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Nonlinear σ model for disordered systems with intrinsic spin-orbit couplingP. Virtanen¹, F. S. Bergeret^{2,3,4} and I. V. Tokatly^{5,6,3,7}¹*Department of Physics and Nanoscience Center, University of Jyväskylä, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*²*Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain*³*Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain*⁴*Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*⁵*Nano-Bio Spectroscopy Group, Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Universidad del País Vasco (UPV/EHU), 20018 Donostia-San Sebastián, Spain*⁶*IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain*⁷*ITMO University, Department of Physics and Engineering, Saint-Petersburg 197101, Russia*

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We derive the nonlinear σ model to describe diffusive transport in normal metals and superconductors with intrinsic spin-orbit coupling (SOC). The SOC is described via an SU(2) gauge field, and we expand the model to the fourth order in gradients to find the leading non-Abelian field-strength contribution. This contribution generates the spin-charge coupling that is responsible for the spin-Hall effect. We discuss how its symmetry differs from the leading quasiclassical higher-order gradient terms. We also derive the corresponding Usadel equation describing the diffusive spin-charge dynamics in superconducting systems. As an example, we apply the obtained equations to describe the anomalous supercurrent in dirty Rashba superconductors at arbitrary temperatures.

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I. INTRODUCTION

The intrinsic spin-Hall effect is a magnetoelectric coupling between spin and charge degrees of freedom, which arises from a geometric property of the electron bands caused by the spin-orbit coupling (SOC) [1–3]. The spin-charge interconversion is the basis of the spin-Hall magnetoresistance [4], the Edelstein [5,6], and spin-galvanic effects [7], observed in a wide variety of systems [8–11].

The counterpart of these effects in superconducting systems with SOC has also been widely studied [12–15]. Supercurrents, i.e., currents without dissipation, can induce a spin density. Reciprocally, a Zeeman or exchange field can cause supercurrents in a superconducting system with strong SOC. An example of the latter is the realization of anomalous Josephson junctions [16,17], where the interplay between the SOC and a spin-splitting field leads to the appearance of spontaneous supercurrents in superconducting loops [18,19]. The charge-spin coupling in superconducting systems with SOC is also at the basis of the superconducting diode effect [20–24], observed experimentally [25,26]. With potential applications in emerging technologies, all these effects are observed in hybrid systems, which combine different materials with disorder. From a theoretical point of view, the formulation of a kinetic theory of electronic transport in the presence of SOC is therefore of extreme importance.

If the system under consideration is described by an effective Hamiltonian with a linear in momentum SOC, the latter can be treated by introducing an SU(2) gauge potential [27–33]. This viewpoint turns out to be fruitful, as the

intrinsic spin-Hall contribution in electron transport theory can be related to the corresponding SU(2) field strength [15,30,32–34]. In superconductors, the magnetoelectric contribution has been considered in various limits [12,15,17,35–38]. One of the questions is the effect of impurity scattering, and the formulation of the transport theory in terms of kinetic equations for the quasiclassical Green's functions (GFs), in superconductors with SOC in the diffusive limit. This type of formulation is the most suitable for the study of realistic mesoscopic systems, such as anomalous Josephson junctions, superconductor-ferromagnet, or superconductor-semiconductor hybrid systems [18,19,26].

Intrinsic magnetoelectric effects in diffusive hybrid systems have been considered mostly in the linearized case, when superconducting correlations are weak either due to large temperature or weak proximity effect [15–17,39]. In such a case, the SU(2)-covariant quasiclassical equation, the Usadel equation, has a similar form as the diffusion equation in a normal system [33] and the anomalous (superconducting) GFs can be treated perturbatively. Going beyond the linearized case is not a trivial task and attempts to obtain the Usadel equation beyond that limit using standard quasiclassical kinetic equation approaches run into technical consistency issues [40]. On the one hand, the spin-Hall effect appears in a subquasiclassical order in the expansions. On the other hand, the resulting Usadel equation needs to preserve a commutator form to ensure the normalization of the quasiclassical GF. An alternative and reliable way to formulate the diffusive limit transport theory is via the nonlinear σ -model approach [41–45]. The saddle-point equation of the nonlinear σ model

is the Usadel equation. We used this approach previously in Ref. [46] to describe the contribution of extrinsic SOC to magnetoelectric effects in superconductors. However, in the case of intrinsic SOC described by SU(2) gauge fields, the number of terms appearing in the naive expansion of the action with respect to the gradients and fields is immense and cannot be treated manually.

In this work we derive the nonlinear σ model for superconducting and normal systems including the intrinsic SOC in the form of an SU(2) gauge field. We identify the leading SU(2) field strength term responsible for the spin-Hall effects in the gradient expansion of the model, and the relevant symmetry properties. We perform the expansion systematically via computer algebra, and also recover other terms, e.g., describing thermoelectric effects [47]. The corresponding saddle-point equations provide a general framework to study magnetoelectric effects in disordered superconductors at arbitrary temperature and generalize the Usadel equation to include the intrinsic spin-Hall effects. Using this equation we determine the anomalous current generated by the interplay between SOC and an exchange field in a proximitized normal metal with Rashba SOC. Our result corrects previous results, and predicts an enhancement of the anomalous current for exchange fields of the order of the superconducting gap.

The paper is structured as follows. In Sec. II we outline the main results of our work, namely the nonlinear σ -model Keldysh action, Eqs. (5)–(7), and its saddle-point equation, the generalized Usadel equation, Eqs. (8)–(11). In Sec. III we discuss the gradient expansion of the nonlinear σ model with SU(2) gauge fields, and derivation of the main results. Explanation of the computer implementation of this calculation is postponed to Appendix. In Sec. IV we derive the kinetic equations found at the saddle point of the model. In Sec. V we provide an example by calculating the anomalous current induced by an exchange field in a Rashba superconducting system. Section VI concludes the discussion.

II. MAIN RESULTS

Consider a normal conductor with linear-in-momentum spin-orbit coupling (SOC) and an exchange field. In the most general case, its Hamiltonian can be written as

$$H_0 = \frac{\hat{p}^2}{2m} - \frac{1}{2m} \mathcal{A}_k^a \hat{p}_k \sigma^a - \frac{1}{2} \mathcal{A}_0^a \sigma^a + V_{\text{imp}}, \quad (1)$$

where the second and third terms describe the SOC and exchange field, respectively, σ^a are Pauli matrices spanning the spin space, and V_{imp} is a random impurity potential. Here and throughout the paper summation over repeated indices is implied. The linear SOC can be related to a local SU(2) gauge invariance of the corresponding Hamiltonian [27,29,30,32,33,39,48] that can be written (up to an irrelevant constant) as

$$H_0 = \frac{1}{2m} (\hat{p}_j - \hat{\mathcal{A}}_j)^2 + V_{\text{imp}} - \hat{\mathcal{A}}_0, \quad (2)$$

where $\hat{\mathcal{A}}_j = \frac{1}{2} \mathcal{A}_j^a \sigma^a$.

To describe superconducting systems with SOC one constructs from the normal state Hamiltonian, Eq. (2), the

Bogoliubov–de Gennes Hamiltonian

$$\mathcal{H} = \tau_3 \left[\frac{[\hat{p} - \check{\mathcal{A}}(\mathbf{r})]^2}{2m} - \mu + V_{\text{imp}}(\mathbf{r}) - \check{\mathcal{A}}_0(\mathbf{r}) - \hat{\Delta}(\mathbf{r}) \right], \quad (3)$$

where $\hat{\Delta}$ is the superconducting anomalous self-energy for s -wave superconductor given by $\hat{\Delta} = \tau_3 \tau_1 \Delta e^{-i\tau_3 \phi}$. Here τ_j are Pauli matrices in the Nambu space. For generality, in Eq. (3) we have included the $U(1)$ scalar and vector electromagnetic potentials, Φ , (A_x, A_y, A_z) , by defining $\check{\mathcal{A}}_i = A_i \tau_3 + \frac{1}{2} \mathcal{A}_i \cdot \boldsymbol{\sigma}$ and $\check{\mathcal{A}}_0 = \Phi + \frac{1}{2} \mathcal{A}_0 \cdot \boldsymbol{\sigma} \tau_3$. The field strength associated with $\check{\mathcal{A}}$ is

$$\check{F}_{\mu\nu} = \partial_\mu \check{\mathcal{A}}_\nu - \partial_\nu \check{\mathcal{A}}_\mu - i[\check{\mathcal{A}}_\mu, \check{\mathcal{A}}_\nu], \quad (4)$$

containing electric and magnetic fields, and their SOC generalizations. Here and below we use Greek indices for the range $\nu = 0, 1, 2, 3$ including the time component, and Latin indices for the spatial components $i = 1, 2, 3$.

Starting from Hamiltonian (3), we derive a disorder-averaged theory describing electron diffusion in such system, valid in the quasiclassical diffusive limit $\xi \gg \ell \gg \lambda_F$, where ξ , ℓ , and λ_F are the superconducting coherence length, the mean free path, and the Fermi wavelength. To obtain the Hall and spin-Hall effects, we include the leading subquasiclassical corrections $\propto (\lambda_F/\ell)^1$. As explained in Sec. III, we formulate the problem as a systematic expansion of Eq. (3) in the small parameters, in the approximation scheme of nonlinear σ models, which concentrates on physics of the low-energy diffusion modes.

A. Keldysh action

Our main result can be compactly expressed as the nonlinear σ -model Keldysh action,

$$S[Q] = S_0[Q] + S_H[Q], \quad (5)$$

$$S_0[Q] = \frac{i\pi v_F}{8} \text{Tr}[D(\hat{\nabla}Q)^2 + 4i(\Omega + \check{\mathcal{A}}_0)Q], \quad (6)$$

$$S_H[Q] = \frac{i\pi v_F D \ell^2}{8 p_F \ell} \text{Tr}[-\check{F}_{ij}Q(\hat{\nabla}_i Q)(\hat{\nabla}_j Q)]. \quad (7)$$

Here $Q(\mathbf{r})$ is a matrix field with $Q(\mathbf{r})^2 = \mathbb{1}$, which describes the low energy diffusion modes, $\hat{\nabla}_i Q = \partial_{r_i} Q - [i\check{\mathcal{A}}_i, Q]$ are its covariant gradients, and $\Omega = i\tau_3 \hat{\epsilon} + \hat{\Delta}$ contains the energy operator and local self-energies. Moreover, v_F is the density of states, and D the diffusion constant. The local gauge symmetry of the original Hamiltonian in Eq. (3) translates to the invariance of the σ model under the (gauge) transformations $Q \mapsto U Q U^{-1}$, $\check{\mathcal{A}}_j \mapsto U \check{\mathcal{A}}_j U^{-1} + iU \partial_j U^{-1}$, $\check{F}_{ij} \mapsto U \check{F}_{ij} U^{-1}$, $\Omega + \check{\mathcal{A}}_0 \mapsto U(\Omega + \check{\mathcal{A}}_0)U^{-1}$.

The action S_0 comprises the previous nonlinear σ -model theory for superconductivity [43,44,49,50] with the spin-dependent gauge fields.

The term S_H contains the leading magnetic field-strength contribution that breaks the symmetry of S_0 , hence bringing in new physical effects related to generalized Hall effects. Indeed that term in the case of two-dimensional (2D) electron gas and $U(1)$ fields has the form of the topological term in Pruisken's action for the integer Hall effect [51–53]. We notice that this

term also appears in the nonlinear σ model for a disordered Weyl semimetal [54,55]. In contrast, the SU(2) counterpart of the Hall term cannot be written as a total derivative, and hence will generate a nontrivial contribution to the saddle-point equation for Q [see Eq. (8)]. S_H describes the spin-Hall effects, i.e., effects caused by the spin-charge coupling.

As discussed later, the action also contains other terms. For example, the gradient expansion also generates formally larger terms that do not break symmetries of S_0 —these will renormalize diffusion, but do not contribute to magneto-electric effects. There are also other terms that break the electron-hole symmetry, associated with thermoelectric effects, previously discussed in Ref. [47]. We recover all these terms from our systematic analysis in Sec. III.

B. Generalized Usadel equation

The saddle-point equation of S_0 is the covariant version of the well-known Usadel diffusion equation [56] for superconducting systems, and Eq. (5) provides its minimal extension including the Hall and intrinsic spin-Hall effects. The Usadel equation is obtained from minimizing the action under the condition $Q^2 = 1$, that is $i(\delta S/\delta Q)|_{Q^2=1} = 0$, and has the form

$$\hat{\nabla}_i \mathcal{J}_i = [i\Omega + i\check{A}_0, Q]. \quad (8)$$

Here \mathcal{J}_μ are the matrix currents, proportional to the variation of S with respect to the matrix-valued vector potential \check{A}_μ . Hence, their different components are directly related to observable charge J^c and spin J^s currents by taking appropriate traces, $J_i^c(t) = -\frac{\pi\nu}{2} \text{tr} \tau_3 \mathcal{J}_i^K(t, t)$, $J_{ij}^s(t) = -\frac{\pi\nu}{2} \text{tr} \sigma_j \mathcal{J}_i^K(t, t)$. Spin density and charge imbalance are given by $S_i = -\frac{\pi\nu}{2} \text{tr} \sigma_i \tau_3 J_0^K(t, t)$ and $\delta\rho = -\frac{\pi\nu}{2} \text{tr} J_0^K(t, t)$. Here K superscript denotes the upper right Keldysh component of the matrix.

The spatial components of the matrix currents can be expressed as

$$\mathcal{J}_i \equiv -\frac{2}{\pi\nu} \frac{\delta S}{\delta \check{A}_i} = \mathcal{J}_i^{(0)} + \mathcal{J}_i^{(H)}, \quad (9)$$

$$\mathcal{J}_i^{(0)} = -DQ\hat{\nabla}_i Q, \quad (10)$$

$$\begin{aligned} \mathcal{J}_i^{(H)} = & -\frac{D\tau}{4m} [\{\check{F}_{ij} + Q\check{F}_{ij}Q, \hat{\nabla}_j Q\} \\ & - i\hat{\nabla}_j(Q[\hat{\nabla}_i Q, \hat{\nabla}_j Q])], \end{aligned} \quad (11)$$

and time component is $\mathcal{J}_0^{(0)} = Q$. The current $\mathcal{J}^{(0)}$ is the standard diffusive current, and $\mathcal{J}^{(H)}$ is the leading contribution from spin-charge coupling. The first term in Eq. (11) becomes the (spin-)Hall current in the normal state, and the remainder gives superconducting corrections. Equation (8) implies a covariant conservation equation of these spin currents [32], where nonconservation of spin current is associated with the $[-i\mathcal{A}, \cdot]$ part of the covariant derivative.

In the next sections we derive the above results.

III. GRADIENT EXPANSION

The starting point is the Keldysh partition function [44,45] expressed via the path integral with the action corresponding

to the Hamiltonian of Eq. (3),

$$S = \int_C dt \bar{\Psi}^T (i\tau_3 \partial_t - \tau_3 \mathcal{H}) \Psi, \quad (12)$$

where $\Psi = (\psi_\uparrow, \psi_\downarrow, \bar{\psi}_\downarrow, -\bar{\psi}_\uparrow)^T / \sqrt{2}$ and $\bar{\Psi} = -i\sigma_y \tau_1 \Psi$ are Nambu spinors of electron fields on the Keldysh contour C . We then perform standard steps in the nonlinear σ -model derivation: (i) averaging the generating function over the Gaussian disorder potential with $\langle V_{\text{imp}}(\mathbf{r}) V_{\text{imp}}(\mathbf{r}') \rangle = \frac{1}{2\pi\nu\tau} \delta(\mathbf{r} - \mathbf{r}')$ where τ and ν are parameters describing the scattering time and density of states, and (ii) decoupling the generated quartic interaction term with a local matrix field Q , $[\bar{\Psi}_i(\mathbf{r}, t) \Psi_j(\mathbf{r}, t')][\Psi_i(\mathbf{r}, t) \bar{\Psi}_j(\mathbf{r}, t')] \mapsto \bar{\Psi}_i(\mathbf{r}, t) Q_{ij}(\mathbf{r}; t, t') \Psi_j(\mathbf{r}, t')$. The details of this procedure in the Keldysh formulation are discussed, e.g., in Refs. [44,45,49,57]. As these steps only involve the disorder term of the action, the gauge fields do not directly affect the procedure at this stage.

After integrating out the fermion fields, the result becomes the nonlinear σ -model action,

$$S = \frac{i\pi\nu_F}{8\tau} \text{Tr} Q^2 - \frac{i}{2} \text{Tr} \ln_\otimes G^{-1}, \quad (13)$$

$$G^{-1} = \Omega + \mu - \frac{1}{2m} (p_k - \check{A}_k)(p_k - \check{A}_k) + \frac{i}{2\tau} Q, \quad (14)$$

where $\Omega = \epsilon\tau_3 + \check{A}_0 + \hat{\Delta}$, $\hat{\epsilon} = i\partial_t \delta(t - t')$, and ν_F is the density of states at the Fermi energy.

In Keldysh theory, $Q(\mathbf{r}; t, t')$ depends on two times, and is a 8×8 matrix, with 4×4 blocks with the Nambu and spin indices, in a 2×2 retarded-advanced-Keldysh structure [58]. Here and below, matrix products and trace also imply integrations over time, $(XY)(t, t') = \int_{-\infty}^{\infty} dt_1 X(t, t_1) Y(t_1, t')$ and $\text{Tr} X = \int_{-\infty}^{\infty} dt d^d r \text{tr} X(t, t)$. In some cases it can be technically advantageous to use the energy representation that is defined as follows: $X(\epsilon, \epsilon') = \int_{-\infty}^{\infty} dt dt' e^{i\epsilon t - i\epsilon' t'} X(t, t')$.

We use here a Wigner representation for the spatial coordinates,

$$G(\mathbf{r}, \mathbf{r}'; t, t') = \sum_{\mathbf{p}} e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} G\left(\frac{\mathbf{r} + \mathbf{r}'}{2}, \mathbf{p}; t, t'\right), \quad (15)$$

in which convolutions $(A \otimes B)(\mathbf{r}, \mathbf{r}'; t, t') = \int d\mathbf{r}_1 dt_1 A(\mathbf{r}, \mathbf{r}_1; t, t_1) B(\mathbf{r}_1, \mathbf{r}'; t_1, t')$ can be expressed by the Moyal product

$$\begin{aligned} (A \otimes B)(\mathbf{r}, \mathbf{p}; t, t') = & \int_{-\infty}^{\infty} dt_1 A(\mathbf{r}, \mathbf{p}; t, t_1) \\ & \times \exp\left[\frac{i}{2} (\overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p - \overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_r)\right] \\ & \times B(\mathbf{r}, \mathbf{p}; t_1, t'). \end{aligned} \quad (16)$$

Here the arrows above the ∇ indicate on which function the derivative operator acts. The trace becomes

$$\text{Tr} X = \int d^d r dt \sum_{\mathbf{p}} \text{tr} X(\mathbf{r}, \mathbf{p}; t, t), \quad (17)$$

where tr is the trace over matrix indices. For brevity, in the following we will not write down the time integrations.

Next, we expand the action of Eq. (13) in gradients of Q and gauge fields \check{A}_μ . This follows a standard approach

in σ models. In this expansion, one usually separates the “transverse” nearly massless modes of the Q field, from the “longitudinal” massive modes. The longitudinal modes usually only renormalize coefficients of the transverse mode theory. Below, we concentrate only on the massless modes, and separate them out by writing $Q = T(\Lambda + B)T^{-1}$ where Λ is the uniform saddle-point solution at $\Omega = \check{A} = 0$ with $\Lambda^2 = 1$, B with $[B, \Lambda] = 0$ describes longitudinal fluctuations, and T parametrizes the remaining rotations around it [59,60]. Since at $\Omega = \check{A} = 0$ all matrices $Q = T\Lambda T^{-1}$ are also saddle-point solutions, the rotations T in general describe the nearly massless modes, whereas the longitudinal modes are suppressed by the impurity scattering energy scale $\frac{1}{\tau}$. We will first neglect the longitudinal corrections and set $B = 0$.

Inserting the parametrization to Eq. (13), the electronic part can be rewritten as

$$\text{Tr} \ln G^{-1} = \text{Tr} \ln_{\otimes} \left[\mu - \frac{(p_k - a_k)(p_k - a_k)}{2m} + \frac{ib}{2\tau} \Lambda + a_0 \right], \quad (18)$$

where

$$a_0 = T^{-1}(\Omega + \check{A}_0)T, \quad (19)$$

$$a_k = iT^{-1}\partial_k T + T^{-1}\check{A}_k T. \quad (20)$$

The expansion in gradients of Q and in \check{A} and Ω now translates to expanding the $\text{Tr} \ln$ in small a_0, a_k . Note that because Ω also contains the energy ϵ , the expansion is valid only at low energies $|\epsilon| \ll \tau^{-1}$, and can be used to describe only the low-energy part of $T(\epsilon, \epsilon')$.

We carry this expansion to fourth order in a_i, a_0 . We also expand the result in the quasiclassical parameter $\psi = p_F \ell \gg 1$. In the end we rewrite the result in terms of the covariant gradients

$$\hat{\nabla}_i Q = T[-ia_i, \Lambda]T^{-1} = \partial_i Q - i[\check{A}_i, Q], \quad (21)$$

$$\hat{\nabla}_0 Q = T[-ia_0, \Lambda]T^{-1} = -[i\Omega + i\check{A}_0, Q], \quad (22)$$

and non-Abelian field strengths

$$T(\partial_i a_j - \partial_j a_i - i[a_i, a_j])T^{-1} = \partial_i \check{A}_j - \partial_j \check{A}_i - i[\check{A}_i, \check{A}_j] = \check{F}_{ij}, \quad (23)$$

$$T(\partial_k a_0 - i[a_k, a_0])T^{-1} = \partial_k \check{A}_0 - \partial_0 \check{A}_k - i[\check{A}_k, \check{A}_0] + \hat{\nabla}_k \check{\Delta} = \check{F}_{k0} + \hat{\nabla}_k \check{\Delta}. \quad (24)$$

By construction, the final result should be formally gauge covariant and therefore it can contain only covariant objects, which is indeed confirmed by explicit calculations.

Expansion of the logarithm, gradient expansion of the Moyal product, calculation of the momentum sum in the Tr , and rewriting the result, is a mechanical calculation, and mainly a bookkeeping problem. We discuss our technical method in Appendix, and concentrate on the results below.

A. Results

The gradient expansion produces the terms

$$\delta S = S_{\text{grad}} + S_{\Omega}, \quad (25)$$

where S_{grad} contains only spatial gradients, and S_{Ω} contains the remaining terms with Ω and \check{A}_0 . The leading part in the expansion of S_{Ω} is well known,

$$S_{\Omega} = \frac{i\pi v_F}{8} \text{Tr} 4i(\Omega + \check{A}_0)Q + \dots \quad (26)$$

The pure spatial gradient terms, up to fourth order in gradients and first order in $1/(p_F \ell)$ in three dimensions, are

$$S_{\text{grad}} = S_2 + S_{4,0} + S_{4,1} + S'_{4,1} + \dots, \quad (27)$$

$$S_2 = \frac{i\pi v_F D}{8} \text{Tr}(\hat{\nabla} Q)^2, \quad (28)$$

$$S_{4,0} = \frac{i\pi v_F D \ell^2}{8} \text{Tr} \left[-\frac{3}{5} \hat{\nabla}_i \hat{\nabla}_i Q \hat{\nabla}_j \hat{\nabla}_j Q + \frac{3}{4} \hat{\nabla}_i Q \hat{\nabla}_i Q \hat{\nabla}_j Q \hat{\nabla}_j Q \right], \quad (29)$$

$$S_{4,1} \equiv S_H = \frac{i\pi v_F D \ell^2}{8 p_F \ell} \text{Tr}[-\check{F}_{ij} Q (\hat{\nabla}_i Q) (\hat{\nabla}_j Q)], \quad (30)$$

$$S'_{4,1} = \frac{i\pi v_F D \ell^2}{8 p_F \ell} \text{Tr}[iQ (\hat{\nabla}_i \hat{\nabla}_j Q) (\hat{\nabla}_i \hat{\nabla}_j Q)]. \quad (31)$$

The double expansion consists of terms $S_{m,n}$ that are of order m in gradients, and order n in $1/(p_F \ell)$. Here, braces in indices denote symmetrization of the tensor, which is defined as the average $X_{(i_1, \dots, i_N)} = \frac{1}{|\mathcal{P}|} \sum_{\sigma \in \mathcal{P}} X_{i_{\sigma(1)}, \dots, i_{\sigma(N)}}$ over all permutations σ , where \mathcal{P} is the set of permutations of $1, \dots, N$ and $|\mathcal{P}| = N!$.

The prefactor of the diffusion term S_2 is connected to the longitudinal Drude conductivity by the Einstein relation $v_F D = e^{-2} \sigma_{xx}$. Similarly, the prefactor of the field strength term $S_{4,1} = S_H$ is related to the transverse Hall conductivity by $v_F D \ell^2 / (p_F \ell) = e^{-3} \frac{d\sigma_{yx}}{dB} |_{B=0}$ where $\sigma_{yx} = \sigma_{xx} \omega_c \tau$ and $\omega_c = \frac{eB}{m}$ is the cyclotron frequency [61]. By the generic gauge structure of the theory, this coefficient is the *same* both for the Hall effect and the spin-Hall effect. One can also note that unlike in the quantum Hall effect [51–53], we are here working in the limit of small field strengths, and so the prefactor is not quantized.

While such physical considerations suggest that the relationship between the coefficients of these two terms is fixed, in general the coefficients of the higher-order gradient terms can be modified by the longitudinal fluctuations of the Q field. Already if we allow for nonzero longitudinal part $B \neq 0$ on the saddle-point level [62], additional corrections of similar order in the small parameters as in $S_{4,0}$ and $S'_{4,1}$ appear and additional considerations are necessary if one wants to derive coefficients of such terms from the microscopic theory. On the saddle-point level, the coefficient of $S_{4,1}$ is not renormalized by them.

The higher-order gradient terms in Eq. (25) are usually not of direct physical interest (see, however, [63,64]), except if they break a symmetry present in the lower-order model S_2 . In that case, they can give rise to new physically interesting phenomena. We discuss the model symmetry in more detail in Sec. III B.

We can recognize that the non-Abelian field strength term $S_{4,1} = S_H$ is a generalization of the spin-Hall term in Ref. [46] from the extrinsic spin-Hall effect to the intrinsic one, with

the correspondence $\check{F}_{ij} \leftrightarrow -\frac{p_F}{\ell} \theta \epsilon_{ijk} \sigma_k$, where θ is the spin-Hall angle. In the equations of motion, this term will lead to conversion between charge and spin currents, a feature that is not present in a model containing only S_2 . The term in $S'_{4,1}$ on the other hand was previously noted in Ref. [47] in the context of thermoelectric effects for $A = F = 0$.

B. Symmetry analysis

Terms in the action S can be classified based on which symmetries they break. A symmetry relevant for magnetoelectric effects is the electron-hole symmetry, or the “quasiclassical” symmetry, which implies [65] a certain lack of coupling between spin and charge transport. The electron-hole symmetry can be understood as one that flips the sign of the electron dispersion $\xi_p = \frac{p^2}{2m} - \mu \mapsto -\xi_p$. On the level of the σ model, this can be expressed as the transformation [65]

$$Q \mapsto \bar{Q} \equiv -\tau_1 \bar{Q} \tau_1 = -\tau_2 \sigma_y Q^T \sigma_y \tau_2, \quad (32)$$

where $\bar{Q} = \tau_3 \sigma_y Q^T \sigma_y \tau_3$ is a time-reversal transformation. Similarly as for Green functions, the transformation swaps the Nambu blocks and reverses time, which corresponds to reversing sign of the “normal” part in the Bogoliubov–de Gennes Hamiltonian while keeping the anomalous unchanged. A similar transformation was used in Ref. [47]; the above is its extension to a superconducting case, which also requires keeping the superconducting anomalous self-energy terms $\propto \text{Tr}[\Delta \tau_3 \tau_1 e^{i\tau_3 \varphi} Q]$ invariant.

In the usual σ model the action S_0 consists of S_2 and the leading term in S_Ω . In the latter term, \check{A}_0 changes sign under the e-h transformation Eq. (32), whereas S_2 remains invariant. This in particular implies that at the level of S_0 , the transformation Eq. (32) defines a mapping between systems with opposite directions of the Zeeman field \mathbf{A}_0 . When combined with the time-reversal symmetry, this mapping forbids the anomalous supercurrent [65,66], which explains the absence of magnetoelectric effects in the theory defined by the leading contribution S_0 to the σ model.

By analyzing the subleading higher gradient terms in Eq. (27), we find that $S_{4,0}$ is invariant under the transformation of Eq. (32), but $S_{4,1} = S_H$ and $S'_{4,1}$ change sign. Expansion of S_Ω (see Appendix A 4) can be classified similarly. Hence, even though $S_{4,0}$ is formally larger in the quasiclassical parameter $p_F \ell \gg 1$, it has the same symmetry as S_2 , and we expect its effect is merely a renormalization of diffusion and not of interest for us here. In contrast, the terms breaking the “quasiclassical” e-h symmetry introduce new physics and qualitatively change the behavior of the system.

The first antisymmetric term $S_{4,1} = S_H$, Eq. (30), introduces the spin-Hall effect. This term is responsible for all magnetoelectric effects mediated by intrinsic SOC, such as direct and inverse spin-galvanic/Edelstein effects in normal conductors and the appearance of anomalous supercurrents and anomalous Josephson effect in superconductors.

The second antisymmetric term $S'_{4,1}$ of Eq. (31) and the term $\frac{i\pi v \ell}{8p_F} \text{Tr} \Omega (\hat{\nabla}_i Q) (\hat{\nabla}_j Q)$ appearing in S_Ω (see Appendix A 4) were previously presented in Ref. [47] providing an extension of the σ model to include thermoelectric effects.

IV. SADDLE POINT

As noted in Sec. II, variation of the action produces the generalized Usadel equation that is the saddle-point condition for $S[Q]$.

Technically, the variation under the condition $Q^2 = 1$ is calculated by writing $Q = T \Lambda T^{-1}$, where Λ is the uniform saddle-point solution, and by observing that $\delta Q = [W, Q]$ with $W = (\delta T) T^{-1}$. A straightforward calculation [62] with subsequent integration by parts then produces the final result, which can however be represented in different forms, reflecting different formal properties of the saddle-point equation. On the one hand, the commutator form of the allowed variations $\delta Q = [W, Q]$ implies that the saddle-point equation also has a commutator form $[\dots, Q] = 0$, which guarantees that it is consistent with the normalization condition $Q^2 = 1$. On the other hand, the gauge invariance of the action implies that the saddle-point equation can be represented in a form of a covariant conservation law,

$$\hat{\nabla}_i \mathcal{J}_i = [i\Omega + i\check{A}_0, Q], \quad (33)$$

where the matrix current \mathcal{J}_i can be expressed as a variational derivative of the action with respect to the gauge potential

$$\mathcal{J}_i \equiv -\frac{2}{\pi v} \frac{\delta S}{\delta \check{A}_i} = \mathcal{J}_i^{(2)} + \mathcal{J}_i^{(4,0)} + \mathcal{J}_i^{(4,1)} + \mathcal{J}_i^{(4,1')}, \quad (34)$$

where from S_2 and $S_{4,1}$ we obtain

$$\mathcal{J}_i^{(2)} = -DQ \hat{\nabla}_i Q, \quad (35)$$

$$\begin{aligned} \mathcal{J}_i^{(4,1)} = & -\frac{D\tau}{4m} [\{\check{F}_{ij} + Q\check{F}_{ij}Q, \hat{\nabla}_j Q\} \\ & - i\hat{\nabla}_j (Q[\hat{\nabla}_i Q, \hat{\nabla}_j Q])]. \end{aligned} \quad (36)$$

Similarly, from $S_{4,0}$ and $S'_{4,1}$:

$$\begin{aligned} \mathcal{J}_i^{(4,0)} = & -\frac{3D\ell^2}{5} \left(Q\hat{\nabla}_i \hat{\nabla}_j \hat{\nabla}_j Q \right. \\ & + Q[\hat{\nabla}_i Q \hat{\nabla}_j \hat{\nabla}_j Q + 2\hat{\nabla}_i \hat{\nabla}_j Q \hat{\nabla}_j Q]Q \\ & \left. + \frac{1}{2} Q\hat{\nabla}_i Q \hat{\nabla}_j Q \hat{\nabla}_j Q \right), \end{aligned} \quad (37)$$

$$\mathcal{J}_i^{(4,1')} = -\frac{D\tau}{2m} [\hat{\nabla}_i Q, \hat{\nabla}_j Q \hat{\nabla}_j Q]. \quad (38)$$

As we noticed before, whereas the numerical prefactors in Eqs. (35) and (36) are not modified on the saddle-point level [62] by the longitudinal corrections, prefactors in the last two equations have to be renormalized.

At this point it is instructive to compare the present covariant theory with intrinsic SOC, and the theory of diffusive systems with SOC of extrinsic origin, such as random impurities [46]. At the level of the nonlinear σ model, the extrinsic and intrinsic theories can be connected by (i) replacing the usual gradients with the covariant gradients, and (ii) identifying $\check{F}_{ij} \leftrightarrow -\frac{p_F}{\ell} \theta \epsilon_{ijk} \sigma_k$ in the spin-Hall term. It is natural to expect that the same replacement rules should work for the Usadel equation. However, this does not look obvious if one naively compares the Usadel equation from Ref. [46] and Eq. (33) with the current given by Eqs. (35) and (36). In the extrinsic case an additional torque term \mathcal{T} appears in

the Usadel equation, while the current has a form that can be identified only with the first term in Eq. (36). This apparent contradiction is resolved by noticing that the expected torque is of course there, but because of the gauge symmetry it must have a form of a covariant divergence. It therefore appears in the Usadel equation as an additional contribution to the current. Indeed, by using the identity $-i[\check{F}_{ij}, f] = [\hat{\nabla}_i, \hat{\nabla}_j]f$ and the replacement $\check{F}_{ij} \mapsto -\frac{p_F}{\ell}\theta\epsilon_{ijk}\sigma_k$, we recover the correct torque \mathcal{T} of the extrinsic theory. Also, in the case of extrinsic SOC, there is a spin relaxation Elliot-Yafet term, in the Usadel equation. In the present case of Eq. (33), the spin relaxation stems from the double covariant gradient term when substituting Eq. (35) into Eq. (33). This term corresponds to the Dyakonov-Perel type of spin relaxation.

Finally we make a connection to the well established theory of normal conductors with SOC. The normal-state diffusion equations can be recovered from Eq. (33) by the replacement

$$Q \mapsto \begin{pmatrix} 1 & 2f \\ 0 & -1 \end{pmatrix}, \quad (39)$$

where the 2×2 matrix is in Keldysh space, and Nambu structure is trivial and we replace $\tau_3 \mapsto 1$. Here $f(\mathbf{r}, t, t') = f_0(\mathbf{r}, t, t') + \boldsymbol{\sigma} \cdot \mathbf{f}(\mathbf{r}, t, t')$ is the spin-dependent distribution function of electrons. The Usadel equation then becomes the diffusion equation

$$[i\hat{\epsilon}, f] = \hat{\nabla}_i \mathcal{J}_i, \quad (40)$$

$$\mathcal{J}_i = -D\hat{\nabla}_i f - \frac{D\tau}{2m}[\check{F}_{ij}, \hat{\nabla}_j f] - \frac{3D\ell^2}{5}\hat{\nabla}_{(i}\hat{\nabla}_j\hat{\nabla}_{j)}f, \quad (41)$$

where we wrote the terms corresponding to the leading term of S_Ω , and the spatial gradient terms S_2 , $S_{4,1}$, and also $S_{4,0}$ which gives a symmetrized derivative term. The other higher-gradient term $S'_{4,1}$ gives no contribution in normal state.

Keeping only the first two terms in Eq. (41), when integrated over the energy, results to the known spin-charge diffusion equations in the case of normal metals with intrinsic SOC [33,67–70]. In the case of $U(1)$ magnetic field strength \mathbf{B} , one can derive the equations describing the ordinary Hall effect.

The last symmetric derivative term in Eq. (41) from $S_{4,0}$ is essentially always neglected in derivations of such normal-state equations, even though it is formally larger by $p_F\ell \gg 1$ than the SOC term. As we argued in Sec. III B, it can however be excluded on symmetry grounds. For completeness, let us show how this term would appear in standard derivations. In the normal state, we can consider the quasiclassical distribution function $f(\hat{p}, \mathbf{r}; t, t')$ on the Fermi level, which depends on the position and momentum direction. It obeys a transport (Eilenberger) equation [71]

$$-\frac{1}{\tau}(f - \langle f \rangle) = (\mathbf{v} \cdot \hat{\nabla} + \partial_t - \partial_{t'})f = \hat{D}f, \quad (42)$$

where $\hat{\nabla}$ is the gauge-invariant gradient and $\mathbf{v}(\hat{p})$ is the velocity. This formulation works on the $1/(p_F\ell)^0$ level, and will not capture magnetoelectric effects. We can formally solve Eq. (42), take the average $\langle \cdot \rangle$ over momentum directions \hat{p} ,

and expand in $\tau \rightarrow 0$ to find

$$0 = \frac{1}{\tau} \langle (1 + \tau\hat{D})^{-1} \langle f \rangle - f \rangle = \frac{1}{\tau} \sum_{n=1}^{\infty} \langle [-\tau\hat{D}]^n \langle f \rangle \rangle. \quad (43)$$

Truncating to fourth order in spatial gradients and first order in time derivative, this gradient expansion becomes

$$\begin{aligned} 0 &= -(\partial_t - \partial_{t'})\langle f \rangle + \tau \langle v_i v_j \rangle \hat{\nabla}_i \hat{\nabla}_j \langle f \rangle \\ &\quad + \tau^3 \langle v_i v_j v_k v_l \rangle \hat{\nabla}_i \hat{\nabla}_j \hat{\nabla}_k \hat{\nabla}_l \langle f \rangle \\ &= -(\partial_t - \partial_{t'})\langle f \rangle + D\hat{\nabla}_i \hat{\nabla}_i \langle f \rangle + \frac{D\ell^2 d}{d+2} \hat{\nabla}_{(i} \hat{\nabla}_i \hat{\nabla}_j \hat{\nabla}_{j)} \langle f \rangle, \end{aligned} \quad (44)$$

where d is the space dimension. The first two terms constitute the standard diffusion equation, and the third term is what appears in Eq. (40), recognizing that $\hat{\nabla}_i \hat{\nabla}_i \hat{\nabla}_j \hat{\nabla}_j = \hat{\nabla}_{(i} \hat{\nabla}_i \hat{\nabla}_j \hat{\nabla}_{j)}$.

V. EXAMPLE: ANOMALOUS CURRENT IN A SUPERCONDUCTING SYSTEM WITH RASHBA SOC

It was predicted first by Edelstein [12,13] that a superconductor with a Rashba SOC supports spontaneous supercurrents in the presence of a Zeeman field. This is nothing but the superconducting version of the spin-galvanic effect predicted in normal systems [34]. Anomalous supercurrents are not only present in superconductors but also in proximitized normal systems and Josephson junctions with SOC [15–19].

The spin-galvanic effect in superconductors has been studied primarily on linear response assuming either a small superconducting gap Δ or a small Zeeman field \mathcal{A}_0 [13, 15–19,72]. Going beyond linear response is not straightforward. The result of Ref. [40] suggested that the spin-galvanic relation between the charge current and the induced spin in a superconductor is identical to that in a normal metal, i.e., that the current induced by the SOC is proportional to the deviation of the spin density from the Pauli response δS . However, as follows from Eq. (11), this statement is incorrect. In this section we determine the anomalous current induced in a Rashba superconductor to all orders in the magnetic field and arbitrary temperatures.

Let us consider a two-dimensional infinite homogeneous normal system with an isotropic Rashba SOC, proximitized by a superconductor. The SOC is described by the $SU(2)$ vector potential with components $\mathcal{A}_x = 2\alpha\sigma_y$ and $\mathcal{A}_y = -2\alpha\sigma_x$. Because the system is homogeneous, no gradient terms enter Eq. (33). Moreover, the term Eq. (36) does not contribute to the Usadel equation which acquires the simple form [40]:

$$D\mathcal{A}^2[\sigma_i, Q[\sigma_i, Q]] = [i\Omega + i\hbar\sigma_x, Q]. \quad (46)$$

The term in the left-hand side is the Dyakonov-Perel relaxation term due to the SOC, and we have assumed that the Zeeman field h points in x direction. From this equation one determines the function Q which in the present situation has the structure

$$Q = \hat{Q}_0 + \hat{Q}_x \sigma_x, \quad (47)$$

where $\hat{Q}_{0,x}$ are 2×2 matrices in Nambu space.

Once the matrix Q is obtained one can determine the Hall matrix current $J^{(H)}$ given by Eq. (11):

$$J_{\text{an}} = -\frac{D\tau}{4m}(i\pi T\nu) \sum_{\omega_n} \text{Tr} \tau_3 \{ \check{F}_{yx} + Q\check{F}_{yx}Q, \hat{V}_x Q \}. \quad (48)$$

Notice that the last term in Eq. (11) does not contribute in the case considered here. This expression has the same structure of the matrix current derived in Ref. [40] after the substitution $\check{F}_{ij} \rightarrow (\check{F}_{ij} + Q\check{F}_{ij}Q)/2$. As we demonstrate next the term $Q\check{F}_{ij}Q$ leads to an enhancement of the anomalous current when $h \sim \Delta$.

First, in order to obtain an analytical result we neglect the relaxation term and obtain for the components of Q in Eq. (47)

$$\hat{Q}_{0,x} = g_{0,x}\tau_3 + f_{0,x}\tau_1 \quad (49)$$

with

$$g_{0,x} = \frac{g_+ \pm g_-}{2}, \quad (50)$$

$$f_{0,x} = \frac{f_+ \pm f_-}{2}, \quad (51)$$

and

$$g_{\pm} = \frac{\omega_n \pm ih}{\sqrt{(\omega_n \pm ih)^2 + \Delta^2}}, \quad (52)$$

$$f_{\pm} = \frac{\Delta}{\sqrt{(\omega_n \pm ih)^2 + \Delta^2}}. \quad (53)$$

We have used the Matsubara representation of the Green's functions, with $\omega_n = \pi T(2n + 1)$, and h is the amplitude of the Zeeman or exchange field.

It is easy to check that the Q defined by Eqs. (47)–(53) satisfied the normalization $Q^2 = 1$. To calculate the charge anomalous current J_{an} one substitutes the above Q in Eq. (48):

$$\begin{aligned} J_{\text{an}} &= -\frac{i\pi TD\tau\alpha^3}{2m} \sum_{\omega_n} (g_+ - g_-)(1 + g_+g_- + f_+f_-) \\ &= \frac{2\pi TD\tau\alpha^3}{m} h\Delta^2 \sum_{\omega_n} \frac{\text{Re}\sqrt{\Delta^2 + (\omega_n + ih)^2}}{h^4 + 2h^2(\omega_n^2 - \Delta^2) + (\omega_n^2 + \Delta^2)^2}. \end{aligned} \quad (54)$$

The value of the maximum of J_{an} at $h = \Delta$ in the limit $T \ll \Delta$ can be found as follows. For small T and $h = \Delta$ the Matsubara sum in Eq. (54) is dominated by $\omega \ll \Delta$. Therefore,

$$\begin{aligned} J_{\text{an}}|_{h=\Delta} &\approx \frac{\pi\Delta D\tau\alpha^3}{m} T \sum_{\omega>0} \frac{\sqrt{\Delta}}{\omega^{3/2}} \\ &= \frac{\pi\Delta D\tau\alpha^3}{m} \frac{2^{3/2} - 1}{(2\pi)^{3/2}} \zeta(3/2) \sqrt{\frac{\Delta}{T}}. \end{aligned} \quad (55)$$

This result holds when neglecting the spin relaxation. If the latter is taken into account, the $1/\sqrt{T}$ divergence at $T \rightarrow 0$ saturates to the value $1/\sqrt{\Gamma_{\text{DP}}}$ at temperatures smaller than the Dyakonov-Perel spin relaxation term $\Gamma_{\text{DP}} = D\alpha^2$.

Inclusion of the spin-relaxation term stemming after substitution of Eq. (11) into Eq. (8) does not allow for a analytical solution for the Green's functions. We therefore calculate

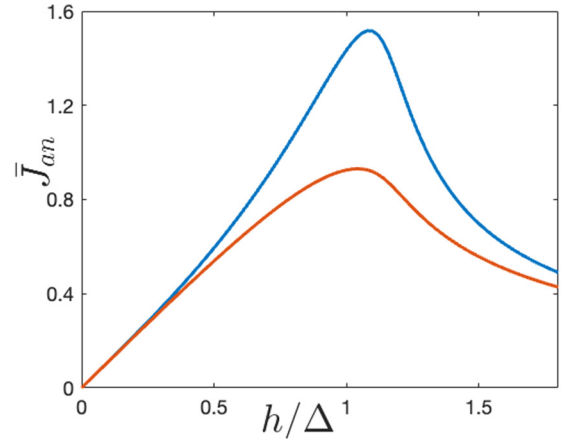


FIG. 1. The anomalous current $\bar{J}_{\text{an}} = J_{\text{an}} 2m / (\pi \Delta \tau \alpha^3)$ (blue solid line) as a function of the field h for $D\alpha^2 = 0.1\Delta$ and $T = 0.02\Delta$. The red line shows the result obtained from Ref. [40].

numerically the anomalous current, Eq. (54). In Fig. 1 we show the result for $D\alpha^2 = 0.1\Delta$ at $T = 0.5\Delta$. The red line shows the result obtained using the expression for the current from Ref. [40], $J_{\text{an}} = -i\pi TD\tau\alpha^3 / (2m) \sum_{\omega_n} (g_+ - g_-)$. Whereas at a small field both results coincide (linear regime), the anomalous current at fields comparable to Δ is clearly larger than the one obtained in that work.

VI. CONCLUSIONS

With the help of computer algebra, we have derived the nonlinear σ model for superconducting and normal systems, including the intrinsic SOC. The latter enters the theory as an effective SU(2) gauge field and therefore appears in the σ model only via gauge covariant combinations, the field strength, and covariant derivatives. We have performed a systematic gradient expansion and identified the spin-Hall term, which is responsible for the spin-Hall effect and other magnetoelectric effects mediated by the intrinsic SOC, such as spin-galvanic/Edelstein effects and anomalous supercurrents in superconductors. In the same order of the gradient expansion, we also recover the previously discussed contribution related to thermoelectricity [47].

The saddle-point equation of the model, Eqs. (33)–(38), which corresponds to the generalized Usadel equation, reveals new terms only present in the superconducting state and in nonlinear regimes, e.g., Eq. (36). We applied the derived equations to compute the anomalous current generated by a Zeeman field in a superconductor with Rashba SOC. We observe a substantial increase in the anomalous current compared to the results of previous incomplete theories, which clearly demonstrates the importance of new nonlinear terms in the saddle-point equations.

The presented generalized nonlinear σ model provides a flexible and convenient tool for studying diffusive superconducting systems with intrinsic SOC. It is expected to be especially useful for analyzing the effects of intrinsic spin-charge coupling in the nonlinear regime at the saddle-point level and for the description of a wide range of fluctuation phenomena.

In our derivation of the σ model we described superconducting correlations at the mean-field level. Apparently the mean-field approximation is not critical for our approach. Both the Cooper channel interaction and the usual Fermi-liquid interactions can be straightforwardly included into the formalism of the σ model without resorting on the mean-field treatment (see, for example, Ref. [73] and references therein). A natural further development of our work is to extend the model beyond the mean-field description of electron-electron interactions in the spirit of Refs. [43,50,73,74] to study the interplay of interactions, spin-charge coupling, and superconductivity.

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APPENDIX: COMPUTER ALGEBRA METHODS

1. Gradient expansion

We compute the expansion of

$$\begin{aligned} \delta S &= -\frac{i}{2} \text{Tr} \ln G^{-1} + \frac{i}{2} \text{Tr} \ln \mathcal{G}^{-1} \\ &= -\frac{i}{2} \text{Tr} \ln \left[1 + \left(\frac{2p_k a_k - a_k a_k}{2m} + a_0 \right) \otimes \mathcal{G} \right] \end{aligned} \quad (\text{A1})$$

in the small parameter a_k , $\partial_k \sim \text{small}$. Here $\mathcal{G}_p^{-1} = \mu - \frac{p^2}{2m} + \frac{i}{2\tau} \Lambda$, and $\Lambda^2 = 1$.

As explained in the main text, we work in the Wigner representation, where the Moyal product has the gradient expansion

$$X \otimes Y = \sum_{n=0}^{\infty} \frac{i^n}{2^n n!} X (\overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p - \overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_r)^n Y \quad (\text{A2})$$

that corresponds to an expansion in “small,” and can be truncated. It is convenient to express the mass $m = \tau \psi / \ell^2$ and the chemical potential $\mu = \psi / (2\tau)$ in terms of the scattering time τ or mean free path ℓ , and the quasiclassical parameter $\psi = p_F \ell$, to express the result as a double expansion in small ℓ and large ψ .

The series expansion of the logarithm and the Moyal product, and (as we see below) calculation of the momentum sum is straightforward. It results to the gradient expanded action, which can in the end be reexpressed in terms of gauge-invariant derivatives $\hat{\nabla}_j Q = \partial_j Q - [iA_j, Q]$ and the field strength $\tilde{F}_{ij} = \partial_i A_j - \partial_j A_i - i[A_i, A_j]$. We truncate the

expansion in order small⁴, which is where the lowest-order spatial field-strength term appears.

As the calculation of many (>100) terms is tedious to do manually, we implement this in computer algebra. The gradient expansion outlined above can be done symbolically by considering an algebra of terms cm consisting of a non-commutative monomial m and a scalar coefficient c , with m consisting of a product of symbols $\{\Lambda, a_i, a_0, \mathcal{G}\}$. The only nonzero momentum derivative of the base symbols is $\partial_{p_i} \mathcal{G} = \frac{p_i}{m} \mathcal{G} \mathcal{G}$. The nonzero spatial derivatives we denote in terms of $a_{X,i} \equiv \partial_i a_X$ where X is some set of indices. Here $a_{ijk\dots}$ are symmetric under exchange of indices, excluding the first index. The order in small of a monomial is equal to the total number of indices in a .

At the end of the expansion the monomials appear under tr , where they can be permuted cyclically. We define an (arbitrary) ordering of monomials $m > m'$, and permute each term to the order where the monomial is minimal. The procedure produces an expansion $\delta S = \text{Tr} \sum_j c_j m_j$ which after momentum integration becomes the local gradient expansion $\delta S = \int d^d r \text{tr} \sum_j c'_j m'_j$. We will also drop total derivative terms. Finally, we reexpress δS in a gauge-invariant form, in terms of monomials of symbols $Q_{X,i} \leftrightarrow \hat{\nabla}_i Q_X$ and \tilde{F}_{ij} .

It is also possible to formulate the expansion in a manifestly gauge-invariant manner, in terms of a gauge-invariant Moyal product. However, the present approach is simpler to implement in computer algebra.

The implementation is written using *SageMath* [78], and is included in the Supplemental Material [62].

2. Momentum integration

The momentum integrals are calculated exactly, and then expanded in series in the quasiclassical parameter $\psi = p_F \ell = 2\mu\tau \gg 1$. Although their analytic evaluation is standard, for completeness we explain it here in a form suitable for straightforward computer implementation.

All expressions generated by the expansion have the form

$$I = \sum_{\mathbf{p}} f(\mathbf{p}) = \int_{-\mu}^{\infty} d\xi \nu(\xi) \langle f(\mathbf{p}(\xi)) \rangle, \quad (\text{A3})$$

$$f(\mathbf{p}) = g(\mathbf{p}) \mathcal{G}_p Z_1 \mathcal{G}_p Z_2 \dots Z_{N-1} \mathcal{G}_p, \quad (\text{A4})$$

where $\mathcal{G}_p^{-1} = -\xi_p + \frac{i}{2\tau} \Lambda$, and we consider a parabolic band $\xi_p = \frac{p^2}{2m} - \mu$ in d dimensions, $\nu(\xi) = (1 + \xi/\mu)^{d/2-1} \nu_F$. Here $g(\mathbf{p})$ is a product of p_i and a \mathbf{p} -independent scalar, and Z_j are momentum independent.

The angular average $\langle \cdot \rangle$ over the $(d-1)$ sphere can be evaluated with a well-known formula, for n even,

$$\int_{S^{d-1}} \frac{dS_p p_{i_1} \dots p_{i_n}}{V(S^{d-1})} = \frac{p^n (d-2)!!}{(n+d-2)!!} \sum_{C \in \mathcal{P}} \prod_{(i_a, i_b) \in C} \delta_{i_a, i_b}, \quad (\text{A5})$$

where \mathcal{P} is the set of all pairings C of the indices $\{i_1, \dots, i_n\}$, and $V(S^d)$ is the sphere surface volume. The result is zero if n is odd. We then get $\langle g(\mathbf{p}) \rangle = g_0 (\frac{p^2}{2m})^\beta$, where β is an integer and g_0 a scalar.

TABLE I. Coefficients $C_{\beta N n}$ in Eq. (A6), for $d = 3$, expanded in $\psi = p_F \ell \gg 1$ up to $O(\psi^1)$.

β, N	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$
0, 1	∞	1	—	—	—
0, 2	$\frac{i\psi}{2}$	0	$-\frac{i\psi}{2}$	—	—
0, 3	$-\frac{3i\psi}{16}$	$\frac{\psi^2}{8}$	$\frac{i\psi}{16}$	$-\frac{3\psi^2}{8}$	—
0, 4	$\frac{i\psi^3}{16} - \frac{5i\psi}{128}$	$-\frac{\psi^2}{32}$	$-\frac{i\psi^3}{16} + \frac{i\psi}{128}$	$\frac{\psi^2}{32}$	$\frac{5i\psi^3}{16} - \frac{i\psi}{128}$
1, 1	∞	∞	—	—	—
1, 2	∞	0	$-\frac{i\psi}{2}$	—	—
1, 3	$-\frac{9i\psi}{16}$	$\frac{\psi^2}{8}$	$\frac{3i\psi}{16}$	$-\frac{3\psi^2}{8}$	—
1, 4	$\frac{i\psi^3}{16} + \frac{15i\psi}{128}$	$-\frac{3\psi^2}{32}$	$-\frac{i\psi^3}{16} - \frac{3i\psi}{128}$	$\frac{3\psi^2}{32}$	$\frac{5i\psi^3}{16} + \frac{3i\psi}{128}$
2, 1	∞	∞	—	—	—
2, 2	∞	∞	$-\frac{i\psi}{2}$	—	—
2, 3	∞	$\frac{\psi^2}{8}$	$\frac{5i\psi}{16}$	$-\frac{3\psi^2}{8}$	—
2, 4	$\frac{i\psi^3}{16} + \frac{75i\psi}{128}$	$-\frac{5\psi^2}{32}$	$-\frac{i\psi^3}{16} - \frac{15i\psi}{128}$	$\frac{5\psi^2}{32}$	$\frac{5i\psi^3}{16} + \frac{15i\psi}{128}$

Using $\Lambda^2 = 1$ and that $\mathcal{G}_p = (-\xi_p - \frac{i}{2\tau}\Lambda)/(\xi_p^2 + \frac{1}{4\tau^2})$, we can rewrite

$$I = -i\pi v_F \mu^{\beta+1-N} g_0 \sum_{\alpha} C_{\beta, N, |\alpha|_1} R_{\alpha}, \quad (\text{A6})$$

$$R_{\alpha} = \Lambda^{\alpha_1} Z_1 \Lambda^{\alpha_2} Z_2 \dots Z_{N-1} \Lambda^{\alpha_N}, \quad (\text{A7})$$

where the sum runs over the multi-index $\alpha = (\alpha_1, \dots, \alpha_N)$, $\alpha_j \in \{0, 1\}$, and $|\alpha|_1 = \sum_j \alpha_j$. The coefficients are given by

$$C_{\beta N n} = \frac{i^{n+1}(-1)^N}{\pi \psi^n} \int_{-1}^{\infty} dz \frac{(1+z)^{\beta+d/2-1} z^{N-n}}{(z^2 + \psi^{-2})^N}, \quad (\text{A8})$$

where $\psi = 2\mu\tau = p_F \ell$.

The integral over z can be evaluated by contour integration, with the help of an analytic function $q(z)$ satisfying a Riemann-Hilbert problem $q(z + i0^+) - q(z - i0^+) = \theta(1 + z)(1 + z)^{d/2-1}$ on a branch cut along the real axis. The result is given by

$$C_{\beta N n} = -2i^n(-1)^N \psi^{-n} \sum_{\pm} \text{Res}_{z=\pm i/\psi} q(z) \frac{(1+z)^{\beta} z^{N-n}}{(z^2 + \psi^{-2})^N}, \quad (\text{A9})$$

where we can take

$$q(z) = \begin{cases} \frac{i}{2\pi} \ln(-1-z)(1+z)^{d/2-1}, & d \text{ even}, \\ \frac{i}{2} \sqrt{-1-z}(1+z)^{(d-1)/2-1}, & d \text{ odd}. \end{cases} \quad (\text{A10})$$

Calculating the residue and expanding the result in series in ψ for $\psi \gg 1$ is straightforward with computer algebra. The values for $C_{\beta N n}$ are shown in Table I for $d = 3$, expanded in series of $\psi \gg 1$ truncated to order ψ^1 . To this order, one can show that the results are the same as from a pole approximation neglecting the band bottom.

The momentum integral converges for $\beta + d/2 < N + n$, and for other values the constants are diverging. Inspection of the gradient expansion indicates that momentum integrals appearing in order $k > d$ of the expansion are all convergent. For $d = 2$ and 3 , a nonconvergent integral appears in the second-order gradient expansion, but can be removed by requiring that the expansion is gauge invariant. Namely, for

constant scalar A_i ,

$$0 = \text{Tr} \ln \mathcal{G}_{p+A}^{-1} - \text{Tr} \ln \mathcal{G}_p^{-1} \simeq -\frac{1}{2m} \text{Tr}[\partial_{p_j}(p_i \mathcal{G})] A_i A_j. \quad (\text{A11})$$

This equation implies a sum rule $C_{120} + \frac{d}{2} C_{010} = -C_{122}$, using which eliminates all divergent constants appearing. This operation corresponds to subtraction of the above total derivative.

The above also allows evaluating the $\Omega = \check{A}_{\mu} = 0$ uniform saddle-point equation of Eq. (13) exactly. Making an ansatz $Q = b\Lambda$ with some scalar b , we have

$$b\Lambda = \frac{i}{\pi v_F} \sum_p' G(p) = \sum_p \frac{\frac{1}{2\pi\tau v_F}}{[\mu - \frac{p^2}{2m}]^2 + \frac{b^2}{4\tau^2}} b\Lambda, \quad (\text{A12})$$

where the primed sum is defined with the trace part subtracted, consistent with $\text{tr} \Lambda = 0$. Hence,

$$b = C_{011} |_{\psi \mapsto \psi/b} = \text{Re} \sqrt{1 + \frac{ib}{\psi}}, \quad (\text{A13})$$

From this it follows $b = 1 + O(\psi^{-2})$, so with the accuracy we work with, we can take $b = 1$.

3. Noncommutative reduction

The final step is rewriting the expansion, which consists of terms with monomials of symbols $\{\Lambda, a_j, a_0\}$, in terms of gauge-invariant derivatives and the field strength. We do this using a similar Gaussian elimination approach as used in noncommutative Gröbner basis constructions [79]. We outline the approach briefly below.

We define additional symbols \bar{Q}_i , \bar{Q}_{ij} , \bar{F}_{ij} , and consider the relations

$$\bar{Q}_i = [-ia_i, \Lambda], \quad (\text{A14})$$

$$\bar{Q}_{ij} = [-ia_{ij}, \Lambda] + [-ia_j, [-ia_i, \Lambda]], \quad (\text{A15})$$

$$\bar{F}_{ij} = a_{ji} - a_{ij} - i[a_i, a_j]. \quad (\text{A16})$$

The relations to the actual Q and field strength are then $\bar{Q}_i = T^{-1} \hat{\nabla}_i Q T$, $\bar{Q}_{ij} = T^{-1} \hat{\nabla}_j \hat{\nabla}_i Q T$, and $\bar{F}_{ij} = T^{-1} F_{ij} T$.

Consider now the problem of rewriting an expression $S = \sum_j c_j m_j$ expressed in terms of a, Λ solely in terms of \bar{Q} , \bar{F} , and Λ . It is understood the expression is under tr , and monomials can be cyclically permuted to their minimal form. Note that the factors of T, T^{-1} cancel under tr in expressions containing only the symbols \bar{Q}, \bar{F} , with replacement $\Lambda \leftrightarrow Q$.

The above relations (A14)–(A16) can be expressed as $g_j = 0$, $j = 1, 2, 3$, where $g_j = \sum_k c'_{jk} m'_{jk}$ are expressions containing symbols $a, \bar{Q}, \bar{F}, \Lambda$. Form then the set I of ideal generators $g'_{kj} = n_k g_j$, where n_k are any monomials such that the maximum order of terms in g' is $\leq M$ where M is a constant; here we can take $M = 6$. We permute all monomials in g'_{kj} cyclically to their minimal form. The set I has a finite number of elements. Obviously each expression g' in I satisfies $\text{tr} g' = 0$ if the definitions of \bar{Q}, \bar{F} symbols hold. Gröbner basis algorithms use a more optimal construction of the set I , although they usually do not consider trace permutations.

Define now a monomial ordering so that all monomials m containing a symbols satisfy $m \succ m'$ for all m' not containing any a symbols. The monomials, ordered from largest to smallest, can be considered as the basis of a vector space: one can then perform Gaussian elimination on the ideal generator set $I = \{g'\}$ and the expression S , to find the scalar coefficients d_j which eliminate the largest terms (in the basis sense) in $S' = S - \sum_j d_j g'_j$. Because a symbols were considered largest, Gaussian elimination removes them first, and the resulting expression S' will not contain them if S is gauge invariant. The results of the transformation are straightforward to verify.

The same approach can be used to rewrite results in terms of the symmetrized gauge-invariant derivatives, by introducing symmetrized derivative symbols ordered smaller than others, and for other forms of symbolic simplification of the noncommutative expressions under trace.

4. Results

We list below the typeset output of the program in the Supplemental Material [62] that performs the computations outlined above. The results are the leading contributions to the local gradient expanded action, written in form $\delta S = -\frac{\pi\nu_F}{2} \int d^3r \text{tr} \bar{S}$ and in units with $\ell = \tau = 1$.

The spatial gradient part, up to order 4 in gradients and to ψ^{-1} in $\psi = p_F \ell$,

$$\bar{S}_{\text{grad}} = \bar{S}_2 + \bar{S}_{4,0} + \frac{1}{\psi} \bar{S}_{4,1}, \quad (\text{A17})$$

$$\bar{S}_2 = -\frac{1}{12} i Q_i Q_i, \quad (\text{A18})$$

$$\bar{S}_{4,0} = \frac{1}{20} i Q_{(ii} Q_{jj)} - \frac{1}{16} i Q_{(i} Q_{(j} Q_{j} Q_{i)}, \quad (\text{A19})$$

$$\bar{S}_{4,1} = -\frac{1}{12} Q_i Q_j Q_{ij} + \frac{1}{12} i F_{ij} Q Q_i Q_j, \quad (\text{A20})$$

Here (...) in indices means tensor symmetrization, $Q = T \Lambda T^{-1}$, and $Q_i = \hat{\nabla}_i Q$, $Q_{ij} = \hat{\nabla}_j \hat{\nabla}_i Q$, and F is the field strength.

The first term in $\bar{S}_{4,1}$ can be written in various forms under trace, using Eqs. (A14) and (A15). For example, $\text{Tr}(Q_i Q_j Q_{ij}) = -\text{Tr}(Q Q_{ij} Q_{ij}) = -\frac{1}{2} \text{Tr}(Q_{ii} Q_j Q_j)$.

The a_0 part, up to fourth order in “small” and to ψ^{-1} in ψ :

$$\bar{S}_\Omega = \sum_{j=0}^4 \left(\bar{S}_{\Omega,j,0} + \frac{1}{\psi} \bar{S}_{\Omega,j,1} \right), \quad (\text{A21})$$

$$\bar{S}_{\Omega,0,0} = 0, \quad (\text{A22})$$

$$\bar{S}_{\Omega,1,0} = C_{010} \Omega + Q \Omega, \quad (\text{A23})$$

$$\bar{S}_{\Omega,2,0} = -\frac{1}{4} i Q_0 Q_0, \quad (\text{A24})$$

$$\bar{S}_{\Omega,3,0} = -\frac{1}{6} F_{0i} Q_i - \frac{1}{4} i Q Q_i Q_{0i} - \frac{1}{4} i Q Q_0 Q_{00}, \quad (\text{A25})$$

$$\begin{aligned} \bar{S}_{\Omega,4,0} = & \frac{1}{6} i F_{0i} F_{0i} + \frac{1}{2} i Q_{0i} Q_{0i} + \frac{1}{4} i Q_{00} Q_{00} + F_{0i} Q Q_{0i} \\ & + \frac{2}{3} F_{0i} Q_0 Q_i + \frac{1}{3} F_{0i} Q_i Q_0 - \frac{5}{16} i Q_0 Q_0 Q_0 Q_0 \\ & - \frac{5}{12} i Q_0 Q_0 Q_i Q_i - \frac{5}{24} i Q_0 Q_i Q_0 Q_i - \frac{1}{6} i F_{0i} Q F_{0i} Q, \end{aligned} \quad (\text{A26})$$

and

$$\bar{S}_{\Omega,0,1} = 0, \quad (\text{A27})$$

$$\bar{S}_{\Omega,1,1} = 0, \quad (\text{A28})$$

$$\bar{S}_{\Omega,2,1} = \frac{1}{2} Q \Omega \Omega, \quad (\text{A29})$$

$$\bar{S}_{\Omega,3,1} = -\frac{1}{4} i Q_0 Q_0 \Omega - \frac{1}{4} i Q_i Q_i \Omega, \quad (\text{A30})$$

$$\begin{aligned} \bar{S}_{\Omega,4,1} = & -i F_{0i} Q_{0i} - \frac{1}{2} F_{0i} Q_i \Omega + \frac{1}{8} Q Q_{0i} Q_{0i} - \frac{3}{8} Q_0 Q_i Q_{0i} \\ & - \frac{1}{2} i F_{0i} Q Q_0 Q_i - \frac{1}{4} i F_{0i} Q Q_i Q_0 - \frac{3}{4} i Q Q_i Q_{0i} \Omega \\ & - \frac{1}{4} i Q Q_0 Q_{00} \Omega, \end{aligned} \quad (\text{A31})$$

where we define $Q_0 = [-i\Omega, Q]$ for the “time derivative,” and $F_{k0} = -F_{0k} = T(a_{0k} - i[a_k, a_0])T^{-1} = \partial_k \Omega - i[A_k, \Omega] = \hat{\nabla}_k \Omega$ for the “field strength.” Above, in contrast to the main text, we set $\dot{A}_0 = 0$. To recover the 0 components of the fields and the field strengths in Eqs. (A21)–(A31), shift $\Omega \mapsto \Omega + \dot{A}_0$ so that also $F_{k0} = -F_{0k} \mapsto \hat{\nabla}_k \Omega + \dot{F}_{k0}$.

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