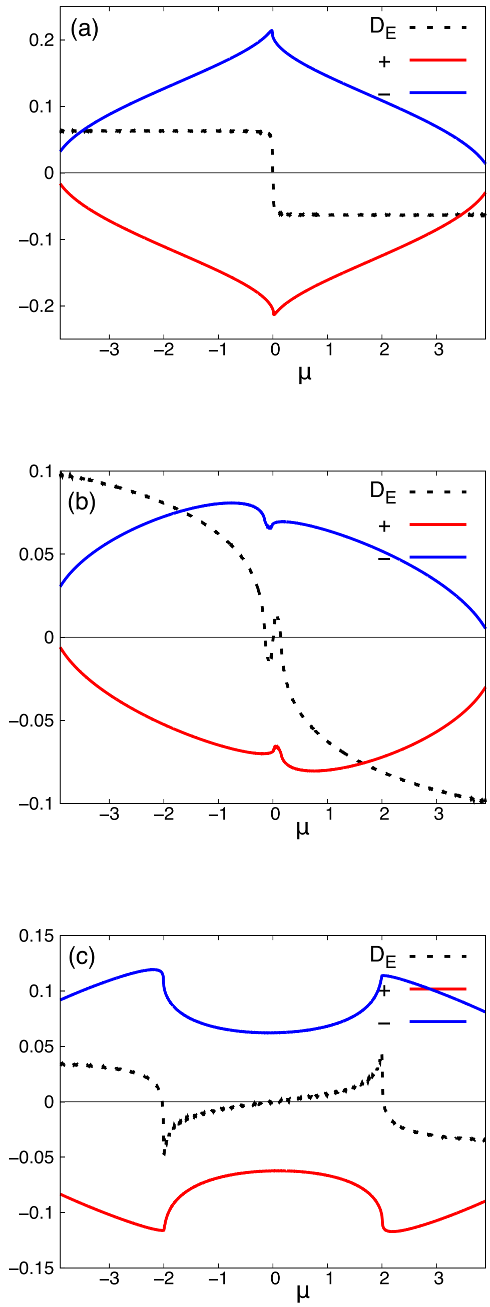

FIG. 6. The two chirality (±) contributions to the Edelstein constant (5) and the total D_E (as in Figs. 3–5, multiplied by a factor of 4 for clarity): (a) $t_x = t_y = 1$ and $\lambda_x = \lambda_y = 0.1$; (b) $t_x = 1$, $t_y = 1$, $\lambda_x = 0.1$, and $\lambda_y = 0.4$; and (c) $t_x = 1$, $t_y = 2$, and $\lambda_x = \lambda_y = 0.1$.

As discussed above, this expression for the imaginary part of the response function can be recast in the form

$$D_E = \sum_{\pm} \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} f_{\mathbf{k}\pm} \left. \frac{\partial^2 \epsilon_{\mathbf{k}\pm}}{\partial h^y \partial \phi_x} \right|_{h^y,\phi_x \to 0}. \tag{5}$$

To evaluate the derivative $\frac{\partial^2 \epsilon_{\mathbf{k}\pm}}{\partial h^y \partial \phi_x}|_{h^y,\phi_x\to 0}$ we add in the Hamiltonian (1) a magnetic field in the $\hat{y}$ direction ($+h^y s^y$), modifying the eigenvalues as

$$\begin{aligned}\epsilon_{\mathbf{k}\pm} &= \epsilon^{(0)}_{\mathbf{k}} \pm 2\sqrt{[\lambda_x \sin(k_x + \phi_x) - h^y/2]^2 + \lambda_y^2 \sin^2 k_y} \\ &= \epsilon^{(0)}_{\mathbf{k}}(\phi_x) \pm \Delta_{\mathbf{k}}(\phi_x, h^y),\end{aligned}$$

and finally obtaining

$$\frac{\partial^2 \epsilon_{\mathbf{k}\pm}}{\partial h^y \partial \phi_x} = (\mp) \frac{(2\lambda_x \cos k_x)(2\lambda_y \sin k_y)^2}{\Delta^3_{\mathbf{k}}\big|_{h^y=0,\phi_x=0}}. \tag{6}$$

Note from (5) and (6) that, inverting $\lambda_x \to -\lambda_x$, $D_E \to -D_E$, while D_E remains invariant changing the sign of λ_y.

As we are interested in probing Fermi surface topological transitions, the derivatives of D_E with respect to chemical potential trace FS topological transitions. At the points where the curvature of D_E as a function of fermion density ρ changes sign, we have the relation

$$\frac{d^2 D_E/d\mu^2}{dD_E/d\mu} = -\frac{d^2\mu/d\rho^2}{(d\mu/d\rho)^2}. \tag{7}$$

The ratio of the derivatives of D_E on the left-hand side probes Fermi surface topological transitions because at $T = 0$ the integrations are along Fermi surface paths within the first BZ:

$$\begin{aligned}\frac{d^2 D_E}{d\mu^2} &= (\mp) \sum_{\pm} \frac{\partial}{\partial \mu} \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} \\ &\quad \times \frac{(2\lambda_x \cos k_x)(2\lambda_y \sin k_y)^2}{\Delta^3_{\mathbf{k}}|_{h^y=0,\phi_x=0}} \delta(\mu - \epsilon_{\mathbf{k}\pm}), \end{aligned} \tag{8}$$

$$\begin{aligned}\frac{dD_E}{d\mu} &= (\mp) \sum_{\pm} \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} \\ &\quad \times \frac{(2\lambda_x \cos k_x)(2\lambda_y \sin k_y)^2}{\Delta^3_{\mathbf{k}}|_{h^y=0,\phi_x=0}} \delta(\mu - \epsilon_{\mathbf{k}\pm}). \end{aligned} \tag{9}$$

Figure 3 shows D_E at zero temperature as a function of fermion density for $t_x = t_y = 1$ and $\lambda_x = \lambda_y = 0.1$. We see that D_E changes sign as we go from a closed to an open Fermi surface. As we noted before, this behavior captures the transition from an electronlike to a holelike pocket. Similarly, Fig. 4 illustrates the same physics for the case of anisotropic spin-orbit coupling, while in Fig. 5 the chosen parameters correspond to anisotropic strength of hopping elements. In Fig. 6 we show separately the opposite contributions of the two chiralities to D_E in (5). We find that D_E is the result of a large cancellation between the two components, each of which however keeps track of the FS topological transitions.

The low density limit $\mathbf{k} \to 0$ can be treated analytically for the isotropic parameters $t_x = t_y = t$ and $\lambda_x = \lambda_y = \lambda$. With $k_x = k\cos\phi$ and $k_y = k\sin\phi$ we obtain $\epsilon_{k\pm} = -4t + tk^2 \pm 2\lambda k$:

$$\begin{aligned}D_E &= \sum_{\pm} \frac{1}{(2\pi)^2} \int_0^{\infty} dk k f_{k\pm} \int_0^{2\pi} d\phi \\ &\quad (\mp) \frac{8\lambda^3(1 - k^2\cos^2\phi/2)k^2\sin^2\phi}{8\lambda^3 k^3} \\ &= -\frac{1}{4\pi} \int_0^{\infty} dk (f_{k+} - f_{k-}) \left(1 - \frac{k^2}{8}\right). \end{aligned} \tag{10}$$

At $T = 0$ the upper cutoff of the integrals becomes $k_{\pm c} = \mp\lambda + \sqrt{(4t+\mu)^2 + \lambda^2}$:

$$D_E = -\frac{1}{4\pi}\left[\left(k_{+c} - \frac{k_{+c}^3}{24}\right) - \left(k_{-c} - \frac{k_{-c}^3}{24}\right)\right]. \tag{11}$$

V. CONCLUSIONS

In this paper we study the effect of spin-orbit interaction on the reactive Hall constant R_H within a noninteracting fermion Hamiltonian model. In particular we show the role of Van Hove singularities in the density of states as cusps in the density dependence of R_H. Furthermore, we introduce the concept of the reactive Edelstein constant, an effect in spin-orbit coupled systems, and derive an expression analogous to the Kohn formula for the reactive response.

The main open question is the effect of interactions, introduced, e.g., by a Hubbard U term in the Hamiltonian. An emerging Mott gap, typically at half filling, leads to a vanishing D as Kohn pointed out, the criterion for a Mott metal-insulator transition. Thus the interaction effects in combination with the presence of (higher order) Van Hove singularities can have drastic consequences on phase formation [41]. At first, this can be studied by a mean field approach [42,43] which essentially leads to effective single-particle states allowing a direct computation of R_H and D_E. Next, the interaction effects can be studied by either numerical simulations or many-body theory techniques [41]. An interesting question is the temperature dependence of the Edelstein constant. While it is known that the Drude weight vanishes at any finite temperature in an interacting system, evidence of dissipation due to interactions, the temperature dependence of D_E is not clear.

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