Localization transitions in non-Hermitian quantum mechanics

Naomichi Hatano* and David R. Nelson
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138

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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 the transverse Meissner effect is accompanied by stretched exponential relaxation of the field into the bulk and a diverging penetration depth at the transition.

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 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 [1]. Although the field component $H_\perp$ parallel to the columns acts like a chemical potential for the bosons, the component perpendicular to the columns results in a constant imaginary vector potential [1].

We study localization in this simple example of non-Hermitian quantum mechanics, and thereby show how a flux line is 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 non-interacting 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 $\mathcal{H} = (p + i\hbar)^2/(2m) + V(x)$, where $p = (h/i) \nabla_x$, and $V(x)$ is a random potential. The non-Hermitian field $\hbar$ originates in the transverse magnetic field as $\hbar = \phi_0 H_\perp/(4\pi)$, where $\phi_0$ is the flux quantum [1]. 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 $L_\tau$ of the superconductor. Interactions between many particles (or flux lines) can be treated approximately by forbidding multiple occupancy of localized state in a tight binding model (see below) [6]. Interactions in the delocalized regime will be discussed in a future publication [3].

Since the field $\hbar$ acts like a vector potential, we define the current operator as $J = -i\partial H/\partial \hbar = (p + i\hbar)/m$. 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 $\tau$ from the bottom surface of the superconductor is given by $(x)_{\tau} = \mathcal{Z}^{-1} (\psi^i e^{-(L_\tau - \tau)H/\hbar} e^{-\tau\hbar/\psi^i})$, where $\psi^i$ and $\psi^f$ describe boundary conditions at the bottom and top surfaces ($\tau = 0, L_\tau$) of the superconductor, respectively. The partition function is $Z = \langle \psi^f e^{-L_\tau H/\hbar}\vert \psi^i \rangle$. The commutation relation $[\mathcal{H}, x] = -i\hbar J$ leads immediately to $(\partial/\partial \tau) (x)_{\tau} = -i (J)_{\tau} = \text{Im} \langle J \rangle_{\tau}$.

The total displacement of the flux line between the bottom and the top surfaces is given by $(x)_{L_\tau} - (x)_0 = \hbar (\partial/\partial \hbar) \ln Z = \text{Im} \int_0^{L_\tau} \langle J \rangle_{\tau} d\tau$. This quantity is an indicator of the delocalization transition: the transverse displacement of a flux line must be 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 $\epsilon_n$ are known for $\hbar = 0$. For small $\hbar$ the right- and left-eigenvectors of $\mathcal{H}$ are given by $\psi_n^R(x; \hbar) = e^{\hbar x/\hbar} \psi_n(x; \hbar = 0)$, and $\psi_n^L(x; \hbar) = e^{-\hbar x/\hbar} \psi_n^*(x; \hbar = 0)$. The energy eigenvalue $\epsilon_n$ is unchanged under this “imaginary” gauge transformation $\mathcal{G}$. The imaginary gauge transformation applies even to many-body eigenvectors of interacting systems [3]. However, the above wave functions $\psi_n^R$ and $\psi_n^L$ may diverge in $|x| \to \infty$, and hence may not be normalizable. The normalizability condition is $|\hbar| < \hbar \kappa_n$, where $\kappa_n$ is the inverse localization length of the state $\psi_n(x; \hbar = 0)$. Then the wave function (with the normalization $\int d^d x \psi_n^R(x) \psi_n^L(x) = 1$) is approximately

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

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

We naturally regard the point |h| = hκn as the delocalization point of the state ψn. In the region |h| ≥ hκn, 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 ψn(Lx/2, y, ...) = ψn(−Lx/2, y, ...), with the x axis parallel to h. The one-dimensional periodic system is realized in the setup shown in Fig. 1. Except for the imaginary vector potential, this setup is the flux-line analogue of a mesoscopic metal ring threaded by a solenoid.

At the boundaries x = ±Lx/2, the wave function of the form (3) has a mismatch of the factor e(−κnx−h/2Lx). In the region h < hκn, this mismatch is exponentially small, and so is the change necessary to meet the periodic boundary condition. In the region h ≥ hκn, however, the wave function changes drastically, and a complex eigenvalue appears. To understand this point, consider the case |h| → ∞, a limit in which the random potential V(x) may be neglected. The periodic boundary condition is satisfied only by the extended function eikx, with kv = 2πν/Lν, where ν is an integer and Lν is the system size in the xν direction. (If a right-eigenvector is eikx, the corresponding left-eigenvector is e−ikx.) The eigenvalue is complex: ε(k) = (h k + iℏ)2/(2m).

The imaginary part of an eigenvalue has the following meaning. The time evolution of an extended state is described by eikx−iτε/h. This must actually be a function of k · (x − τ Im(J)), because the corresponding flux line has the tilt slope Im(J). (The angular brackets here denote the expectation value with respect to the state with energy ε.) We hence expect the relation Im(ε) ≃ ℏk · Im(J) ≡ −ℏk · (ℏ/∂x) Re(ε). 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: H = −(ℏN− ℏ)2/(2m) − Vδ(x). We first solve H(φ)(x) = εφ(x) for x ≠ 0 to obtain the two degenerate solutions φ±(x) = e±iκx+κε/ℏ, and then write the general solution as ψ = Aφ+ + Bφ−. We impose the periodic boundary condition ψ(Lx) = ψ(0) and the condition for the delta potential, ψ′(Lx) − ψ′(0) = (2mVb/h2)ψ(0). A nontrivial solution arises whenever k[cos(Lx h/ℏ) − cos(Lx k)] + (mVb/h2)sin(Lx k) = 0. The ground state (defined by the lowest real part of the eigenvalue) is localized only for h < hκgs = mVb/ℏ. All the other states are extended. The localized ground-state energy is εgs = −mVb2/(2ℏ2), and the wave function takes the form ψgs(x) = √nπgs e−κgs x+|hκgs x/Lx} as Lx → ∞. The localization length in the direction of h grows as (hκgs − h)−1, and the state goes through a delocalization transition at h = hκgs. The ground state for h > hκgs is extended with the energy −ℏ2/(2m). The corresponding flux line has the tilt slope h/ℏ, 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 eiknx/√Lx with kν = nπ/Lν, where n is odd for h < hκgs, and is even for h > hκgs. They also have the reflection term e−iknx+2ℏx 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

\[ H = \frac{i}{2} \sum_{\mathbf{x}} \sum_{\nu=1}^{d} \left( e^{i \mathbf{e}_\nu \mathbf{b}^\dagger_{\mathbf{x}+\mathbf{e}_\nu} \mathbf{b}_{\mathbf{x}} + e^{-i \mathbf{e}_\nu \mathbf{b}^\dagger_{\mathbf{x}+\mathbf{e}_\nu} \mathbf{b}_{\mathbf{x}} + \mathbf{e}_\nu} \right) + \sum_{\mathbf{x}} V_{\mathbf{x}} \mathbf{b}^\dagger_{\mathbf{x}} \mathbf{b}_{\mathbf{x}}, \]

where the \{b^\dagger_{\mathbf{x}}, b_{\mathbf{x}}\} are boson creation and annihilation operators, and the \{e_\nu\} are the unit lattice vectors. The hopping element is approximately given by \( t \sim V_{\text{bind}} \exp(-\sqrt{2m}V_{\text{bind}}a/\hbar) \), where Vbind is the binding energy in the tight-binding approximation, and a is the lattice spacing. We apply the periodic boundary conditions \( b_{\mathbf{x}+N} e_\nu = b_{\mathbf{x}} \) 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 ψR, 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 \(\mathcal{H}(\mathbf{h})^T = \mathcal{H}(-\mathbf{h})\). Because of this symmetry, a right-eigenvector of \(\mathcal{H}(\mathbf{h})\) equals to the left-eigenvector of \(\mathcal{H}(-\mathbf{h})\) with the same eigenvalue. If \(V_x \equiv 0\), the eigenvalues are \(\varepsilon = -t \sum_{\nu=1}^{d} \cos[(k_{\nu} + i h_{\nu}/h)a]\) with \(k_{\nu} = 2n_{\nu}\pi/L_{\nu}\), where \(n_{\nu}\) is an integer. The eigenfunction takes the form \(\psi^R(x) \propto \exp(ik \cdot x)\). Numerical calculations for \(V_x \neq 0\) were carried out assuming that the random potential \(V_x\) is uncorrelated in space, and uniformly distributed in the range \([-\Delta, \Delta]\). Results for random hopping models, with no site randomness, are qualitatively similar [3].

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 \(\mathbf{h}\). 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 \(\mathbf{h} = 0\). According to the delocalization criterion \(h_{\nu} = h_\kappa\), a region of delocalized states should appear as \(\mathbf{h}\) increases first at the band center and then move 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 \(\mathbf{h}\), 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 \(\mathbf{h}\). We conclude on the basis of the following argument that the former is the case. If the field \(\mathbf{h}\) 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 \(L_x^{-1/2} e^{i k_x x} \phi(y)\) 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 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 \(\mathbf{h}\) is more readily observed numerically for \(\mathbf{h}\) along the diagonal of a square lattice than for \(\mathbf{h}\) parallel to \(e_x\) or \(e_y\) [3].

Spectra such as those in Fig. 2 (a) at intermediate values of \(\mathbf{h}\) 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 [3]. The system is then characterized by an average chemical potential \(\mu = \langle H \rangle\) which controls the flux-line density and separates occupied from unoccupied

FIG. 2. (a) Im \(\varepsilon\) vs. 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 a cross +. Plots for different \(\mathbf{h}\) are offset for clarity. (b) Im \(J\) (fluxon tilt) vs. Re \(\varepsilon\) for the same sample as in (a). The inset shows \(\kappa a\) vs. Re \(\varepsilon\) for \(\Delta/t = 1\), \(L_x = 500a\) and \(\mathbf{h} = 0\), averaged over one hundred samples binned with energy window 0.04t.
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.

Consider the probability distribution of a flux line near a free surface. At the distance $\tau$ from the bottom surface of the superconductor this probability may be written

$$P(x; \tau) \propto Z^{-1} \langle x | e^{-(x-L_{\tau})/\hbar} | x \rangle e^{-\tau|\Delta\epsilon_1|/\hbar} \langle x | \psi \rangle$$

where we assume free boundary conditions at the bottom and the top surfaces: $\langle \psi \rangle = |\psi \rangle = \int dx |x\rangle$. 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 $\epsilon = \mu$, $P(x; L_{\tau}) \propto \langle x | \psi_{\mu} \rangle = \psi_{\mu}^R(x)$, while the distribution at the bottom surface is proportional to the left-eigenvector of the same state, $P(x; 0) \propto \langle \psi_{\mu} | x \rangle = \psi_{\mu}^L(x)$. The distribution far from these surfaces is given by $P(x; L_{\tau}/2) = \psi_{\mu}^R(x)\psi_{\mu}^L(x)$. In the localized regime, the imaginary gauge transformation for $\psi_{\mu}^R$ and $\psi_{\mu}^L$ describes the displacement of the flux line at the surfaces, while the bulk distribution $P(x; L_{\tau}/2)$ is independent of $\hbar$, consistent with the transverse Meissner effect. 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 $\tau^*$. 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 $\langle x \rangle - \langle x \rangle_{\infty} \propto e^{-\tau|\Delta\epsilon_1|/\hbar}$, where $\Delta\epsilon_1$ 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 the displacement has the stretched exponential form

$$\langle x \rangle - \langle x \rangle_{\infty} \propto e^{-\tau|\Delta\epsilon_1|/\hbar} \exp[-a(\tau/\tau^*)^{1/(d+1)}],$$

where $\langle x \rangle$ is the center of the localized state in the bulk, the penetration depth is given by $\tau^* \equiv g(\mu)\hbar^{d+1}/(\hbar\kappa(\mu) - \hbar)^d$, 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 $\tau^* \sim \xi^\perp_1$, where $\xi^\perp_1 \sim 1/(\hbar\kappa - \hbar)$ is the diverging surface localization length near the transition.

For the derivation of the above, we expand $P(x; \tau)$ with respect to the eigenfunctions. In the limit $L_{\tau} \to \infty$, we have

$$P(x; \tau) \simeq \langle x | \psi_{\mu} | x \rangle \sum_n c_n \exp[-\tau|\Delta\epsilon_n|/\hbar]$$

where $\Delta\epsilon_n \equiv \epsilon_n - \mu$. $\langle \psi_{\mu} | x \rangle = \psi_{\mu}^L(x)$ 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 $\sum_{\infty}$ is restricted to states with energies $\epsilon > \mu$. The asymptotic form for localized states now leads to

$$\langle x \rangle - \langle x \rangle_{\infty} \sim \sum_n c_n e^{-f_n/\hbar},$$

where $f_n(\tau) \equiv \langle \hbar x_n - \hbar \cos \theta_n | x_n + \tau \Delta\epsilon_n, r_n \equiv |x_n - x_n|, \cos \theta_n \equiv \hbar \cdot (x_n - x_n)/|h| r_n$, and the $\{c_n\}$ are additional constant factors. Upon setting $g(\mu)\hbar^{d+1}/\hbar\kappa(\mu) - \hbar)^d \sim 1$, we find that the two terms in $f_n$ compete with each other; in other words, the further the flux line hops, 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 $\theta_n$, we arrive at Eq. (3). We expect that a similar relaxation process governs lines relaxing from the surface to occupied states with $\epsilon < \mu$ as $\tau \to \infty$. For $d = 1$ and randomly distributed column positions, rare events like exceptionally small hopping matrix elements will alter Eq. (3) for very large $\tau$, similar to flux lines pinned by parallel, randomly placed grain boundaries.

The behavior of the flux-line tilt modulus (inverse boson superfluid density) and flux-flow resistivity above the mobility edge may be obtained using the methods of Ref. [1].

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*On leave of absence from Department of Physics, University of Tokyo, Hongo, Bunkyo, Tokyo 113, Japan.

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