Berry Curvature Effects on Quasiparticle Dynamics in Superconductors

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We construct a theory for the semiclassical dynamics of superconducting quasiparticles by following their wave packet motion and reveal rich contents of Berry curvature effects in the phase space spanned by position and momentum. These Berry curvatures are traced back to the characteristics of superconductivity, including the nontrivial momentum-space geometry of superconducting pairing, the real-space supercurrent, and the charge dipole of quasiparticles. The Berry-curvature effects strongly influence the spectroscopic and transport properties of superconductors, such as the local density of states and the thermal Hall conductivity. As a model illustration, we apply the theory to study the twisted bilayer graphene with a $d_{x^2+y^2} + id_{xy}$ superconducting gap function and demonstrate Berry-curvature induced effects.

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Introduction.—The Chern number of Bogoliubov–de Gennes band structure has commonly been used to characterize the topology of exotic superconductors [1–5], while much less attention has been given to the physical effect of the momentum-space Berry curvature that makes up the Chern number [6,7]. In the presence of inhomogeneity due to external fields or a supercurrent, we may also expect to find other components of the Berry curvature in the phase space, such as those in the real space, as well as in the cross planes of position and momentum [8]. Phase-space Berry curvatures are known to be important on the dynamics of Bloch electrons, ubiquitously affecting equilibrium and transport properties of solids [9–16]. It is therefore highly desirable to construct a semiclassical theory for quasiparticle dynamics in superconductors, which systematically takes into account these Berry curvatures, in order to provide an intuitive and effective basis for analyzing various response properties of superconductors.

In this Letter, we introduce the semiclassical quasiparticle as a wave packet in the background of slowly varying gauge potentials and the superconducting order parameter. Apart from Berry curvatures inherited from the parent Bloch states, we identify new contributions due to the phase space structure of the order parameter, which is nontrivial in all but the conventional s-wave superconductors. The quasiparticle also naturally possesses a charge dipole moment, which can couple to a magnetic field through the Lorentz force and induce field-dependent Berry curvatures.

To demonstrate the utility of the developed theory, we discuss how these Berry curvatures modify the phase-space density of states of the quasiparticles and the impact on tunneling spectroscopic measurements. We also present a semiclassical approach to the intrinsic thermal Hall conductivity due to quasiparticles without requiring nontrivial calculations of energy magnetization [17–20] and reveal its relationship with the topological contribution from condensate [21,22]. We illustrate our results in several model systems, including a twisted-bilayer graphene model [23] with a $d + id$ superconducting order parameter.

Quasiparticle wave packet in second quantization formalism.—In order for a semiclassical theory of superconducting quasiparticles to be feasible, we assume that all the possible inhomogeneities in the considered system are smooth in the spread (much larger than the coherence length [24]) of a quasiparticle wave packet, whose center position is marked as $\boldsymbol{r}_c$. For example, in the mixed states of type-II superconductors, we focus only on the region far away from the vortex core, where the pairing potential can be perceived as slowly varying. A local Hamiltonian description of the wave packet hence emerges, namely $H_c = \int d\boldsymbol{r} c^\dagger_{\sigma\boldsymbol{r}}(\hat{h}_c - \mu)c_{\sigma\boldsymbol{r}} - \int d\boldsymbol{r} d\boldsymbol{r}' g(\boldsymbol{r}_c, \boldsymbol{r}-\boldsymbol{r}')c^\dagger_{\uparrow\boldsymbol{r}}c^\dagger_{\downarrow\boldsymbol{r}'}c_{\downarrow\boldsymbol{r}'}c_{\uparrow\boldsymbol{r}}$, where $c^\dagger_{\sigma\boldsymbol{r}}$ is the creation operator for an electron with spin $\sigma(=\uparrow,\downarrow)$ at position $\boldsymbol{r}$, $\hat{h}_c \equiv h_0(\boldsymbol{r}, -i\nabla_{\boldsymbol{r}} - e\boldsymbol{A}(\boldsymbol{r}_c, t); \{\beta_i(\boldsymbol{r}_c)\})$ is the spin degenerate single-electron Hamiltonian in the local approximation (set $\hbar = 1$), μ is the chemical potential, and g is the effective attractive interaction between electrons. We only consider spin-singlet superconductors with intraband pairing and without spin-orbit coupling for simplicity. The slowly varying perturbation fields $\{\beta_i\}$ ($i = 1, 2, \ldots$) and the electromagnetic vector potential $\boldsymbol{A}$ are represented by their values at $\boldsymbol{r}_c$. $\hat{h}_c$ possesses local eigenfunctions $e^{ie\boldsymbol{A}(\boldsymbol{r}_c,t)\cdot\boldsymbol{r}}\psi_{n\sigma\boldsymbol{k};\boldsymbol{r}_c}(\boldsymbol{r})$, where $\psi_{n\sigma\boldsymbol{k};\boldsymbol{r}_c}(\boldsymbol{r})$ are the local Bloch functions of $h_0(\boldsymbol{r}, -i\nabla_{\boldsymbol{r}}; \{\beta_i(\boldsymbol{r}_c)\})$, with local Bloch bands $\xi_{n\boldsymbol{k};\boldsymbol{r}_c}$. Here n and $\boldsymbol{k}$ are the indices for band (with twofold spin degeneracy) and wave vector, respectively, and $\boldsymbol{r}_c$ enters in the eigenstates parametrically as a character of the local description.

The interaction term can be treated within a mean-field approach, ending with [25]

$$H_c = \sum_{n\sigma\boldsymbol{k}} E_{n\boldsymbol{k};\boldsymbol{r}_c} \gamma^{\dagger}_{n\sigma\boldsymbol{k};\boldsymbol{r}_c} \gamma_{n\sigma\boldsymbol{k};\boldsymbol{r}_c}, \tag{1}$$

where the creation and annihilation operators for the local eigenstate are introduced by the Bogoliubov transformation, e.g., $\gamma^{\dagger}_{n\uparrow\boldsymbol{k};\boldsymbol{r}_c} = \mu^*_{n\boldsymbol{k};\boldsymbol{r}_c} c^{\dagger}_{n\uparrow\boldsymbol{k};\boldsymbol{r}_c} - \nu^*_{n\boldsymbol{k};\boldsymbol{r}_c} c_{n\downarrow-\boldsymbol{k};\boldsymbol{r}_c}$. Here $c^{\dagger}_{n\sigma\boldsymbol{k};\boldsymbol{r}_c} = \int d\boldsymbol{r} e^{ie\boldsymbol{A}(\boldsymbol{r}_c,t)\cdot\boldsymbol{r}} \psi_{n\sigma\boldsymbol{k};\boldsymbol{r}_c}(\boldsymbol{r}) c^{\dagger}_{\sigma\boldsymbol{r}}$ creates the local Bloch eigenstates of $\hat{h}_c$, whereas $(\mu_{n\boldsymbol{k};\boldsymbol{r}_c}, \nu_{n\boldsymbol{k};\boldsymbol{r}_c})^T$ and $E_{n\boldsymbol{k};\boldsymbol{r}_c} = \sqrt{\xi^2_{n\boldsymbol{k};\boldsymbol{r}_c} + |\Delta_{n\boldsymbol{k};\boldsymbol{r}_c}|^2}$ are the Bogoliubov wave function in this local Bloch representation and the eigenenergy, respectively, and $\Delta_{n\boldsymbol{k};\boldsymbol{r}_c}$ is the local momentum-space superconducting pairing function. The quasiparticle operators not only define the excitations of the local Hamiltonian, but also determine the ground state of the local Hamiltonian with annihilation operators $|G\rangle = \mathcal{N} \prod_{n\sigma\boldsymbol{k}} \gamma_{n\sigma\boldsymbol{k};\boldsymbol{r}_c} |0\rangle$. Here $\mathcal{N}$ is the normalization factor and $|0\rangle$ is the vacuum for electrons.

Now we construct a quasiparticle wave packet centered around $(\boldsymbol{r}_c, \boldsymbol{k}_c)$, with the local creation operators acting on the superconducting ground state [24],

$$|\Psi_{n\uparrow}(\boldsymbol{r}_c, \boldsymbol{k}_c, t)\rangle = \int [d\boldsymbol{k}] \alpha(\boldsymbol{k}, t) \gamma^{\dagger}_{n\uparrow\boldsymbol{k};\boldsymbol{r}_c} |G\rangle, \tag{2}$$

where $\int [d\boldsymbol{k}]$ is shorthand for $\int d^m k/(2\pi)^m$ with m the dimension of the system. The envelope function $\alpha(\boldsymbol{k}, t)$ is sharply distributed in reciprocal space so that it makes sense to speak of the wave vector $\boldsymbol{k}_c = \int [d\boldsymbol{k}] |\alpha(\boldsymbol{k}, t)|^2 \boldsymbol{k}$ of the wave packet. With the SU(2) spin rotation symmetry, the equations of motion for quasiparticles of up and down spins take the same form. Thus we only demonstrate the spin-up wave packet. Before proceeding we also note that, while the momentum-space Berry curvature can be reconstructed from the Bogoliubov–de Gennes formalism in the Nambu form [7,21], the superconductivity induced phase-space Berry phase effects related to the charge dipole, gauge field, and supercurrent addressed below have not been presented previously.

Spin center and charge dipole of the wave packet.—For Bloch electrons, the wave packet center is simply the charge center. However, for superconducting quasiparticles, the charge center is elusive, as the mean-field (bare) quasiparticles are momentum-dependent mixture of electrons and holes, with vanishing effective charge at the excitation gap. Moreover, if the Coulomb interaction is considered, it was shown that the renormalized quasiparticles are charge neutral [24,26]. On the other hand, spin is a conserved quantity in the absence of spin-orbit coupling, hence the spin center serves physically as the center of a wave packet. For this purpose, we consider the spin density operator $\hat{S}(\boldsymbol{r}) = c^{\dagger}_{\uparrow,\boldsymbol{r}} c_{\uparrow,\boldsymbol{r}} - c^{\dagger}_{\downarrow,\boldsymbol{r}} c_{\downarrow,\boldsymbol{r}}$ and calculate its wave packet averaging $S(\boldsymbol{r}) = \langle\Psi|\hat{S}(\boldsymbol{r})|\Psi\rangle - \langle G|\hat{S}(\boldsymbol{r})|G\rangle$. This gives the distribution of spin on the wave packet, and its center, the spin center, is given by [25]

$$\boldsymbol{r}_c \equiv \int d\boldsymbol{r} S(\boldsymbol{r}) \boldsymbol{r} = \frac{\partial \gamma_c}{\partial \boldsymbol{k}_c} + \langle\phi|i\nabla_{\boldsymbol{k}_c}\phi\rangle - \rho_c \nabla_{\boldsymbol{k}_c} \theta_c, \tag{3}$$

where $\theta_c = \frac{1}{2} \arg \Delta_{n\boldsymbol{k}_c;\boldsymbol{r}_c}$ is related to the phase of the superconducting order parameter, $\rho_c = \xi_{n\boldsymbol{k}_c;\boldsymbol{r}_c}/E_{n\boldsymbol{k}_c;\boldsymbol{r}_c}$ measures the charge of mean-field quasiparticles, $|\phi\rangle$ is the periodic part of the Bloch state $|\psi_{n\sigma\boldsymbol{k}_c;\boldsymbol{r}_c}\rangle$, and $\gamma_c = -\arg \alpha(\boldsymbol{k}_c, t)$ is the phase of the envelope function. The Berry connections contain not only the Bloch part $\mathcal{A}^b_{\boldsymbol{k}_c} = \langle\phi|i\nabla_{\boldsymbol{k}_c}\phi\rangle$ from the single-electron band structure, but also the superconducting part $\mathcal{A}^{sc}_{\boldsymbol{k}_c} = -\rho_c \nabla_{\boldsymbol{k}_c} \theta_c$ from the momentum dependence of the superconducting order parameter. Note that a similar but different construction involving the momentum-space gradient of the phase of the order parameter was studied in [27].

The spin center is not sufficient to describe the coupling of quasiparticles with electromagnetic fields, which would inevitably involve information on the charge distribution upon the spread of a wave packet. Since the charge distribution is not centered at $\boldsymbol{r}_c$, there should be a charge dipole moment associated with a wave packet. Indeed one can consider the charge density operator $\hat{Q}(\boldsymbol{r}) = e(c^{\dagger}_{\uparrow\boldsymbol{r}} c_{\uparrow\boldsymbol{r}} + c^{\dagger}_{\downarrow\boldsymbol{r}} c_{\downarrow\boldsymbol{r}})$, and its wave packet averaging $Q(\boldsymbol{r}) = \langle\Psi|\hat{Q}(\boldsymbol{r})|\Psi\rangle - \langle G|\hat{Q}(\boldsymbol{r})|G\rangle$ provides a proper definition for the charge dipole moment [25]

$$\boldsymbol{d} \equiv \int d\boldsymbol{r} Q(\boldsymbol{r})(\boldsymbol{r} - \boldsymbol{r}_c) = e(\rho_c^2 - 1) \frac{\partial \theta_c}{\partial \boldsymbol{k}_c}. \tag{4}$$

It is nonzero only in the case of a momentum-dependent phase of superconducting order parameter. Furthermore, if the external-field-free system has either time-reversal (space-inversion) symmetry, $\boldsymbol{d}$ is an even (odd) function in momentum space, as can be inspected from the semiclassical equations of motion proposed later.

Berry curvatures and semiclassical dynamics.—The distinctive properties of the wave packet are anticipated to strongly affect its semiclassical dynamics determined by the Lagrangian $\mathcal{L} = \langle\Psi|i(d/dt) - \hat{H}_c|\Psi\rangle - \langle G|i(d/dt) - \hat{H}_c|G\rangle$ [9] and should be embodied in various Berry curvatures characterizing the dynamical structure. Adopting the circular gauge $\boldsymbol{A}(\boldsymbol{r}_c) = \frac{1}{2} \boldsymbol{B} \times \boldsymbol{r}_c$, which is suitable for the approximately uniform magnetic field in regions far away from vortex lines, after some algebra we get [25] (hereafter the wave packet center label c is omitted for simplicity)

$$\mathcal{L} = -E + \boldsymbol{k}\cdot\dot{\boldsymbol{r}} + (\mathcal{A}_{\boldsymbol{r}}^{b} - \rho\boldsymbol{v}^{s} + \boldsymbol{B}\times\tilde{\boldsymbol{d}})\cdot\dot{\boldsymbol{r}} + (\mathcal{A}_{\boldsymbol{k}}^{b} - \rho\nabla_{\boldsymbol{k}}\theta)\cdot\dot{\boldsymbol{k}}. \tag{5}$$

Here the coupling of the wave packet to the magnetic field involves the charge dipole and gives $\boldsymbol{B}\times\tilde{\boldsymbol{d}}$, with $\tilde{\boldsymbol{d}} = \boldsymbol{d}/2$. Additionally, $\boldsymbol{v}^{s} = \nabla_{\boldsymbol{r}}\theta - e\boldsymbol{A}$ is half of the gauge invariant supercurrent velocity, and $\mathcal{A}_{\boldsymbol{r}}^{b} = \langle\phi|i\nabla_{\boldsymbol{r}}\phi\rangle$ is the real-space Berry connection of the single-electron wave function.

The structure of the Lagrangian implies that the total Berry connections in the momentum and real space take the forms of $\mathcal{A}_{\boldsymbol{k}} = \mathcal{A}_{\boldsymbol{k}}^{b} - \rho\nabla_{\boldsymbol{k}}\theta$ and $\mathcal{A}_{\boldsymbol{r}} = \mathcal{A}_{\boldsymbol{r}}^{b} - \rho\boldsymbol{v}^{s} + \boldsymbol{B}\times\tilde{\boldsymbol{d}}$, respectively. Various Berry curvatures are then formed as $\Omega_{\lambda_\alpha\lambda_\beta} = \partial_{\lambda_\alpha}\mathcal{A}_{\lambda_\beta} - \partial_{\lambda_\beta}\mathcal{A}_{\lambda_\alpha}$, where $\boldsymbol{\lambda} = \boldsymbol{r}, \boldsymbol{k}$, and α and β are Cartesian indices. In particular, $\Omega_{k_\alpha k_\beta}$ and $\Omega_{r_\alpha r_\beta}$ are antisymmetric tensors, whose vector forms read, respectively,

$$\boldsymbol{\Omega}_{\boldsymbol{k}} = i\langle\nabla_{\boldsymbol{k}}\phi|\times|\nabla_{\boldsymbol{k}}\phi\rangle - \nabla_{\boldsymbol{k}}\rho\times\nabla_{\boldsymbol{k}}\theta \tag{6}$$

and

$$\boldsymbol{\Omega}_{\boldsymbol{r}} = i\langle\nabla_{\boldsymbol{r}}\phi|\times|\nabla_{\boldsymbol{r}}\phi\rangle + e\rho\boldsymbol{B} - \nabla_{\boldsymbol{r}}\rho\times\boldsymbol{v}^{s} + \nabla_{\boldsymbol{r}}\times(\boldsymbol{B}\times\tilde{\boldsymbol{d}}). \tag{7}$$

The first terms in these two equations are the familiar Berry curvatures from the single-electron band structure [9], while other terms involve superconductivity. One can readily verify that the superconductivity induced $\boldsymbol{\Omega}_{\boldsymbol{k}}$ coincides with that obtained from the Bogoliubov–de Gennes equation [7]. Moreover, the charge dipole and supercurrent are embedded in the superconductivity induced $\boldsymbol{\Omega}_{\boldsymbol{r}}$.

Regarding the phase-space Berry curvature $\boldsymbol{\Omega}_{\boldsymbol{kr}}$, there are remarkable qualitative differences from that for Bloch electrons, namely $\boldsymbol{\Omega}_{\boldsymbol{kr}} = 0$ and $\boldsymbol{\Omega}_{\boldsymbol{kr}} \neq 0$, respectively, in normal and superconducting states subjected to scalar perturbations. The physics can be easily understood by thinking with the Nambu space, in which the scalar perturbation in the electronic Hamiltonian is endowed with a spin structure. Thus, the usual scalar field felt by electrons is no longer scalar for superconducting quasiparticles. Nonzero $\boldsymbol{\Omega}_{\boldsymbol{kr}}$ will play a vital role in a number of experimental measurables [9]. For example, in the presence of pure magnetic perturbations, its trace reads

$$\mathrm{Tr}[\boldsymbol{\Omega}_{\boldsymbol{kr}}] = -\nabla_{\boldsymbol{k}}\rho\cdot\boldsymbol{v}^{s} - e\rho\boldsymbol{B}\cdot(\nabla_{\boldsymbol{k}}\rho\times\nabla_{\boldsymbol{k}}\theta). \tag{8}$$

As will be shown later, this trace of the Berry-curvature tensor plays an important role in the geometric modulations to the quasiparticle density of states [9].

With the above Berry curvatures, the Euler-Lagrange equations of motion for superconducting quasiparticles possess the same noncanonical structure as for Bloch electrons [9]. Having realized this, we neglect the Berry curvatures from Bloch band structures for simplicity and focus on those originated from superconductivity. Thus, the equations of motion read

$$\begin{aligned}\dot{\boldsymbol{r}} &= \nabla_{\boldsymbol{k}}E + \dot{\boldsymbol{k}}\times(\nabla_{\boldsymbol{k}}\rho\times\nabla_{\boldsymbol{k}}\theta) + \nabla_{\boldsymbol{k}}(\rho\boldsymbol{v}^{s} - \boldsymbol{B}\times\tilde{\boldsymbol{d}})\cdot\dot{\boldsymbol{r}} - \dot{\boldsymbol{r}}\cdot\nabla_{\boldsymbol{r}}(\rho\nabla_{\boldsymbol{k}}\theta),\\ \dot{\boldsymbol{k}} &= -\nabla_{\boldsymbol{r}}E + \dot{\boldsymbol{r}}\times(e\rho\boldsymbol{B} - \nabla_{\boldsymbol{r}}\rho\times\boldsymbol{v}^{s} + \nabla_{\boldsymbol{r}}\times(\boldsymbol{B}\times\tilde{\boldsymbol{d}})) - \nabla_{\boldsymbol{r}}(\rho\nabla_{\boldsymbol{k}}\theta)\cdot\dot{\boldsymbol{k}} + \dot{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}(\rho\boldsymbol{v}^{s} - \boldsymbol{B}\times\tilde{\boldsymbol{d}}).\end{aligned} \tag{9}$$

In the absence of superconductivity, $\rho = 1$, $\tilde{\boldsymbol{d}} = 0$, and $\theta = 0$ are all constants, and all the derivatives with respect to these quantities in Eq. (9) vanishes. Hence the equations of motion reduce to the usual ones for electrons [8]. For trivial superconducting pairing, the momentum-space Berry connection vanishes but the real-space one may still survive due to the supercurrent velocity: $\mathcal{A}_{\boldsymbol{r}} = -\rho\boldsymbol{v}^{s}$. The resulting Berry curvature in real space is given by $\boldsymbol{\Omega}_{\boldsymbol{r}} = e\rho\boldsymbol{B} + \nabla_{\boldsymbol{r}}\rho\times\boldsymbol{v}^{s}$. The equations of motion describe the quasiparticle dynamics subjected to background superflow and take a similar form to those for bosonic Bogoliubov quasiparticles in a Bose-Einstein condensate with a vortex [28].

Equation (9) is the central result of this Letter. It provides a framework to understand quasiparticle dynamics in superconductors subjected to various perturbations. In the following, we apply this semiclassical theory to calculate several properties of superconductors.

Density of states.—A most direct consequence of the Berry curvatures appearing in the equations of motion is the breakdown of the phase-space volume conservation. As a result, the phase-space measure $\mathcal{D}(\boldsymbol{r},\boldsymbol{k})$ is modified by Berry curvatures [11], which to the first order of the spatial inhomogeneity can be expressed as

$$\mathcal{D}(\boldsymbol{r},\boldsymbol{k}) = 1 + \mathrm{Tr}\boldsymbol{\Omega}_{\boldsymbol{kr}} - \boldsymbol{\Omega}_{\boldsymbol{r}}\cdot\boldsymbol{\Omega}_{\boldsymbol{k}}. \tag{10}$$

The modification may originate from various perturbations, such as the supercurrent and magnetic field. We note that $\partial\mathcal{D}/\partial\boldsymbol{B} = 0$, since the relevant terms in $\mathrm{Tr}\boldsymbol{\Omega}_{\boldsymbol{kr}}$ and $\boldsymbol{\Omega}_{\boldsymbol{r}}\cdot\boldsymbol{\Omega}_{\boldsymbol{k}}$ cancel each other, in sharp contrast to the case of Bloch electrons [11]

$\mathcal{D}$ would influence the local density of states, which is the momentum integration of the quasiparticle spectra function

$$n(\boldsymbol{r},\omega) = \int[d\boldsymbol{k}]\mathcal{D}(\boldsymbol{r},\boldsymbol{k})[|\mu|^2\delta(\omega - E) + |\nu|^2\delta(\omega + E)]. \tag{11}$$

This local density of states is proportional to the differential conductance, which can be directly measured by scanning tunneling microscopy [29]. $\mathcal{D}$ would also influence the momentum-space density of states

$$n(\boldsymbol{k}) = \iint d\omega d\boldsymbol{r} \mathcal{D}(\boldsymbol{r},\boldsymbol{k})[|\mu|^2\delta(\omega - E) + |\nu|^2\delta(\omega + E)] \tag{12}$$

given by the real-space and frequency integrations of the spectra function, which can be measured by the momentum and energy resolved tunneling spectroscopy [30]. In particular, in the case of a small supercurrent, we have $\mathcal{D} = 1 - \nabla_{\boldsymbol{k}}\rho \cdot \boldsymbol{v}^s$ according to Eq. (8). This deviation of $\mathcal{D}$ from unity leads to the following modifications to the aforementioned densities of states: $\delta n(\boldsymbol{r},\omega) = -\int[d\boldsymbol{k}]\boldsymbol{v}^s \cdot \nabla_{\boldsymbol{k}}\rho[|\mu|^2\delta(\omega - E_{\boldsymbol{r},\boldsymbol{k}}) + |\nu|^2\delta(\omega + E_{\boldsymbol{r},\boldsymbol{k}})]$ and $\delta n(\boldsymbol{k}) = -\int[d\boldsymbol{r}]\boldsymbol{v}^s \cdot \nabla_{\boldsymbol{k}}\rho$. These modifications depend on the direction of the supercurrent and hence could be experimentally verified by injecting supercurrent on different directions.

Thermal Hall transport.—The semiclassical theory can also be employed to study transport properties in superconductors such as the intrinsic thermal Hall effect. Compared to the edge-state analysis [21,22], our theory not only yields the quantized thermal Hall conductivity contributed by topological edge states but also renders information on bulk quasiparticles in intrinsic thermal transport. Compared to Green's function method [18–20], the semiclassical theory has a remarkable advantage of obtaining the transport component of the current [17,31] without requiring exact but involved determination of the energy magnetization of superconducting quasiparticles.

Here we sketch the key steps from the semiclassical equations toward the thermal Hall transport. We start from the semiclassical expression for the local energy current density $\boldsymbol{j}^Q = \int[d\boldsymbol{k}]\mathcal{D}(\boldsymbol{k})f(E_{\boldsymbol{k}}, T)E_{\boldsymbol{k}}\dot{\boldsymbol{r}}$ [32] where $f(E_{\boldsymbol{k}}, T)$ is the Fermi-Dirac distribution at temperature T. Then we substitute the equation of motion for $\dot{\boldsymbol{r}}$ in the absence of magnetic field and find $\boldsymbol{j}^Q = -\nabla T \times (\partial/\partial T)\int[d\boldsymbol{k}]h\boldsymbol{\Omega}_{\boldsymbol{k}} + \nabla \times \int[d\boldsymbol{k}]h\boldsymbol{\Omega}_{\boldsymbol{k}}$, where we introduce the auxiliary function $h(E_{\boldsymbol{k}}, T) = -\int_{E_{\boldsymbol{k}}}^{\infty} d\eta f(\eta, T)\eta$. Now the second term is a circulating current that should be discounted, leaving the transport current $\boldsymbol{j}^{Q\mathrm{tr}} = \int[d\boldsymbol{k}](\partial h/\partial T)\boldsymbol{\Omega}_{\boldsymbol{k}} \times \nabla T$. The Hall response of this current is given by

$$\kappa_{xy}^q = \frac{2}{T}\int[d\boldsymbol{k}](\boldsymbol{\Omega}_{\boldsymbol{k}})_z\int_{E_{\boldsymbol{k}}}^{\infty} d\eta\eta^2 f'(\eta, T), \tag{13}$$

where the factor 2 denotes the spin degeneracy.

The above formula accounts for the contribution from quasiparticles beyond the superconducting condensate. It is physically reasonable to make the connection $\kappa_0 + \kappa_{xy}^q = \kappa_{xy}^{\mathrm{BdG}}$ between this "quasiparticle plus condensate" description and the Bogoliubov–de Gennes (BdG) one [20]. Here κ_0 is the thermal Hall conductivity contributed by the condensate and $\kappa_{xy}^{\mathrm{BdG}} = (1/T)\int[d\boldsymbol{k}](\boldsymbol{\Omega}_{\boldsymbol{k}})_z(\int_{E_{\boldsymbol{k}}}^{\infty} - \int_{-E_{\boldsymbol{k}}}^{\infty})d\eta\eta^2 f'(\eta, T)$ is the conductivity obtained using the particle-hole symmetric BdG bands. In $\kappa_{xy}^{\mathrm{BdG}}$ the spin degeneracy and the particle-hole redundancy cancel out, and $-E_{\boldsymbol{k}}$ means the BdG "valence band" whose Berry curvature is $-(\boldsymbol{\Omega}_{\boldsymbol{k}})_z$. The above connection enables us to obtain the condensate contribution $\kappa_0 = -(1/T)\int[d\boldsymbol{k}](\boldsymbol{\Omega}_{\boldsymbol{k}})_z\int_{-\infty}^{\infty} d\eta\eta^2 f'(\eta, T) = \pi C_1 k_B^2 T/6\hbar$, with the Chern number C_1.

Model illustration: Twisted-bilayer graphene with $d + id$ superconductivity.—To illustrate the application of the semiclassical theory, we consider the twisted-bilayer graphene system that has been proposed to support a topological chiral d-wave superconducting state [33–36]. We take the following effective four-band tight-binding Hamiltonian [23]:

$$H = -\mu\sum_i \tilde{c}_i^\dagger\tilde{c}_i + t_1\sum_{\langle i,j\rangle}\tilde{c}_i^\dagger\tilde{c}_j + \sum_{[i,j]}\tilde{c}_i^\dagger[(t_2\sigma_0 + it_3\sigma_y) \otimes \sigma_0]\tilde{c}_j + \mathrm{H.c.}, \tag{14}$$

where $\tilde{c}_i^\dagger \equiv (c_{i,x,\uparrow}^\dagger, c_{i,y,\uparrow}^\dagger, c_{i,x,\downarrow}^\dagger, c_{i,y,\downarrow}^\dagger)$ is the electron creation operator with two distinct orbitals $\alpha = (p_x, p_y)$, $\sigma_{0,y}$ are the Pauli matrices, t_i ($i = 1$, 2, 3) are hopping parameters, and $\langle i, j\rangle$ and $[i, j]$ represent the summations over the nearest and next-nearest neighbors within the same sublattice, respectively. We diagonalize this Hamiltonian and find two bands that intersect with the chemical potential [25]. Superconductivity in twisted-bilayer graphene with $d_{x^2-y^2} + id_{xy}$ pairing symmetry can be described by the superconducting gap function in the form of [2,37,38] $\Delta(\boldsymbol{k}) = \sum_{i=1}^3 \Delta_i\cos(\boldsymbol{k}\cdot\boldsymbol{R}_i - \varphi_{\boldsymbol{k}})$, with Δ_i, $\varphi_{\boldsymbol{k}}$ and $\boldsymbol{R}_i$ detailed in the Supplemental Material [25].

First we calculate the momentum-space Berry curvature by Eq. (6) for this tight-binding model. In Fig. 1(a), we demonstrate the Berry curvature for one band with typical band parameters given in Ref. [23] and symmetric $d_{x^2-y^2}$ and d_{xy} gaps. The band structure of the tight-binding model has trivial topology, and the Berry curvatures are entirely contributed by the superconducting gap function. Because of the particle-hole symmetry in superconductors, the Berry curvatures concentrate around the Fermi surface. The distribution has symmetric peaks reflecting the D_3 symmetry of the lattice structure and the gap function.

The temperature dependence of the quasiparticle thermal Hall conductivity is shown in Fig. 1(b). It has a near exponential dependence on the temperature at the low temperature regime and becomes an approximated linear function at higher temperatures. We also show the modulation to the momentum-space density of states due to a uniform supercurrent in Fig. 1(c), which concentrates around the Fermi surface. This modulation depends on both the amplitude and direction of the supercurrent (details

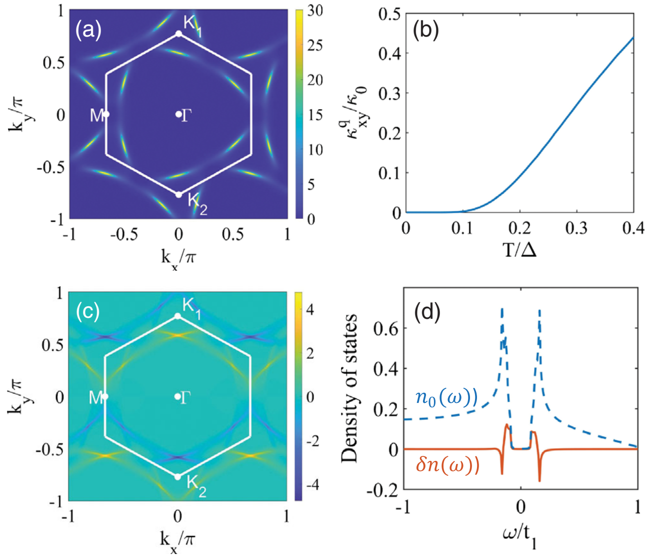

FIG. 1. (a) Berry curvatures of the tight-binding model for twisted-bilayer graphene with $d_{x^2-y^2}$ and id_{xy} superconducting gaps. (b) The quasiparticle thermal Hall conductivity as a function of temperature. Berry-curvature modifications to the momentum space (c) and local (d) density of states with a constant supercurrent $\nabla_{\boldsymbol{r}}\theta = (\sqrt{2}\pi/10)\hat{x}$. In (d) only the result for one of the two bands at the Fermi surface is plotted (solid line). The conventional density of states $n_0(\omega)$ is demonstrated for comparison. Model parameters are taken as $t_2/t_1 = 0.05$, $t_3/t_1 = 0.2$, $\mu = -0.9t_1$, and $\Delta/t_1 = 0.1$.

in the Supplemental Material [25]). These features would be helpful for identifying the $d + id$ pairing in twisted-bilayer graphene systems.

Finally, we consider the local density of states modulations from a supercurrent. In Fig. 1(d), only the contribution from one of the two bands at the Fermi surface is shown, and the contributions by the two bands cancel out for this toy model. Given that these two bands originate from chiral p orbitals with opposite chirality [23], by constructing a junction between a two-dimensional system with asymmetric valleys and the twisted-bilayer graphene, it is possible to achieve a chirality-sensitive tunneling measurement to observe the modulation by one band. On the other hand, we also show in detail in the Supplemental Material [25] that there are other model systems with nonzero local density of states modulations.

Conclusion.—In summary, we derived the semiclassical equations of motion for superconducting quasiparticle wave packets and identified various Berry curvature contributions in momentum space, real space, and phase space. We demonstrated the power of the theory with examples such as the density of states modulation and the thermal Hall transport and applied the theory to several model systems. Our theory opens up a new route to study rich Berry-phase effects on equilibrium and transport properties of superconducting quasiparticles. A subject of particular interest is the charge current [39,40]. As the charge current carried by bare mean-field quasiparticles is nonconserved [39], to make a conserved current entails an elaborate account of the condensate backflow [24]. Indeed, the idea and ingredients of our theory, such as the charge dipole and Berry curvature, have been shown recently to play a role in discussing a conserved charge current at equilibrium [41]. Besides, it is interesting to study effects due to higher moments of a quasiparticle wave packet, which may depend on its shape [42].

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[1] X.-L. Qi and S.-C. Zhang, Topological insulators and superconductors, Rev. Mod. Phys. **83**, 1057 (2011).
[2] A. M. Black-Schaffer and C. Honerkamp, Chiral d-wave superconductivity in doped graphene, J. Phys. Condens. Matter **26**, 423201 (2014).
[3] M. Sato and Y. Ando, Topological superconductors: A review, Rep. Prog. Phys. **80**, 076501 (2017).
[4] F. Liu, C.-C. Liu, K. Wu, F. Yang, and Y. Yao, $d + id'$ Chiral Superconductivity in Bilayer Silicene, Phys. Rev. Lett. **111**, 066804 (2013).
[5] Z. Yang, S. Qin, Q. Zhang, C. Fang, and J. Hu, $\pi/2$-Josephson junction as a topological superconductor, Phys. Rev. B **98**, 104515 (2018).
[6] V. Cvetkovic and O. Vafek, Berry phases and the intrinsic thermal Hall effect in high-temperature cuprate superconductors, Nat. Commun. **6**, 6518 (2015).
[7] L. Liang, S. Peotta, A. Harju, and P. Törmä, Wave-packet dynamics of Bogoliubov quasiparticles: Quantum metric effects, Phys. Rev. B **96**, 064511 (2017).
[8] G. Sundaram and Q. Niu, Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and berry-phase effects, Phys. Rev. B **59**, 14915 (1999).
[9] D. Xiao, M.-C. Chang, and Q. Niu, Berry phase effects on electronic properties, Rev. Mod. Phys. **82**, 1959 (2010).
[10] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Anomalous Hall effect, Rev. Mod. Phys. **82**, 1539 (2010).
[11] D. Xiao, J. Shi, and Q. Niu, Berry Phase Correction to Electron Density of States in Solids, Phys. Rev. Lett. **95**, 137204 (2005).
[12] I. Sodemann and L. Fu, Quantum Nonlinear Hall Effect Induced by Berry Curvature Dipole in Time-Reversal Invariant Materials, Phys. Rev. Lett. **115**, 216806 (2015).

[13] J. E. Moore and J. Orenstein, Confinement-Induced Berry Phase and Helicity-Dependent Photocurrents, Phys. Rev. Lett. **105**, 026805 (2010).

[14] D. Xiao, G.-B. Liu, W. Feng, X. Xu, and W. Yao, Coupled Spin and Valley Physics in Monolayers of MoS_2 and Other Group-VI Dichalcogenides, Phys. Rev. Lett. **108**, 196802 (2012).

[15] F. Freimuth, R. Bamler, Y. Mokrousov, and A. Rosch, Phase-space berry phases in chiral magnets: Dzyaloshinskii-Moriya interaction and the charge of skyrmions, Phys. Rev. B **88**, 214409 (2013).

[16] L. Dong, C. Xiao, B. Xiong, and Q. Niu, Berry Phase Effects in Dipole Density and the Mott Relation, Phys. Rev. Lett. **124**, 066601 (2020).

[17] N. R. Cooper, B. I. Halperin, and I. M. Ruzin, Thermoelectric response of an interacting two-dimensional electron gas in a quantizing magnetic field, Phys. Rev. B **55**, 2344 (1997).

[18] T. Qin, Q. Niu, and J. Shi, Energy Magnetization and the Thermal Hall Effect, Phys. Rev. Lett. **107**, 236601 (2011).

[19] K. Nomura, S. Ryu, A. Furusaki, and N. Nagaosa, Cross-Correlated Responses of Topological Superconductors and Superfluids, Phys. Rev. Lett. **108**, 026802 (2012).

[20] H. Sumiyoshi and S. Fujimoto, Quantum thermal Hall effect in a time-reversal-symmetry-broken topological superconductor in two dimensions: Approach from bulk calculations, J. Phys. Soc. Jpn. **82**, 023602 (2013).

[21] T. Senthil, J. B. Marston, and M. P. A. Fisher, Spin quantum Hall effect in unconventional superconductors, Phys. Rev. B **60**, 4245 (1999).

[22] N. Read and D. Green, Paired states of fermions in two dimensions with breaking of parity and time-reversal symmetries and the fractional quantum Hall effect, Phys. Rev. B **61**, 10267 (2000).

[23] N. F. Q. Yuan and L. Fu, Model for the metal-insulator transition in graphene superlattices and beyond, Phys. Rev. B **98**, 045103 (2018).

[24] S. A. Parameswaran, S. A. Kivelson, R. Shankar, S. L. Sondhi, and B. Z. Spivak, Microscopic Model of Quasiparticle Wave Packets in Superfluids, Superconductors, and Paired Hall States, Phys. Rev. Lett. **109**, 237004 (2012).

[25] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.126.187001 for the detailed derivation of the wave packet theory of semiclassical superconducting quasiparticle dynamics, derivation for the thermal Hall conductivity based on wave packet theory, details of the toy model for the twisted-bilayer graphene and the change of momentum-space density of states with the direction of supercurrent, and modulated local density of states in $d + id$ models of square lattice and of single-layer honeycomb lattice.

[26] S. A. Kivelson and D. S. Rokhsar, Bogoliubov quasiparticles, spinons, and spin-charge decoupling in superconductors, Phys. Rev. B **41**, 11693 (1990).

[27] S. Murakami and N. Nagaosa, Berry Phase in Magnetic Superconductors, Phys. Rev. Lett. **90**, 057002 (2003).

[28] C. Zhang, A. M. Dudarev, and Q. Niu, Berry Phase Effects on the Dynamics of Quasiparticles in a Superfluid with a Vortex, Phys. Rev. Lett. **97**, 040401 (2006).

[29] O. Fischer, M. Kugler, I. Maggio-Aprile, C. Berthod, and C. Renner, Scanning tunneling spectroscopy of high-temperature superconductors, Rev. Mod. Phys. **79**, 353 (2007).

[30] J. Jang, H. M. Yoo, L. N. Pfeiffer, K. W. West, K. W. Baldwin, and R. C. Ashoori, Full momentum- and energy-resolved spectral function of a 2d electronic system, Science **358**, 901 (2017).

[31] C. Xiao and Q. Niu, Unified bulk semiclassical theory for intrinsic thermal transport and magnetization currents, Phys. Rev. B **101**, 235430 (2020).

[32] This expression neglects the finite size of the wave packet, but is reasonable when one aims only at obtaining the transport current, because the neglected is a part of the magnetization current arising from the self-rotation of the wave packet. See Ref. [31] for details.

[33] L. Balents, C. R. Dean, D. K. Efetov, and A. F. Young, Superconductivity and strong correlations in Moiré flat bands, Nat. Phys. **16**, 725 (2020).

[34] H. Guo, X. Zhu, S. Feng, and R. T. Scalettar, Pairing symmetry of interacting fermions on a twisted bilayer graphene superlattice, Phys. Rev. B **97**, 235453 (2018).

[35] C.-C. Liu, L.-D. Zhang, W.-Q. Chen, and F. Yang, Chiral Spin Density Wave and $d + id$ Superconductivity in the Magic-Angle-Twisted Bilayer Graphene, Phys. Rev. Lett. **121**, 217001 (2018).

[36] W. Chen, Y. Chu, T. Huang, and T. Ma, Metal-insulator transition and dominant $d + id$ pairing symmetry in twisted bilayer graphene, Phys. Rev. B **101**, 155413 (2020).

[37] Y. Jiang, D.-X. Yao, E. W. Carlson, H.-D. Chen, and J. P. Hu, Andreev conductance in the $d + id'$-wave superconducting states of graphene, Phys. Rev. B **77**, 235420 (2008).

[38] R. Nandkishore, L. S. Levitov, and A. V. Chubukov, Chiral superconductivity from repulsive interactions in doped graphene, Nat. Phys. **8**, 158 (2012).

[39] Y. Nambu, Quasi-particles and gauge invariance in the theory of superconductivity, Phys. Rev. **117**, 648 (1960).

[40] A. Aronov, Y. Gal̑perin, V. Gurevich, and V. Kozub, The Boltzmann-equation description of transport in superconductors, Adv. Phys. **30**, 539 (1981).

[41] C. Xiao and Q. Niu, Conserved current of nonconserved quantities, arXiv:2009.12058.

[42] A. R. Bishop, P. S. Lomdahl, J. R. Schrieffer, and S. A. Trugman, Pairing-Bag Excitations in Small-Coherence-Length Superconductors, Phys. Rev. Lett. **61**, 2709 (1988).