Geometric phases of *d*-wave vortices in a model of lattice fermions

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We study the local and topological features of Berry phases associated with the adiabatic transport of vortices in a *d*-wave superconductor of lattice fermions. At half filling, where the local Berry curvature must vanish due to symmetries, the phase associated with the exchange of two vortices is found to vanish as well, implying that vortices behave as bosons. Away from half filling, and in the limit where the magnetic length is large compared to the lattice constant, the local Berry curvature gives rise to an intricate flux pattern within the large magnetic unit cell. This renders the Berry phase associated with an exchange of two vortices highly path dependent. However, it is shown that "statistical" fluxes attached to the vortex positions are still absent. Despite the complicated profile of the Berry curvature away from half filling, we show that the average flux density associated with this curvature is tied to the average particle density. This is familiar from dual theories of bosonic systems, even though in the present case, the underlying particles are fermions.

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Introduction. A phenomenology based on a BCS-like pairing state with *d*-wave symmetry has led to considerable success in understanding the properties of quasiparticles in high-T_c superconducting cuprates. This includes the mixed state of these systems, where a magnetic field $H_{c_1} < H < H_{c_2}$ is applied and leads to the presence of an Abrikosov vortex lattice. Effective models[1–15] have been developed that describe the dynamics of the quasiparticles under the simultaneous influence of magnetic field, the supercurrent flow due to the vortices, and in some cases the underlying microscopic lattice. The vortices of the mixed state are usually assumed to be static, i.e., frozen into the Abrikosov lattice. However, it has been argued[16] that both as a result of the small coherence length ξ, and possibly the proximity to an insulating state, fluctuations of vortices may play a fundamental role. Moreover, at sufficiently high magnetic fields below H_{c_2}, it has been predicted that thermal and/or quantum fluctuations may melt the vortex lattice or glass, leading to a "vortex liquid" regime.[17] For all these reasons, it is desirable to construct effective theories that include the vortices as fundamental dynamical degrees of freedom.[18] Such a construction is readily available in systems where the constituent particles are bosons, through the well-known Kramers-Wannier duality.[19] In Fermi systems, however, the vortex degrees of freedom only exist as dual partners of bosonic Cooper pairs that are themselves emergent particles. This arguably complicates the task of passing directly from a microscopic description in terms of electrons to an effective theory in terms of vortices, requiring more *ad hoc* assumptions. Such effective theories have been previously discussed in a continuum formalism.[16] In this Rapid Communication, we aim to establish some key parameters of these theories in a microscopic lattice model. This is similar in spirit, but physically different, from earlier considerations for bosons in the absence of a lattice.[20] These defining parameters include the quantum curvature felt by the vortices in the condensate, that is, the effective magnetic field experienced by them, and their mutual statistics. Specifically in the *d*-wave pairing case, where the continuum description of vortices is somewhat plagued by subtleties concerning self-adjoint extensions,[8] our

microscopic starting point also serves as lattice regularization,[4] which allows for a controlled study of the desired universal properties.

Model description. We will study the Berry phases[21] of vortices in the *BCS-Hofstadter* model, which has been used previously as a microscopic description of the mixed state in the cuprates:[5]

$$H = \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \left[-t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma'} + \frac{\Delta_{\mathbf{r}\mathbf{r}'}}{2} (c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}'\uparrow}^\dagger + c_{\mathbf{r}'\downarrow}^\dagger c_{\mathbf{r}\uparrow}^\dagger) + \text{H.c.} \right] - \mu N. \tag{1}$$

In the above, the sum $\langle \mathbf{r}\mathbf{r}' \rangle$ is over the nearest neighbors, and the hopping terms are just those of the Hofstadter model, to be described below. The corresponding uniform magnetic flux through the plaquettes of the lattice mirrors the fact that the penetration depth is much larger than the coherence length, as befits a type II superconductor. Assuming symmetric gauge $\mathbf{A}(\mathbf{r}) = (-y/2, x/2)\Phi$, where Φ the magnetic flux per plaquette, the hopping amplitude assumes the form

$$t_{\mathbf{r}\mathbf{r}'} = t \, e^{-i \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{A} \cdot d\mathbf{l}}, \tag{2}$$

where $\mathbf{r}$ refers to the discrete sites of the lattice. The *d*-wave paring term is defined as

$$\Delta_{\mathbf{r}\mathbf{r}'} = \eta_{\mathbf{r}-\mathbf{r}'} \Delta_{0,\mathbf{r}\mathbf{r}'} e^{i\theta_{\mathbf{r}\mathbf{r}'}}, \tag{3}$$

$$\eta_{\mathbf{r}-\mathbf{r}'} = +/- \quad \text{if } (\mathbf{r} - \mathbf{r}') \parallel \hat{\mathbf{x}}/\hat{\mathbf{y}}. \tag{4}$$

Here, $\eta_{\mathbf{r}-\mathbf{r}'}$ encodes the *d*-wave symmetry. $\Delta_{0,\mathbf{r}\mathbf{r}'}$ is essentially constant, except for a suppression of amplitude near the vortex core. We follow Ref. 6 in defining the pairing phase factor $e^{\theta_{\mathbf{r}\mathbf{r}'}}$ via

$$e^{i\theta_{\mathbf{r}\mathbf{r}'}} \equiv \frac{e^{i\phi(\mathbf{r})} + e^{i\phi(\mathbf{r}')}}{|e^{i\phi(\mathbf{r})} + e^{i\phi(\mathbf{r}')}|}, \tag{5}$$

i.e., as a link-centered average of a field $\phi(r)$ that satisfies the following continuum equations,

$$\nabla \times \nabla \phi(\mathbf{r}) = 2\pi \hat{z} \sum_i \delta(\mathbf{r} - \mathbf{r}_i), \qquad (6a)$$

$$\nabla \cdot \nabla \phi(\mathbf{r}) = \mathbf{0}, \qquad (6b)$$

where the $\mathbf{r}_i$ denote the vortex positions, which can take on continuous values. The total number of vortices n_V is equal to the number of half flux-quanta Φ_0, $l_x l_y \Phi = n_V \Phi_0$, where $\Phi_0 = \pi$ in natural units, and l_x, l_y are the number of unit cells in the x and y direction, respectively. Equation (6) can be solved[9] via

$$\phi(\mathbf{r}) = \sum_i \{\arg[\sigma(z - z_i, \omega, \omega')]$$
$$+ 2\gamma(x - x_i)(y - y_i) + \mathbf{v}_0 \cdot \mathbf{r}\}, \qquad (7)$$

where $\sigma(z, \omega, \omega')$ is the Weierstrass sigma function with half periods $\omega = l_x/2$, $\omega' = i l_y/2$, $z = x + iy$, and the sum is over vortex positions. Integration constants $\mathbf{v}_0 = 2\sum_i \mathbf{A}(\mathbf{r}_i)$ and $\gamma = \frac{\pi}{2 l_x l_y} - \frac{\eta}{l_x}$ have been chosen such that the superfluid velocity $\mathbf{v}_S = \nabla\phi/2 - \mathbf{A}$ satisfies periodic boundary conditions, and averages to zero over the magnetic unit cell,[6] and $\eta = \zeta(\omega)$ is pure imaginary, with ζ the Weierstrass zeta function.

The pairing phase factor $e^{i\theta_{\mathbf{rr}'}}$ in Eq. (5) is ill defined when the denominator goes to 0. This is unacceptable since we mean to continuously change vortex coordinates in the following. To remove this singularity, we define $\Delta_{0,\mathbf{rr}'}$ as

$$\Delta_{0,\mathbf{rr}'} \equiv \Delta_0 \left[1 - \exp\left(-\frac{|e^{i\phi(\mathbf{r})} + e^{i\phi(\mathbf{r}')}|}{\xi}\right)\right], \qquad (8)$$

where Δ_0 and ξ are constant parameters. This leads to a suppression of pairing amplitude on links near the vortex, hence ξ may be thought of as a core radius.

We further impose periodic magnetic boundary conditions on our model as follows:

$$c_{\mathbf{r}} = T_x^{l_x} c_{\mathbf{r}} (T_x^\dagger)^{l_x} = T_y^{l_y} c_{\mathbf{r}} (T_y^\dagger)^{l_y}, \qquad (9)$$

$$T_{\mathbf{R}} c_{\mathbf{r}} T_{\mathbf{R}}^\dagger = c_{\mathbf{r}+\mathbf{R}} e^{i \int_{\mathbf{r}}^{\mathbf{r}+\mathbf{R}} \mathbf{A} \cdot d\mathbf{l} + i \mathbf{R} \times \mathbf{r} \Phi}. \qquad (10)$$

In the above, the magnetic translation operators T_x and T_y are defined by letting $\mathbf{R} = \hat{x}$ or $\hat{y}$. We note that with the boundary conditions (9) imposed on electron operators, the physics is also periodic in the vortex positions $\mathbf{r}_i$. That is, one may see that the formal replacements $\mathbf{r}_i \to \mathbf{r}_i + l_x\hat{x}$, $\mathbf{r}_i \to \mathbf{r}_i + l_y\hat{y}$ affect the Hamiltonian by a unitary transformation, as given explicitly below. In particular, the quasiparticle spectrum is invariant under such replacements.

Calculation of the Berry phase. In the following, we will consider the model Eqs. (1)–(9) as a function of vortex positions $\{\mathbf{r}_i\}$. We note that the simultaneous presence of the magnetic field and the discrete ionic lattice generically opens up a gap in the quasiparticle spectrum of the d-wave superconductor, except for special vortex configurations that respect inversion symmetry.[10] The Berry phase associated with the motion of vortices is thus well defined. We further remark that the model defined above is traditionally studied by means of a singular gauge transformation,[2] that, on average, removes the magnetic field. This is inconvenient for present purposes,

since the precise transformation depends on vortex positions, and the Berry phase is clearly not invariant under unitary transformations that vary along the particular path in question. We thus need to stay within the present framework of magnetic translations and associated boundary conditions.

To study the Berry phases associated with the motion of vortices, we first note that within our model the vortex positions are well-defined continuous parameters that are, at least for large enough lattice, entirely encoded in the pairing amplitudes $\Delta_{\mathbf{rr}'}$. The Berry phase associated with vortex motion along closed paths may be computed via

$$e^{i\gamma} \approx \langle\Omega_1|\Omega_m\rangle \cdot \ldots \cdot \langle\Omega_3|\Omega_2\rangle \cdot \langle\Omega_2|\Omega_1\rangle, \qquad (11)$$

where the $|\Omega_i\rangle$ are the ground states of the system along a reasonably fine discretization of the path. The above formula has the advantage (over the standard integral formula) that a random, discontinuous phase that each $|\Omega_i\rangle$ acquires in numerical diagonalization automatically cancels. Each ground state is constructed as the vacuum of Bogoliubov operators

$$\gamma_{n\uparrow} = \sum_{\mathbf{r}} [u_n^*(\mathbf{r}) c_{\mathbf{r}\uparrow} - v_n^*(\mathbf{r}) c_{\mathbf{r}\downarrow}^\dagger], \qquad (12)$$

$$\gamma_{n\downarrow} = \sum_{\mathbf{r}} [u_n^*(\mathbf{r}) c_{\mathbf{r}\downarrow} + v_n^*(\mathbf{r}) c_{\mathbf{r}\uparrow}^\dagger], \qquad (13)$$

where the matrices $U_{\mathbf{r}n} = u_n(\mathbf{r})$, $V_{\mathbf{r}n} = v_n(\mathbf{r})$, satisfy Bogoliubov–de Gennes equations

$$\begin{pmatrix} -t - \mu & -\Delta \\ -\Delta^* & t^* + \mu \end{pmatrix} \begin{pmatrix} U \\ -V \end{pmatrix} = E_n \begin{pmatrix} U \\ -V \end{pmatrix} \qquad (14)$$

for non-negative eigenvalues E_n. It is clear from Eq. (12) that the state $|\tilde{0}\rangle = \prod_{\mathbf{r}} c_{\mathbf{r}\downarrow}^\dagger |0\rangle$ is a vacuum of both the operators $\gamma_{n\uparrow}$ and $\gamma_{n\downarrow}^\dagger$, where $|0\rangle$ is the vacuum of the $c_{\mathbf{r}\sigma}$ operators. The ground state of the Hamiltonian thus can be constructed as

$$|\Omega\rangle = \prod_n \gamma_{n\downarrow} |\tilde{0}\rangle. \qquad (15)$$

Using this last relation, and the inverse of Eq. (12), one readily obtains

$$\langle\Omega_i|\Omega_j\rangle = \det(U_i U_j^\dagger + V_i V_j^\dagger). \qquad (16)$$

Results. We first consider the important special case of Eq. (1) with $\mu = 0$, or half filling. In this case the Hamiltonian is invariant under the *antiunitary* charge conjugation operator defined via $\mathcal{C} c_{\mathbf{r}\sigma} \mathcal{C} = (-1)^{\mathbf{r}} c_{\mathbf{r}\sigma}^\dagger$, and the unique ground state $|\Omega\rangle$ is then invariant under $\mathcal{C}$ as well (up to a phase that can be made trivial). It then follows directly from Eq. (11) that $e^{i\gamma} = \pm 1$. The first immediate conclusion from this is that as long as vortices are moved along contractible paths, the Berry phase must be $+1$ for continuity reasons. If vortices were hard-core particles, this would, in principle, still leave the possibility of fermionic statistics. However, careful examination shows that the Hamiltonian can be analytically continued without difficulty into configurations were two vortices fuse into a double vortex at a given location. Exchange paths are thus contractible, and hence vortices must satisfy bosonic statistics. We have tested this for various lattice sizes and exchange paths. The model does, however, become singular when vortex positions are formally approaching lattice sites [see Eq. (7)].

It is thus possible that lattice sites carry an effective π flux felt by vortices encircling such sites. We have carefully checked that this is not the case in our model. Hence at half filling, all Berry phases are unity. The above observations also hold for the *s*-wave case.

The observation that vortices are bosonic is nontrivial, since time reversal symmetry is absent, and hence generically in two spatial dimensions even non-Abelian statistics are possible, as is the case if the pairing symmetry is $p + ip$.[22] Indeed, when we move away from half filling, there is no longer any symmetry that requires the Berry phase to be trivial. We will now show that this situation leads to a very intricate landscape of nontrivial quantum curvature.

The Berry curvature is defined as the Berry phase around an infinitesimal area, divided by the size of this area. In the following, we consider a lattice containing only two vortices in the presence of the periodic boundary condition. One vortex remains fixed, while for any point within the unit cell, we calculate the Berry curvature associated with the motion of the other vortex according to Eq. (11). The Berry phase around arbitrary loops can be obtained as the integral of the Berry curvature over the enclosed area. The result for a 12×10 lattice at $\mu = 0.05$ is presented in Fig. 1(a). It is apparent that the Berry curvature in this model is a highly nontrivial function of position for any $\mu \neq 0$. One observes that the curvature is conspicuously concentrated on the links and the sites of the lattice, even though the vortex positions themselves are formally not tied to the discrete lattice. Singular structures form in particular around the lattice sites. These are described by $B(\mathbf{r}) \sim a_i \delta(\mathbf{r} - \mathbf{r}_i) + f_i(\theta)/r$, where $B(\mathbf{r})$ is the curvature, and θ, r refer to polar coordinates with the lattice site $\mathbf{r}_i$ at the origin. The parameters a_i and the functions f_i depend sensitively on details such as the lattice size, μ, the site index i, and the position of the other, fixed vortex. Yet another interesting feature is the structure seen in the vicinity of the fixed vortex, which is somewhat reminiscent of the shape of a $d_{x^2-y^2}$ orbital. However, this structure does not seem to be reflective of by the pairing symmetry, but rather more the lattice symmetry, as similar calculations for the *s*-wave case show. We note that again no singularity indicative of a flux tube carried by the fixed vortex appears in Fig. 1(b) at the position of this vortex. This implies that we should still think of these vortices as bosons, which move in an effective background magnetic field.

The complex nature of these features and the strong sensitivity on model parameters are likely yet another facet of the fractal nature of the physics of the Hofstadter model. To wit, in view of the fractal nature of the wave-vector dependence of spectral features of the Hofstadter model, it is reasonable to expect that the response to a spatially inhomogeneous perturbation (coupling to many different wave vectors) is characterized by complicated and possibly chaotic spatial modulations. The addition of a pairing order parameter with vortices clearly represents such a perturbation. Here we are mostly interested in how to reconcile the complex features seen at $\mu \neq 0$ with the trivial ones seen at $\mu = 0$. It is clear that our ability to precisely define the vortex position on scales below the lattice constant is dependent on conventions, even though in the present case a natural convention is available, since our ground states are naturally parametrized by the
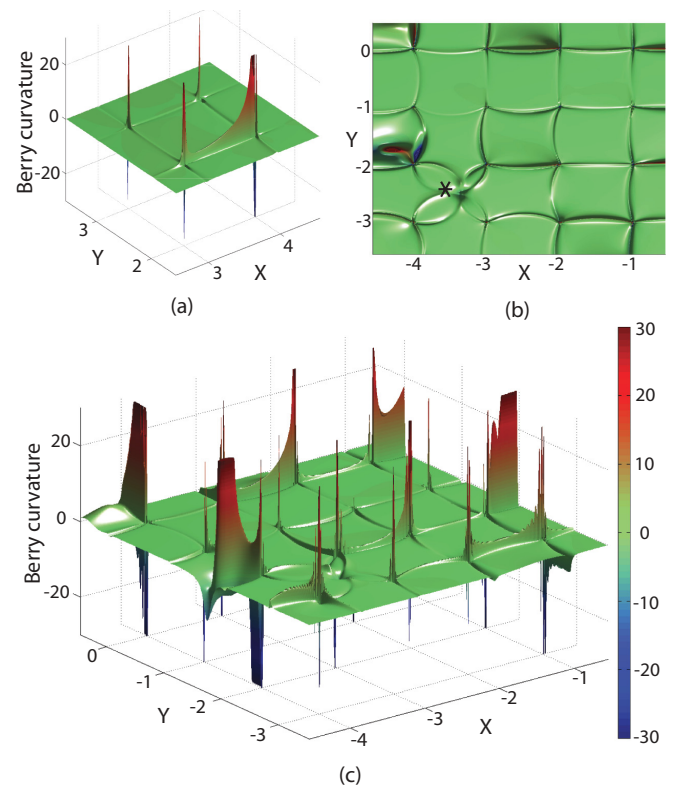

(a)

(b)

(c)

FIG. 1. (Color online) Berry curvature for 12×10 lattice in the presence of two vortices, for $\mu = 0.05$. The calculated curvature at a given location is associated with the motion of one of the vortices at this location, while the position of other vortex is held fixed. (a) Three-dimensional (3D) view of the Berry curvature in the vicinity of one plaquette. Lattice sites and links are clearly visible, since the curvature is chiefly concentrated on the latter, with singularities at the sites. The remaining space within the plaquettes is nearly flat. (b) Top view of the lattice. The position of the fixed vortex is noted by an asterisk. No singularity is present at this position. However, an interesting structure reminiscent of the shape of a $d_{x^2-y^2}$ orbital appears in the vicinity. (c) 3D view of the entire lattice. Detailed features appear highly irregular, except for the fact that the curvature is everywhere concentrated on the sites and the links of the lattice, and on the structure seen around the position of the fixed vortex.

vortex positions in the continuum field (6) used to define the Hamiltonian. We have, however, tested the robustness of the qualitative features shown in Fig. 1 by varying the precise form of the pairing order parameter Eq. (3). In particular, we have varied the core parameter ξ in Eq. (8), and tested various alternative forms for Eq. (5). We also introduced variations in the boundary conditions described above. In all cases we found that the qualitative features of the Berry curvature remained unaltered. Although we believe that the curvature landscape of Fig. 1(c) is interesting in its own right, it is appropriate to make this landscape subject to some coarse graining procedure. It is interesting to ask whether such coarse graining leads to a recovery of one of the basic facts suggested by conventional wisdom about vortex-boson duality, namely, that the curvature discussed above is directly tied to particle (here, Cooper-pair) density. We will show in the following that this statement is recovered when the Berry curvature is averaged over the

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magnetic unit cell (as opposed to the, typically much smaller, lattice unit cell). To this end, we again consider a lattice containing only two vortices within a single magnetic unit cell, subject to the boundary conditions (9).

Let the coordinates of the "moving" vortex be $\mathbf{r} = (x, y)$. As remarked initially, a formal shift of x by l_x changes the Hamiltonian by a gauge transformation. We have $H \to U_x^\dagger H U_x$ with $U_x = e^{i\pi(1-y/l_y)\hat{N}/2}$, where $\hat{N}$ is the particle number operator. Analogous relations hold for $y \to y + l_y$, with $U_y = e^{i\pi(1+x/l_x)\hat{N}/2}$. We now calculate the Berry phase associated with a rectangular path of dimensions l_x, l_y around the lattice. We may then choose a ground state phase convention $|\Omega(\mathbf{r})\rangle$ along the path satisfying

$$|\Omega(\mathbf{r} + l_y \hat{y})\rangle = U_y^\dagger |\Omega(\mathbf{r})\rangle,$$

$$|\Omega(\mathbf{r} + l_x \hat{x})\rangle = U_x^\dagger |\Omega(\mathbf{r})\rangle, \qquad (17)$$

along the horizontal and vertical path segments, respectively. The consistency of Eq. (17) with the continuity of $|\Omega(\mathbf{r})\rangle$ along the path follows from the observation that for any ground state, $U_y^\dagger U_x^\dagger U_y U_x |\Omega\rangle = |\Omega\rangle$. The latter holds because $U_y^\dagger U_x^\dagger U_y U_x = \exp(i\pi \hat{N})$ and because the ground state Eq. (15) always has even particle number parity. We determine the Berry phase for the rectangular path as the integral over the Berry connection, $\langle \Omega(\mathbf{r}) | \nabla | \Omega(\mathbf{r}) \rangle$, where we observe that

$$\langle \Omega(\mathbf{r} + l_x \hat{x}) | \nabla | \Omega(\mathbf{r} + l_x \hat{x}) \rangle$$

$$= \langle \Omega(\mathbf{r}) | U_x \nabla U_x^\dagger | \Omega(\mathbf{r}) \rangle$$

$$= \langle \Omega(\mathbf{r}) | \nabla | \Omega(\mathbf{r}) \rangle + \frac{i\pi}{2l_y} \langle \hat{N} \rangle \hat{y}. \qquad (18)$$

It is clear that only the last term survives a cancellation between the vertical path segments, giving $i\pi \langle \hat{N} \rangle / 2$. The same contribution is obtained from the horizontal segment. We thus obtain $\gamma = \pi \langle \hat{N} \rangle$, or 2π times the number of Cooper pairs in the system, in agreement with general expectations based on duality arguments applied to Cooper pairs.[16] It is worth noting that the quantity γ, when expressed as an integral of the Berry curvature over the entire lattice, is formally reminiscent of a Chern number. It is not truly a Chern number, though, since the boundary conditions (17) do not quite allow one to make contact with one-dimensional vector bundles over the torus. Indeed, γ is not quantized, as $\langle \hat{N} \rangle$ may take on arbitrary values in $[0, 2l_x l_y]$. We note that the derivation above is independent of the pairing symmetry.

Conclusion. The present study establishes several aspects of Berry phases associated with vortex motion in a microscopic model of superconducting lattice fermions. It is shown that these vortices behave as bosons which, away from half filling, are subject to a nontrivial effective magnetic field. In an average sense, it has been shown that this effective field is tied to the density of Cooper pairs. This is expected based on boson-vortex duality, and was seen to emerge here in a microscopic model of fermions. We emphasize that the simple relation between Cooper-pair density and effective field is only seen to emerge after averaging over a magnetic unit cell. This may be used to justify a direct proportionality between Cooper-pair density and Berry curvature in the long wavelength effective theory. However, our results also indicate that care must be used in order to justify such a relationship in general. On the one hand, this is true because of the relatively large nonuniformity of the observed Berry curvature within the magnetic unit cell. Moreover, in the presence of particle hole symmetry we have found that the Berry phase associated with closed paths is always zero, and thus corresponds to π times the average enclosed particle number only for such paths that happen to enclose an even number of lattice sites. In this case, the background field appearing in the effective theory should clearly be zero, and should not follow the total Cooper-pair density. This result will be robust to small perturbations respecting particle hole symmetry, and is thus true for a wide class of microscopic models. We conjecture that the complex landscape of the Berry curvature away from half filling is a facet of the fractal properties of the Hofstadter model, and believe that it is worthy of further investigation.

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