Localization Transitions in Non-Hermitian Quantum Mechanics

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We study the localization transitions which arise in both one and two dimensions when quantum mechanical particles described by a random Schrödinger equation are subjected to a constant imaginary vector potential. A path-integral formulation relates the transition to flux lines depinned from columnar defects by a transverse magnetic field in superconductors. The theory predicts that, close to the depinning transition, the transverse Meissner effect is accompanied by stretched exponential relaxation of the field into the bulk and a diverging penetration depth. [S0031-9007(96)00677-1]

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Although forbidden in conventional quantum mechanics, exponentiated non-Hermitian quantum Hamiltonians do appear in the transfer matrices of classical statistical mechanics problems. A nonequilibrium process can be described as the time evolution of a non-Hermitian system [1]. Another example is the *XXZ* spin chain mapped onto the asymmetric six-vertex model [2].

In this Letter, we investigate a non-Hermitian quantum Hamiltonian with randomness. The study is motivated by a mapping of flux lines in a $(d + 1)$-dimensional superconductor to the world lines of d-dimensional bosons. Columnar defects in the superconductor, which were introduced experimentally in order to pin the flux lines [3], give rise to random potential in the boson system [4]. Although the field component H_z parallel to the columns acts as a chemical potential for the bosons, the component perpendicular to the columns results in a constant imaginary vector potential [5].

We study localization in this simple example of non-Hermitian quantum mechanics, and show how flux lines are depinned from columnar defects by an increasing perpendicular magnetic field $H_\perp$. It is generally believed that all eigenstates are localized in conventional one- and two-dimensional noninteracting quantum systems with randomness. On the other hand, it is almost obvious that a flux line is depinned from defects by a strong perpendicular field component. This indicates that the present non-Hermitian system has extended states in a large $H_\perp$ region, and that there must be a delocalization transition at a certain strength of $H_\perp$.

The non-Hermitian Hamiltonian treated hereafter has the form $\mathcal{H} \equiv (p + ih)^2/(2m) + V(x)$, where $p \equiv (\hbar/i)\nabla$ and $V(x)$ is a random potential. The non-Hermitian field h originates in the transverse magnetic field as $h = \phi_0 H_\perp/4\pi$. The flux quantum $\phi_0 = 2\pi\hbar c/2e$ plays the role of a charge and the non-Hermitian factor $i = \sqrt{-1}$ arises from the mapping onto imaginary time quantum mechanics [4,5]. Figure 1 shows a vortex whose "world line" is described by this Hamiltonian with periodic boundary conditions in one dimension. The mass m is equivalent to the tilt modulus of the flux line. The Planck parameter $\hbar$ corresponds to the temperature of the superconductor, while the inverse temperature of the quantum system corresponds to the thickness L_τ of the sample along H_z. Interactions between many particles (or flux lines) can be treated approximately by forbidding multiple occupancy of localized states in a tight-binding model (see below) [4]. Interactions in the delocalized regime are described by a non-Hermitian boson Hubbard model, and will be discussed in a future publication [6].

Since the field h acts as a vector potential, we define the current operator as $J \equiv -i\partial\mathcal{H}/\partial h = (p + ih)/m$. The imaginary part of the current describes the tilt slope of a flux line. To see this, note first that the position of the flux line x at the distance τ from the bottom surface of the superconductor is given by $\langle x \rangle_\tau \equiv Z^{-1} \times \langle \psi^f | e^{-(L_\tau-\tau)\mathcal{H}/\hbar} x e^{-\tau\mathcal{H}/\hbar} | \psi^i \rangle$, where ψ^i and ψ^f describe boundary conditions at the bottom and top surfaces ($\tau = 0, L_\tau$) of the superconductor, respectively.
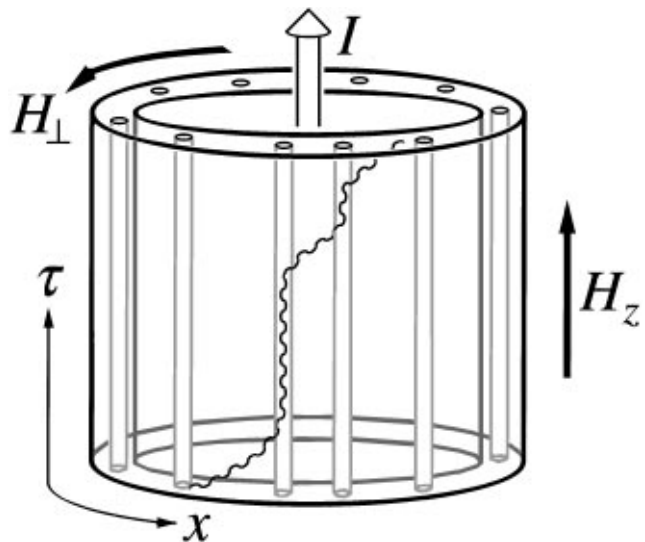

FIG. 1. One flux line (wavy curve) induced by the field H_z and interacting with columnar pins in a cylindrical superconducting shell with radial thickness smaller than the penetration depth of the defect-free material. The field $H_\perp$ is generated by the current I threading the ring.

The partition function is $Z \equiv \langle \psi^f | e^{-L_\tau \mathcal{H}/\hbar} | \psi^i \rangle$. The commutation relation $[\mathcal{H}, x] = -i\hbar J$ leads immediately to $(\partial/\partial \tau) \langle x \rangle_\tau = -i \langle J \rangle_\tau = \mathrm{Im} \langle J \rangle_\tau$.

The total displacement of the flux line between the bottom and the top surfaces is given by $\langle x \rangle_{L_\tau} - \langle x \rangle_0 = \hbar (\partial/\partial h) \ln Z = \mathrm{Im} \int_0^{L_\tau} \langle J \rangle_\tau d\tau$. This quantity is an indicator of the delocalization transition; the transverse displacement of a flux line must be order of the system size when it is depinned.

Let us first consider localized states in a small perpendicular field. Assume the eigenfunctions $\psi_n(x)$ and the eigenvalues ε_n are known for $h = 0$. For small h the right and left eigenvectors of $\mathcal{H}$ are given by $\psi_n^R(x; h) = e^{h \cdot x/\hbar} \psi_n(x; h = 0)$ and $\psi_n^L(x; h) = e^{-h \cdot x/\hbar} \psi_n^*(x; h = 0)$. The energy eigenvalue ε_n is unchanged under this "imaginary" gauge transformation [7]. The imaginary gauge transformation applies even to many-body eigenvectors of interacting systems [6]. However, the above wave functions ψ_n^R and ψ_n^L may diverge as $|x| \to \infty$, and hence may not be normalizable. The normalizability condition is $|h| < \hbar \kappa_n$, where κ_n is the inverse localization length of the state $\psi_n(x; h = 0)$. Then the wave function [with the normalization $\int d^d x\, \psi_n^R(x) \psi_n^L(x) = 1$] is approximately

$$\psi_n^R(x) \simeq \sqrt{\frac{(2\kappa_n)^d}{\Gamma(d)\Omega_d}}\, e^{h \cdot (x - x_n)/\hbar - \kappa_n |x - x_n|}, \qquad (1)$$

where x_n is the localization center for $h = 0$ and Ω_d is the total solid angle of the d-dimensional space.

The point $|h| = \hbar \kappa_n$ is the delocalization point of the state ψ_n^R: In the region $|h| \geq \hbar \kappa_n$, the eigenfunction becomes extended. Hence we need to specify the boundary conditions in order to obtain a well-defined wave function in the thermodynamic limit.

Let us consider imposing the periodic boundary condition $\psi_n^R(L_x/2, y, \ldots) = \psi_n^R(-L_x/2, y, \ldots)$, with the x axis parallel to h. The one-dimensional periodic system is shown in Fig. 1. Except for the *imaginary* vector potential, this setup is the flux-line analog of a mesoscopic metal ring threaded by a solenoid. At the boundaries $x = \pm L_x/2$, the wave function (1) has a mismatch of order $e^{-(\kappa_n - h/\hbar)L_x}$. In the region $h < \hbar \kappa_n$, this mismatch is exponentially small, as is the change necessary to meet the periodic boundary condition. In the region $h \geq \hbar \kappa_n$, however, the wave function changes drastically, and a complex eigenvalue appears. To understand this point, consider the case $|h| \to \infty$, a limit in which the random potential $V(x)$ may be neglected [6]. The periodic boundary condition is satisfied only by the extended function $e^{ik \cdot x}$ with $k_\nu = 2n_\nu \pi/L_\nu$, where n_ν is an integer and L_ν is the system size in the x_ν direction. (If a right eigenvector is $e^{ik \cdot x}$, the corresponding left eigenvector is $e^{-ik \cdot x}$.) The eigenvalue is complex: $\varepsilon(k) = (\hbar k + ih)^2/2m$.

The imaginary part of an eigenvalue has the following meaning. The time evolution of an extended state is described as $e^{ik \cdot x - \tau \varepsilon/\hbar}$. This must actually be a function of $k \cdot (x - \tau \mathrm{Im} \langle J \rangle)$, because the corresponding flux line has the tilt slope $\mathrm{Im} \langle J \rangle$. (The angular brackets here denote the expectation value with respect to the state with energy ε.) We hence expect the relation $\mathrm{Im} \varepsilon \simeq \hbar k \cdot \mathrm{Im} \langle J \rangle \equiv -\hbar k \cdot (\partial/\partial h) \mathrm{Re} \varepsilon$. Thus appearance of a complex eigenvalue is another indicator of the delocalization transition.

It is instructive to solve the one-dimensional system with a single attractive impurity: $\mathcal{H} \equiv -(\hbar \nabla - h)^2/2m - V_0 \delta(x)$. We first solve $\mathcal{H} \phi(x) = \varepsilon \phi(x)$ for $x \neq 0$ to obtain the two degenerate solutions $\phi_\pm(x) = e^{\pm ikx + hx/\hbar}$, and then write the general solution as $\psi = A\phi_+ + B\phi_-$. We impose the periodic boundary condition $\psi(L_x) = \psi(0)$ and the condition for the delta potential, $\psi'(L_x) - \psi'(0) = (2mV_0/\hbar^2)\psi(0)$. A nontrivial solution arises whenever $k[\cosh(L_x h/\hbar) - \cos(L_x k)] + (mV_0/\hbar^2)\sin(L_x k) = 0$. The ground state (the state which minimizes $\mathrm{Re}\,\varepsilon$) is localized only for $h < \hbar \kappa_{gs} = mV_0/\hbar$. All the other states are extended. The localized ground-state energy is $\varepsilon_{gs} = -mV_0^2/2\hbar^2$, and the wave function takes the form $\psi_{gs}^R(x) = \sqrt{\kappa_{gs}}\, e^{-\kappa_{gs}|x| + hx/\hbar}$ as $L_x \to \infty$. The localization length in the direction of h grows as $(\hbar \kappa_{gs} - h)^{-1}$, and the state goes through a delocalization transition at $h = \hbar \kappa_{gs}$. The ground state for $h > \hbar \kappa_{gs}$ is extended with the energy $-h^2/2m$. The corresponding flux line has the tilt slope h/m, which is equal to the value in the impurity-free case. The tilt slope of the ground state has a jump at the delocalization point.

Extended states in the thermodynamic limit have a form close to the pure case. The leading term is $e^{ik_n x}/\sqrt{L_x}$ with $k_n = n\pi/L_x$, where n is odd for $h < \hbar \kappa_{gs}$, and is even for $h > \hbar \kappa_{gs}$. There is a reflection term $e^{-ik_n x + 2hx}$ in the region $x < 0$. The energy eigenvalue takes the same form as the pure system. The above solution shows that a depinned flux line almost ignores the columnar defect.

Now we move on to the case of random potential. For the purpose of numerical calculations, it is convenient to introduce the non-Hermitian tight-binding model. The second-quantized Hamiltonian is written in the form

$$\mathcal{H} \equiv -\frac{t}{2} \sum_x \sum_{\nu=1}^d (e^{h \cdot e_\nu/\hbar} b_{x+e_\nu}^\dagger b_x + e^{-h \cdot e_\nu/\hbar} b_x^\dagger b_{x+e_\nu}) + \sum_x V_x b_x^\dagger b_x, \qquad (2)$$

where the $\{b_x^\dagger, b_x\}$ are boson creation and annihilation operators [8], and the $\{e_\nu\}$ are the unit lattice vectors. The hopping element is approximately given by [4] $t \sim V_{bind} \exp(-\sqrt{2mV_{bind}}\, a/\hbar)$, where V_{bind} is a typical binding energy of the columnar defect, and a is the lattice spacing. We apply the periodic boundary conditions $b_{x+N_\nu e_\nu} = b_x$ for $\nu = 1, 2, \ldots, d$, where $N_\nu \equiv L_\nu/a$. The complex eigenvalues in this non-Hermitian system always appear in conjugate pairs; if there is a complex eigenvalue ε with a right eigenvector ψ^R, there is also the eigenvalue ε^* with the right eigenvector $(\psi^R)^*$. This symmetry ensures that the partition function Z is real.

Another symmetry is $\mathcal{H}(\boldsymbol{h})^T = \mathcal{H}(-\boldsymbol{h})$. Because of this symmetry, a right eigenfunction of $\mathcal{H}(\boldsymbol{h})$ equals the left eigenfunction of $\mathcal{H}(-\boldsymbol{h})$ with the same eigenvalue. If $V_{\boldsymbol{x}} \equiv 0$, the eigenvalues are $\varepsilon = -t \sum_{\nu=1}^{d} \cos[(k_\nu + ih_\nu/\hbar)a]$ with $k_\nu = 2n_\nu\pi/L_\nu$, where n_ν is an integer. The eigenfunction takes the form $\psi^R(\boldsymbol{x}) \propto \exp(i\boldsymbol{k}\cdot\boldsymbol{x})$. Numerical calculations for $V_{\boldsymbol{x}} \neq 0$ were carried out assuming that the random potential $V_{\boldsymbol{x}}$ is uncorrelated in space, and uniformly distributed in the range $[-\Delta, \Delta]$. Results for random hopping models, with *no* site randomness, are qualitatively similar [6].

Figure 2(a) shows the eigenvalue spectrum for $d = 1$. The real eigenvalues indicate localized states, while the complex eigenvalues indicate delocalized ones. As discussed above, the eigenvalues for the localized states are
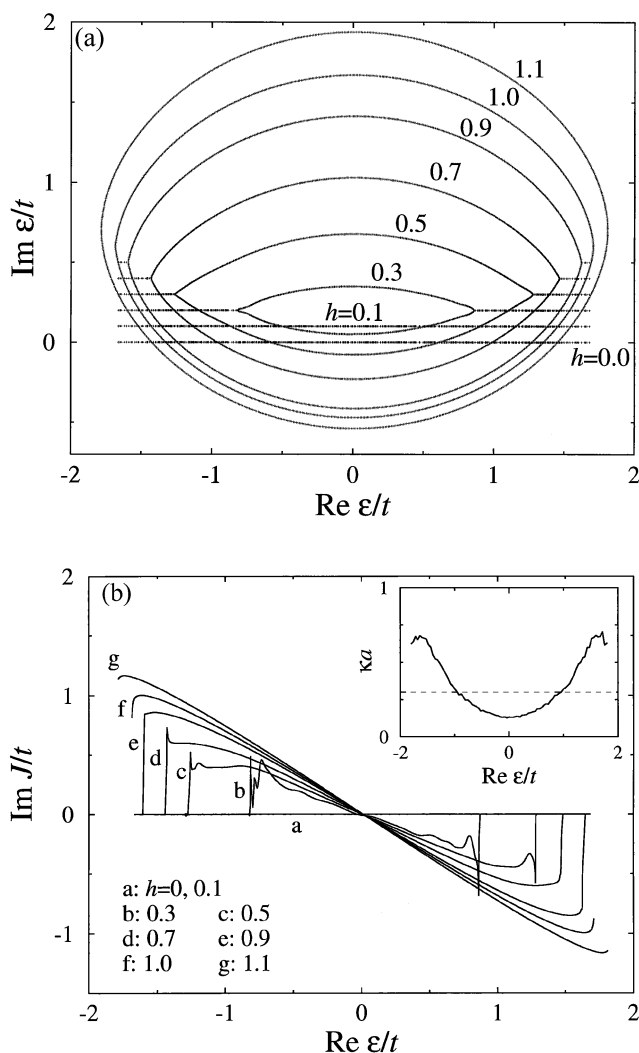

indeed independent of $\boldsymbol{h}$. The behavior of the delocalized states, on the other hand, is similar to impurity-free systems except near the mobility edges. Figure 2(b) shows the imaginary part of the current, or the tilt slope of the corresponding flux line plotted against the real part of the energy. The tilt slope has a jump at the mobility edges as in the one-impurity case. The inset to Fig. 2(b) shows the inverse localization length for this problem when $\boldsymbol{h} = 0$. (We calculated the approximate inverse localization length from the second moment of the wave function.) According to the delocalization criterion $h_c = \hbar\kappa$, a region of delocalized states should appear as h increases, first at the band center and then moving outwards, as we observe.

In two dimensions we again find bands of localized energies bounded by a mobility edge, although extended and localized states are apparently *mixed* in a complicated way near the band center. Extended states again almost ignore impurities. The case of an attractive impurity shows that the localized ground state exists in a certain region of small $\boldsymbol{h}$, and that the energy spectrum of the extended states is close to the impurity-free case.

An interesting question in the two-dimensional random case is whether a delocalized state is extended in both the x and y directions, or extended only in the direction of $\boldsymbol{h}$. We believe delocalization must occur in *both* directions: If the field $\boldsymbol{h}$ is parallel to the x axis and a state is extended in this direction, we may assume that the wave function has the approximate form $L_x^{-1/2}e^{ik_x x}\phi(y)$ in order to accommodate periodic boundary conditions. This is indeed an eigenfunction of the partial Hamiltonian which has only the kinetic term in the x direction. We then calculate the effective Hamiltonian for $\phi(y)$ in degenerate perturbation theory, taking the kinetic term in the y direction and the random potential term as the perturbation. We find that the effective Hamiltonian for $\phi(y)$ has a random potential term of the form $L_x^{-1} \int V(x, y)\, dx$. The width of the probability distribution of this effective random potential, however, vanishes as $L_x^{-1/2}$ in the limit $L_x \to \infty$. The flux line is a random walker in the y direction, and hence $\phi(y)$ is an extended state. Delocalization in directions both parallel and perpendicular to $\boldsymbol{h}$ is more readily observed numerically for $\boldsymbol{h}$ along the *diagonal* of a square lattice than for $\boldsymbol{h}$ parallel to $\boldsymbol{e}_x$ or $\boldsymbol{e}_y$ [6].

Spectra such as those in Fig. 2(a) at intermediate values of $\boldsymbol{h}$ are relevant at low but *finite* concentrations of interacting flux lines, provided that we fill up the localized states in order of increasing energy up to energy $\varepsilon = \mu$, thus forbidding multiple occupancy of a single localized state [4]. The system is then characterized by an average chemical potential $\mu = \mu(H_z)$ which controls the flux-line density and separates occupied from unoccupied levels. Once this chemical potential exceeds the mobility edge, however, we expect spiral trajectories and "Bose condensation" of delocalized flux lines into the lowest-energy extended state; more sophisticated methods of dealing with interactions are then required [6,9].

FIG. 2. (a) $\mathrm{Im}\varepsilon$ vs $\mathrm{Re}\varepsilon$ for a particular sample of the $d = 1$ tight-binding model with $\Delta/t = 1$ and $L_x = 1000a$. Each eigenstate is marked by $+$. Plots for different $\boldsymbol{h}$ are offset for clarity. (b) $\mathrm{Im}J$ (fluxon tilt) vs $\mathrm{Re}\varepsilon$ for the same sample as in (a). The inset shows κa vs $\mathrm{Re}\varepsilon$ for $\Delta/t = 1$, $L_x = 500a$, and $\boldsymbol{h} = 0$, averaged over one hundred samples binned with energy window $0.04t$. The dashed line indicates a particular value of $ha/\hbar$. The states below the dashed line become extended.

Consider the probability distribution of a flux line near a free surface. At the distance τ from the bottom surface of the superconductor this probability may be written $P(\boldsymbol{x}; \tau) \equiv Z^{-1} \langle \psi^f | e^{-(L_\tau - \tau)\mathcal{H}/\hbar} | \boldsymbol{x} \rangle \langle \boldsymbol{x} | e^{-\tau\mathcal{H}/\hbar} | \psi^i \rangle$, where we assume free boundary conditions at the bottom and the top surfaces: $|\psi^i\rangle = |\psi^f\rangle = \int d^d \boldsymbol{x}' |\boldsymbol{x}'\rangle$. In the limit $L_\tau \to \infty$, the probability distribution of the most weakly bound flux line at the top surface is proportional to the right eigenvector with the eigenvalue $\varepsilon = \mu$, $P(\boldsymbol{x}; L_\tau) \propto \langle \boldsymbol{x} | \psi_\mu \rangle = \psi_\mu^R(\boldsymbol{x})$, while the distribution at the bottom surface is proportional to the left eigenvector of the same state, $P(\boldsymbol{x}; 0) \propto \langle \psi_\mu | \boldsymbol{x} \rangle = \psi_\mu^L(\boldsymbol{x})$. The distribution far from these surfaces is given by $P(\boldsymbol{x}; L_\tau/2) = \psi_\mu^R(\boldsymbol{x})\psi_\mu^L(\boldsymbol{x})$. In the localized regime, the imaginary gauge transformation for ψ_μ^R and ψ_μ^L describes the displacement of the flux line at the surfaces, while the bulk distribution $P(\boldsymbol{x}; L_\tau/2)$ is independent of $\boldsymbol{h}$, consistent with the transverse Meissner effect [4]. These statements are approximate because we have neglected excitations of occupied states. They are exact for the ground state. The displacement of the flux lines near the top and bottom surfaces allows partial penetration of the transverse component of the magnetic field, characterized by a transverse London penetration depth τ^*.

In the case of one columnar defect (or a single impurity in a tight-binding model), the displacement of a flux line takes the form $(\langle \boldsymbol{x} \rangle_\tau - \langle \boldsymbol{x} \rangle_\infty) \cdot \boldsymbol{h} \sim e^{-\tau \Delta\varepsilon_1/\hbar}$, where $\Delta\varepsilon_1$ is the energy gap between the localized ground state and the extended first excited state. In the random case with finite concentration of flux lines, we consider the relaxation near a free surface $\tau = 0$ of the most weakly bound line to the highest-energy occupied state. We show below that, close to the delocalization transition, the displacement has the stretched exponential form

$$\overline{(\langle \boldsymbol{x} \rangle_\tau - \langle \boldsymbol{x} \rangle_\infty)} \cdot \boldsymbol{h} \underset{\tau \to \infty}{\sim} \exp[-a(\tau/\tau^*)^{1/(d+1)}], \quad (3)$$

where $\langle \boldsymbol{x} \rangle_\infty$ is the center of the localized state in the bulk, the overbar denotes the random average, the penetration depth is given by $\tau^* \equiv g(\mu)\hbar^{d+1}/[\hbar\kappa(\mu) - h]^d$, and a is a constant of order of unity. Here $g(\mu)$ and $\kappa(\mu)$ are, respectively, the density of states and the inverse localization length at the chemical potential. Note that $\tau^* \sim \xi_\perp^d$, where $\xi_\perp \sim 1/(\hbar\kappa - h)$ is the diverging surface localization length near the transition.

For the derivation of the above, we expand $P(\boldsymbol{x}; \tau)$ with respect to the eigenfunctions. In the limit $L_\tau \to \infty$, we have $P(\boldsymbol{x}; \tau) \simeq \langle \psi_\mu | \boldsymbol{x} \rangle \sum_n' c_n \langle \boldsymbol{x} | \psi_n \rangle e^{-\tau \Delta\varepsilon_n/\hbar}$, where $\Delta\varepsilon_n \equiv \varepsilon_n - \mu$, $\langle \psi_\mu | \boldsymbol{x} \rangle = \psi_\mu^L(\boldsymbol{x})$ is the left eigenvector describing the shifted probability distribution of the surface, and the $\{c_n\}$ are certain constants coming from the normalization factor. The summation $\sum_n'$ is restricted to states with energies $\varepsilon > \mu$. For $h \lesssim \hbar\kappa(\mu)$, many

of these excited states will contribute to the relaxation process. The asymptotic form (1) for localized states now leads to $|\langle \boldsymbol{x} \rangle_\tau - \langle \boldsymbol{x} \rangle_\infty| \sim \sum_n' \tilde{c}_n e^{-f_n/\hbar}$, where $f_n(\tau) \equiv (\hbar\kappa_n - h\cos\theta_n)r_n + \tau\Delta\varepsilon_n$, $r_n \equiv |\boldsymbol{x}_n - \boldsymbol{x}_\mu|$, $\cos\theta_n \equiv \boldsymbol{h} \cdot (\boldsymbol{x}_\mu - \boldsymbol{x}_n)/|\boldsymbol{h}|r_n$ and the $\{\tilde{c}_n\}$ are additional constant factors. Upon setting $g(\mu)r_n^d\Delta\varepsilon_n \sim 1$ [4], we find that the two terms in f_n compete with each other; in other words, the further the flux line hops, the more the kink energy costs, but the lower the binding energy of the state n is. Minimizing f_n with respect to r_n and θ_n, we arrive at Eq. (3). We expect that a similar relaxation process governs lines relaxing from the surface to all occupied states with $\varepsilon < \mu$ as $\tau \to \infty$. For $d = 1$ and randomly distributed column *positions,* rare events such as exceptionally small hopping matrix elements will alter Eq. (3) for very large τ, similar to flux lines pinned by parallel, randomly placed grain boundaries [10].

The behavior of the flux-line tilt modulus (inverse boson superfluid density) and flux-flow resistivity *above* the mobility edge may be obtained [6] using the methods of Ref. [9].

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