Beroy phases and the intrinsic thermal Hall effect in high-temperature cuprate superconductors

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Bogolyubov quasiparticles move in a practically uniform magnetic field in the vortex state of high-temperature cuprate superconductors. When set in motion by an externally applied heat current, the quasiparticles' trajectories may bend, causing a temperature gradient perpendicular to the heat current and the applied magnetic field, resulting in the thermal Hall effect. Here we relate this effect to the Berry curvature of quasiparticle magnetic sub-bands, and calculate the dependence of the intrinsic thermal Hall conductivity on superconductor's temperature, magnetic field and the amplitude of the d-wave pairing. The intrinsic contribution to thermal Hall conductivity displays a rapid onset with increasing temperature, which compares favourably with existing experiments at high magnetic field on the highest purity samples. Because such temperature onset is related to the pairing amplitude, our finding may help to settle a much-debated question of the bulk value of the pairing strength in cuprate superconductors in magnetic field.
ow-energy excitations of a superconductor, the Bogolyubov quasiparticles (QPs), are quantum mechanically coherent superpositions of an electron and its absence, the hole. Therefore, QPs do not carry a fixed electrical charge. In the vortex state of extreme type-II superconductors, such as high transition temperature cuprates, the externally applied magnetic field $H$ penetrates the sample in the form of flux tubes, whose width is set by the material-specific parameter named penetration depth. For essentially the entire range of $H$ fields applied in a typical experiment, the cuprates’ penetration depth is much larger than the inter-vortex separation, the latter being set by the material-specific parameter named penetration depth. For experiment, the cuprates’ penetration depth is much larger than the inter-vortex separation, the latter being set by the material-specific parameter named penetration depth.

In this work, we present results of an extensive numerical calculation providing detailed $T$, $H$ and $\Delta$ dependence of the intrinsic contribution to $\kappa_{xy}$. Because $\kappa_{xy}$ is perpendicular to the thermal Hall gradient, the thermal Hall effect does not contribute to entropy production, $dS/dt = -\int d\langle \nabla T / T^2 \rangle \cdot \mathbf{J}(r)$. Therefore, there is an intrinsic contribution to the corresponding non-dissipative transport coefficient, independent of the details of the relaxation processes, which return the system to equilibrium. Such an intrinsic contribution to $\kappa_{xy}$, which we expect to dominate in the clean limit, is a direct consequence of the QP wavefunctions acquiring a non-trivial Berry curvature upon adiabatic changes of the vortex crystal momentum. We thus calculate $\kappa_{xy}$ using the tight-binding regularization for a $d$-wave superconductor—whose $H = 0$ pairing function is $2\Delta (\cos k_x - \cos k_y)$—and for a variety of $H$ values and vortex lattice geometries. Our main finding is that, when properly rescaled by its value in the normal state, which is also assumed to be in the clean limit, $\kappa_{xy}$ does not depend on the structure of the vortex lattice or $H$, assuming of course that $H$ is not large enough to destroy superconductivity. When $T$ is reported in units of $\Delta$, here varied independently of $H$, the important dimensionless quantity determining the $T$ dependence of $\kappa_{xy}$ is the anisotropy of the dispersion near the gap node, $\zeta_D$, and even here the dependence is weak. The scaling collapse thus attained clearly displays the rapid temperature onset at a small fraction of $\Delta$ followed by an almost linear $T$ dependence. This finding may establish measurements of $\kappa_{xy}$ as a means to obtain bulk spectroscopic information about high-temperature superconductors, and provide an avenue for resolving the pressing question regarding the overall strength of Cooper pairing in high magnetic field.

Results

The QP density of states and the $\kappa_{xy}$ scaling. We motivate the description of the details of the model and its analysis by first showing the main results, which were obtained using the Hamiltonian in equation (1). Figure 1 shows the QP density of states per area at energy $\epsilon$, $N(\epsilon)$, integrated from $\epsilon = 0$ up to $\epsilon = E$. The reason for plotting the integrated density of states (IDOSs), as opposed to $N(\epsilon)$, is that the QP spectrum is described by a large number of magnetic sub-bands whose number grows with decreasing magnetic field as $1/H$. Being in two space dimensions, each one of the sub-bands harbours at least one van Hove singularity with a logarithmic divergence of $N(\epsilon)$. Thus, plotting the contribution from each sub-band to $N(\epsilon)$ leads to large variations of the resulting $\epsilon$ dependence, obscuring the main physical effect. On the other hand, the IDOS simply counts the number of eigenstates between 0 and $E$, which is smoother, and lends itself more readily to physical insight. Indeed, the $H$-induced increase in the number of states at low energy is clearly seen on the scaling plot marked by various symbols in Fig. 1, when compared with the result at $H = 0$ shown as the solid black line. At $H = 0$, $N(\epsilon) \sim \epsilon$ at small $\epsilon$, and therefore $\int_0^\epsilon N(\epsilon) d\epsilon \sim E^2$; this can be graphed on the scaling plot assuming increasingly small $E$ and increasingly large $\ell_H$, such that $E \ell_H$ is finite, because
only the quadratic term in the Taylor expansion of IDOS in $E$ survives in this limit. The low-energy portion of the spectrum is thus seen to obey Simon and Lee scaling\(^{4}\) to a very good approximation. Furthermore, Volovik’s result\(^{2}\), $N(\varepsilon \to 0) \propto \sqrt{H}$, appears as the linear dependence of the scaled IDOS marked by the red line. The key point here is that, on average, the external magnetic field increases the number of QP states at low energy. The next question that we address is their contribution to the intrinsic $\kappa_{xy}$.

The principal result of this paper is shown in Fig. 2. $\kappa_{xy}$ was calculated for several values of $H$ and vortex lattice geometries as indicated in the legend by the values of the dimensions of the magnetic unit cell $L_x \times L_y$, given in the units of the underlying tight-binding lattice spacing, $a$. We made sure that the values of $L_x$ and $L_y$ were chosen to be sufficiently large so that the low-energy IDOS collapses on the scaling curve shown in the Fig. 1. Within our model, the normal state value, $\kappa_{xy}(T, 0, H)$, is also computed in the clean limit: in the low $T$ regime where $T \ll H$, $\kappa_{xy}(H) \propto 1/H$. The plot of the ratio $\kappa_{xy}(T, H)/\kappa_{xy}(0, H)$ versus $T/H$ is shown by the solid lines in each panel for six different values of the nodal dispersion anisotropy $\Delta_0 = v_F \sqrt{\Lambda}$ indicated next to each solid line. In addition, for fixed $\Delta_0 = 7.1$, the $\kappa_{xy}$ ratio is shown using various symbols for different values of $H$ and vortex lattice geometries, as indicated by the three columns in the legend. The quality of the collapse for $\Delta_0 = 7.1$ is representative of the scaling at different values of $\Delta_0$, which we do not show to avoid clutter. The $\kappa_{xy}$ ratio is seen to collapse quite well onto a single curve for each of the nodal velocity anisotropy, $\Delta_0$, and to approach $1$ with increasing $k_B T/H$, independent of the vortex lattice geometry; here $k_B$ is the Boltzmann constant. Moreover, the rapid $T$ onset occurs at the value of $T$ set predominantly by (a fraction of) the value of $\Lambda$, with a weak residual dependence on $\Delta_0$. This is followed by the regime of approximately $T$ linear dependence with a negative extrapolated vertical intercept. These theoretical results indicate that experimental measurements of the onset $T$ for fixed values of $H$ can therefore be translated to the $H$ dependence of the maximum magnitude of the $d$-wave Cooper pair amplitude. This would provide highly desirable information on the suppression (or lack thereof) of the superconducting order parameter amplitude by the external magnetic field.

The model Hamiltonian. We work on a two-dimensional square lattice of spacing $a$—that we set to unity—and $H$ perpendicular to it. Our tight-binding Hamiltonian describing excitations of the $d$-wave superconductor in the vortex state is

$$H = \sum_{\mathbf{r}} \left( \sum_{j=1}^{N_{\text{el}}} \epsilon_j c_{\mathbf{r}+\mathbf{j}}^\dagger c_{\mathbf{r}+\mathbf{j}} + \Delta_{\mathbf{r}+\mathbf{\delta}} (c_{\mathbf{r}+\mathbf{\delta}+\mathbf{\alpha}}^\dagger c_{\mathbf{r}+\mathbf{\alpha}} + h.c.) - \mu c_{\mathbf{r}+\mathbf{\alpha}}^\dagger c_{\mathbf{r}+\mathbf{\alpha}} \right).$$

(1)

This model has been discussed extensively elsewhere\(^{5,11,15}\); $c_{\mathbf{r}+\mathbf{\alpha}}$ is the electron annihilation operator, the sum over the spin projection $\sigma = \uparrow$ or $\downarrow$ in the first and the last terms is implicit, $\epsilon_j = -t \pm \Delta$ and $c_{\mathbf{r}+\mathbf{\delta}}$ stands for Hermitian conjugation. The chemical potential and the Zeeman coupling enter via $\mu = \mu \pm \hbar \Delta$. The magnetic flux $\Phi$ through an elementary plaquette enters the Peierls factors as $A_{\mathbf{r}+\mathbf{\delta}} = -\pi \delta \Phi/\phi_0$, and $A_{\mathbf{r}+\mathbf{\delta}} = \pi \pi \Phi/\phi_0$, where $\phi_0 = hc/\varepsilon_0$. The ansatz for the pairing term is $\Delta_{\mathbf{r}+\mathbf{\delta}} = \Delta e^{i\theta(r)} \exp \left( \frac{\pi}{2} \int_{\mathbf{r}+\mathbf{\delta}} d\mathbf{\theta} \right)$, where the d-wave amplitude $\Delta_0 = \Delta_0$ and the line integral is along the nearest neighbour link. Vertex positions, $r_i$, residing in the centres of (some of) the elementary plaquettes, enter the pairing term through $\theta(r)$, which is chosen to be the solution of the (continuum) London’s equations $\nabla \times \nabla \theta(r) = 2\pi \sum_{i} \delta(r - r_i)$, $\nabla \cdot \nabla \theta(r) = 0$. The closed form solution for $\theta(r)$ can be found in the Methods section. Vortices are arranged within the magnetic
in metals, any intrinsic \( \kappa_{xy} \) is therefore driven by Berry phase mechanisms.

The Heisenberg equations of motion, \( i\hbar \frac{\partial}{\partial t} \psi_{\mathbf{k}, \sigma}(\mathbf{k}) = [H(\mathbf{k})] \psi_{\mathbf{k}, \sigma}(\mathbf{k}) \), define the single particle Bloch Hamiltonian, \( H(\mathbf{k}) \), whose discrete eigenvalues, \( E(\mathbf{k}, \sigma) \), and eigenstates, \( | \mathbf{k}, \sigma \rangle \), are labelled by a discrete magnetic sub-band index, \( m \).

For \( H \neq 0 \) and \( \Delta = 0 \), the model in equation (1) reduces to the well-known square lattice Hofstadter ‘butterfly’ problem,\(^{17} \) with flux per plaquette \( \Phi/\phi_0 = L_{H}^{-2} \), where \( L_{H} \) is the size of the lattice. Momentarily ignoring the twofold spin degeneracy, the Chern integers \( \nu_{\mathbf{k}} \), determining the electrical Hall conductivity \( \sigma_{xy}^{(c)} = \nu_{\mathbf{k}} \), are found to be \( \nu_{\mathbf{k}} = \mathbb{D} \cdot \mathbf{k} \), associated with \( M \) filled sub-bands, obey the Diophantine equation\(^{18,19} \)

\[ M = s \frac{L_{H}}{2} + b, \]

where \( s \) is an integer and where \( b \) is subject to the restriction \( |b| \leq L_{H}^{-2}/2 \). Solving for \( b \), we find that\(^{19} \) (for even \( L_{H} \)) the lowest, and each of the highest, \( L_{H}^{-2}/2 \) sub-bands carry the Chern number \( b - b_{1} = +1 \). In addition, there is a pair of touching sub-bands straddling the midline of the energy spectrum, which carries the (large) Chern number 2, \( b - b_{1} = -1 \), equally divided between the two anomalous sub-bands.\(^{19} \) Near the \( H = 0 \) band extrema, the (Landau) energy gaps between the magnetic sub-bands are \( \hbar \omega_{L} = 4\gamma L_{H}^{2} \), because there the \( H = 0 \) energy dispersion is parabolic.

For \( H = 0 \) and \( \Delta \neq 0 \), the \( \text{QP} \) spectrum of \( H \) is

\[ E(\mathbf{k}) = \pm \sqrt{\epsilon(\mathbf{k})^2 + \Delta(\mathbf{k})^2}, \]

with \( \epsilon(\mathbf{k}) = -2t(\cos k_{x} + \cos k_{y}) - \mu \) and \( \Delta(\mathbf{k}) = 2\Delta(\cos k_{x} - \cos k_{y}) \). There are four gapless Dirac points in the first Brillouin zone, with the velocity anisotropy \( v_{y} = v_{x} = t/\Delta \), which dominate the low-temperature thermodynamics.

Thus, the pairing term in \( H \) mixes \( \sim 4\Delta(\mathbf{k})^{2}/(\pi \omega_{L}) \) sub-bands near the Fermi level. In the physically relevant situation, each of these magnetic sub-bands mixed by \( \Delta \) carries a unit Chern number, thus resembling Landau levels of a continuum problem. Moreover, the number of such occupied sub-bands should be large compared with \( L_{H}^{2}/(\pi \omega_{L}) \). Therefore,
we choose to set \( \mu = 2t \), corresponding to \( \approx 0.37 \) holes per site. With this choice the pairing term does not mix the anomalous band with the large Chern number, while at the same time the pairing term remains small compared with the Fermi energy.

We now turn to \( H \neq 0 \) and \( \Delta \neq 0 \). In the semiclassical approximation of Volovik\(^1\), the spatially varying phase \( \theta(r) \) induces a finite zero-energy density of states, \( N(\varepsilon) = 0 \), which scales as \( \sqrt{H} \). More generally, the scaling expected\(^4,8\) from the approximate Dirac model is \( N(\varepsilon) = \frac{1}{\beta_{\text{vol}}/\sqrt{2}} F'(\varepsilon/\beta_{\text{vol}}/2\pi) \).

As shown in Fig. 1, up to small variations\(^6\), we indeed recover this scaling in our model when \( L_x^2/(\pi^2) \gg 1 \). The IDOSs per area, per spin, per layer is seen to follow the scaling \( \int_0^L N(\varepsilon)d\varepsilon = \sqrt{\pi^2/\beta_{\text{vol}}} F(x) \), where \( F(x) \approx bx \) for \( x \ll 1 \) with \( b \approx 0.9 \) and \( F(x) \approx x^2/\pi \) for \( x \gg 1 \), regardless of the shape of the vortex lattice, as long as \( \Delta_D \gg 3 \). This implies that the low-\( T \) specific heat per mol of formula unit is \( C/T = 0.33 \cdot n_{\text{layers}} \cdot \text{Area} [\text{nm}^2] \cdot \sqrt{\pi^2/\beta_{\text{vol}}} \text{ mJ}^{-1} \text{ K}^{-2} \). For example, in YBa\(_2\)Cu\(_3\)O\(_7-\delta\) \( n_{\text{layers}} = 2 \) because there are two CuO\(_2\) layers per unit cell whose Area\([\text{nm}^2]\) \( \approx 0.149 \).

Intrinsic contribution to \( \kappa_{xy} \). It has long been known that for \( H \neq 0 \) the thermal transport coefficients cannot be calculated using the Kubo formula alone\(^10,20–23\). Rather, \( \kappa_{xy} \) is given by\(^10,22\)

\[
\kappa_{xy} = \frac{1}{hT} \int_{-\infty}^{\infty} d\xi \frac{\xi^2}{2} \left( -\frac{\partial f(\xi)}{\partial \xi} \right) \tilde{\sigma}(\xi),
\]

where \( f(\xi) = 1/(e^{\xi/k_BT} + 1) \) and

\[
\tilde{\sigma}(\xi) = \frac{1}{i} \int \frac{d^2k}{4\pi^2} \sum_{E_m(\xi) < E_E(\xi)} \frac{\langle mk | \frac{\partial E_m(\xi)}{\partial nk} | nk \rangle}{(E_m(k) - E_E(k))^2}.
\]

The double sum over \( m \) and \( n \) is to be performed subject to the stated constraint on the eigenenergy. It is well known that \( \tilde{\sigma}(\xi) \approx \sum_m \Omega_m(\xi) \), where \( \Omega_m(\xi) \) is the integral over the Berry curvature of the \( m \)th magnetic sub-band over the parts of the magnetic Brillouin zone, which are below the energy \( \xi \). If the QP sub-band is fully occupied then the integral over the Berry curvature is the first Chern number, which is to say, an integer\(^10,18\).

Our main result is shown in Fig. 2. The rapid onset of \( \kappa_{xy} \) with increasing \( T \) can be understood from the \( \xi \) dependence of \( \tilde{\sigma}(\xi) \) and the formula in equation (3). The quantity \( \tilde{\sigma}(\xi) \), shown in Fig. 3, has a simple physical interpretation: it is proportional to the QP contribution to the \( T = 0 \) spin Hall conductivity\(^10\) if all the QP sub-bands below the energy \( \xi \) are occupied. In addition, for \( \Delta = 0 \) it can be related to the usual electrical Hall conductivity due to, say, spin up electrons only, \( \sigma_{xy}^{(d)}(E_F) \) at the Fermi energy \( E_F \). Indeed, for \( \Delta = 0 \), \( \tilde{\sigma}(\xi) = \frac{1}{i} (\sigma_{xy}^{(d)}(\mu + \zeta) + \sigma_{xy}^{(d)}(\mu - \zeta)) \), where the first term corresponds to the contribution of the spin-up electrons and the second to the spin-down holes moving in the opposite magnetic field. We see that for \( \Delta = 0 \), the quantity \( \zeta \) can be interpreted as a fictitious Zeeman energy splitting. Therefore, the loss of the total Chern number in the minority band is largely compensated by the gain in the majority band, and for \( \Delta = 0 \), \( \tilde{\sigma}(\xi) \) is essentially independent of \( \zeta \). For a range of \( \zeta \)'s near zero, its value is approximately \( 2n_l/h_2 \), that is to say the solution of the mentioned Diophantine equation determining the normal state electrical conductivity at \( \mu \) (see \( 1/2\pi = 0 \) curve in the Fig. 3 for small \( \zeta \)). This is expected, as an analogous formula to equation (3) holds in the normal state as well\(^22\), in which case it relates the electrical Hall conductivity to the thermal Hall conductivity.

For \( \Delta \neq 0 \), the \( \tilde{\sigma}(\xi) \) still reaches the value \( \approx 2n_l \), which is of order \( L_x^2 \), when \( \xi \gg \Delta \). This happens because for \( \xi \) large compared with \( \Delta \), the contribution to the Chern numbers comes predominantly from the QP bands, which are weakly affected by the pairing term. On the other hand, when \( \xi \ll \Delta \), then \( \sigma_{xy}(\xi) \) becomes small, non-universal and its value oscillates around zero. This trend is displayed in Fig. 3, where the \( \xi \) dependence of \( \sigma_{xy}(\xi) \), rescaled by its value in the normal state and \( \xi = 0 \), is shown for various values of \( 1/\Delta_D = \Delta/T \). Such a precipitous drop near \( \xi = 0 \) is a consequence of the QP states near zero energy being an almost equal superposition of the electron and a hole, riding the sub-bands of the Berry curvature. It is fully consistent with the previous result\(^11\) where the value of \( \sigma_{xy}(0) \), small compared with \( L_x^2 \), was obtained near \( \mu = 0 \). Convolving such \( \xi \) dependence of \( \sigma_{xy}(\xi) \) with the thermal factor in equation (3) at low \( T \) results in a vanishingly small \( \kappa_{xy} \). As the temperature increases, the thermal function broadens, and the rapid increase of \( \sigma_{xy}(\xi) \) with increasing \( \xi \) is mirrored by the rapid increase of \( \kappa_{xy} \) with increasing \( T \). We restrict \( k_B T \ll \xi \) in Fig. 2, guaranteeing that in the normal state (\( \Delta = 0 \)), \( \kappa_{xy} \) is linear in \( T \).

The \( \mathbf{H} \) dependence follows readily from the above discussion as well. Since for \( \xi \gg \Delta \), \( \tilde{\sigma}(\xi) \sim L_x^2 \sim 1/\mathbf{H} \), we find that the \( \mathbf{H} \) dependence of \( \kappa_{xy}(\Delta = 0) \) is determined by the \( \mathbf{H} \) dependence of \( \kappa_{xy}(\Delta = 0) \sim 1/\mathbf{H} \). We also find the dependence of \( \kappa_{xy}(\Delta = 0) \) on the Zeeman coupling, \( h_2 \), to be barely observable when \( h_2 \ll \Delta \). This is due to the fact that, with the Zeeman term, we convolve the average of \( \tilde{\sigma}(\xi + h_2) \) instead of \( \tilde{\sigma}(\xi) \). For any \( h_2 << \Delta \), the main effect of the averaging is to smear the fluctuations in \( \tilde{\sigma}(\xi) \), whereas the overall shape of the curve remains essentially unchanged. Similarly, we find negligible dependence on the size of the vortex core as long as it is small compared with the inter-vortex separation.

**Discussion**

The importance and the novelty of our results stem from the role that the overall d-wave pairing strength, \( \Delta \), plays in determining...
the temperature scale at which $\kappa_{xy}$ rapidly increases from a negligibly small value at low $T$. It may therefore serve as an important probe of the cuprate superconductors, and perhaps other materials as well, and provide a means of measuring $\Delta$ via a bulk transport measurement. In the clean limit, this method could become very attractive as, unlike the specific heat, $\kappa_{xy}$ is not contaminated by other degrees, notably phonons which are electrically neutral and whose trajectories do not bend by the Lorentz force. Moreover, the measurement can be performed at a high magnetic field, which can be held constant, and the onset temperature measured by sweeping $T$. It would be very interesting to measure the $H$ dependence of the onset temperature starting from the small values of $H$ well inside the superconducting state all the way to (and past) the resistive field, $H_{tr}$, which marks the transition from the superconductor to a vacuum, and presently poorly understood, resistive low $T$ state of electronic matter. Is the onset temperature gradually suppressed by $H$, making it vanish in some smooth fashion at the $H_{tr}$, does it remain finite above $H_{tr}$, or does it collapse discontinuously? Experimental answers to these questions would provide important clues as to the nature of the resistive high field, low temperature, state.

**Methods**

**Determination of the phase field.** The closed form solution of London’s equations for the pairing phase field with the periodic arrangement of vortices is

$$ \theta(r) = \sum_{j=1}^{m} \text{arg} \left[ \varepsilon(z_j - r; \alpha') \right] + \frac{1}{4\pi} (z - z_j)^{-1} \left[ (z - z_j)^{-1} - (z' - z_j)^{-1} \right] + \frac{1}{2\pi} \left( z_j - z_j' \right)^{-1}. \quad (5) $$

Here, using the complex notation, $z = x + iy$, and the summation over $j$ accounts for the position of the vortices within the magnetic unit cell $z_j = x_j + iy_j$ of which there are two for the configurations shown in the legend of Fig. 2. Therefore, in our case $n_0 = 2$. $(z_j - z_j', \alpha')$ is the Weierstrass $\varepsilon$ function with periods $\omega_L$ and $\omega_F$, respectively. Constants $\gamma$ and $\delta$ are determined by the boundary conditions. In order to ensure that the superfluid velocity $\mathbf{v}_s$, the Hamiltonian in equation (2) possesses symmetries, which consist of either point group operations alone or point group operations combined with the time reversal and/or gauge transformations. These symmetries are reflected in the solution for the phase field, equation (5), and thereby in the hopping amplitudes. From there on one can show that only certain single particle Hamiltonians $\mathcal{H}(k)$ and $\mathcal{H}(k)$, defined below the equation (2), are related by an unitary or an anti-unitary operation, which $\mathbf{k}$ and $\mathbf{k}'$ are symmetry related. It is not necessary to take advantage of these symmetries, but the numerical calculation is faster by about an order of magnitude if this is done.

**Numerical evaluation of $\delta_{xy}(\mathbf{k})$.** The expression in equation (4) can be written as

$$ F_{\mathbf{k}}(E) = \frac{1}{2\pi i} \sum_{E_m(E_0) < E < E_n(E_0)} \frac{V^{\text{vm}}(E) V^{\text{vm}}(E) - V^{\text{vm}}(E) V^{\text{vm}}(E)}{(E_m(E_0) - E_n(E_0))^2}. \quad (6) $$

Thus, we are left with only 2$\mathcal{L}_2$ - 1 terms to sum over. Therefore, if we build the lookup table by recursively adding the result of equation (7) for $F_{\mathbf{k}}(E)$, we obtain $F_{\mathbf{k}}(E + \hbar \omega)$, remembering that $F_{\mathbf{k}}(E) = 0$ for $E < E_g$, so we sum only $O(\mathcal{L}_2)$ terms for each lookup table entry instead of $O(\mathcal{L}_1^2)$. This leads to a further computational time by another $O(\mathcal{L}_1)$ factor. The computation of $\delta_{xy}^\text{vm}(\mathbf{k})$ can be further optimized by noticing that, once $\mathbf{k}$ is fixed, we can find $\frac{1}{\sqrt{2\pi}} v_{\mathbf{k}'}(\mathbf{k})$, store the two vectors for $\mu = x, y$, and use them to compute $\delta_{\mu\nu}^\text{vm}(\mathbf{k})$ and $V^{\text{vm}}(\mathbf{k})$ faster.

Overall, we find that the computational complexity of the lookup table creation is $O(m^2)$, whereas with these improvements. From the expression $\delta_{xy}(\mathbf{k}) = \frac{1}{\sqrt{2\pi}} \int d\mathbf{k} F_{\mathbf{k}}(\mathbf{k})$, we see that $\delta_{xy}(\mathbf{k})$ can be approximated and calculated by expressing it as a Riemann sum. $\delta_{xy}(\mathbf{k}) = \frac{1}{\sqrt{2\pi}} \sum_{n=1}^{N} \frac{1}{N} \int d\mathbf{k} F_{\mathbf{k}}(\mathbf{k})$ where the integration domain, in our case the magnetic BZ (or fraction thereof if symmetries are used), is partitioned into $s$ non-overlapping patches, each with area $A_s$. For each patch, the Berry curvature is calculated at some point $\mathbf{k}_0$ within that patch. We partitioned the integration domain using an adaptive mesh integration method. This method starts with a coarse mesh of $\mathbf{k}$ points and then refines the mesh by increasing the density of $\mathbf{k}$ points in the patches where the absolute errors are the largest. In this manner, the overall error is minimized using the fewest number, $s$, of $k$ points where $\delta_{xy}(\mathbf{k})$ is calculated.

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**Author contributions**

V.C. and O.V. jointly identified the problem, performed the analysis and wrote the paper.

**Additional information**

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