Non-Hermitian delocalization from Hermitian Hamiltonians

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Here we show that using Galilean transformations the non-Hermitian delocalization phenomenon, which is relevant in different fields, such as bacteria population (e.g., Bacillus subtilis), vortex pinning in superconductors, and stability solutions of hydrodynamical problems discovered by Hatano and Nelson [Phys. Rev. Lett. **77**, 5706 (1996)], can be obtained from solutions of the time-dependent Schrödinger equation with a Hermitian Hamiltonian. Using our approach, one avoids the numerical complications and instabilities which result form the calculations of left and right eigenfunctions of the non-Hermitian Hamiltonian which are associated with the non-Hermitian delocalization phenomenon. One also avoids the need to replace the non-Hermitian Hamiltonian $\hat{\mathcal{H}}$ by a supermatrix with twice the dimension of $\hat{\mathcal{H}}$, where the complex frequencies serve as variational parameters rather than eigenvalues of $\hat{\mathcal{H}}$.

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Nelson and co-workers [1–3] and Feinberg and Zee [4] studied the time evolution of spatial fluctuations in inhomogeneous systems by solving the time-dependent Schrödinger-like equation

$$\hat{\mathcal{H}}\psi = -\frac{\partial \psi}{\partial t}, \tag{1}$$

where $\hat{\mathcal{H}}$ is a non-Hermitian ''Hamiltonian'' and $\psi(\mathbf{x},t)$ is the vector of reactants (e.g., species of bacteria, nutrients, etc). The non-Hermitian ''Hamiltonian'' is given by

$$\hat{\mathcal{H}} = -D\boldsymbol{\nabla}^2 + \mathbf{v}\cdot\boldsymbol{\nabla} + V(\mathbf{x}), \tag{2}$$

where $V(\mathbf{x})$ is chosen so that *all* growth eigenvalues of $\hat{\mathcal{H}}$ are positive when $\mathbf{v}=0$. For mobile bacteria, D is an effective diffusion constant, whereas for superconductor systems $D=(2m)^{-1}$ and m is the mass of the electron. $\mathbf{v}$ is a drift velocity in studies of water flow in aqueous media, winds, etc., or a non-Hermitian external field originating from the transverse magnetic field [1].

To solve Eqs. (1) and (2) for a square-integrable initial state, $\psi_0 \equiv \psi(\mathbf{x},0)$, one should use the general definition of the inner product $(f|g)$ rather than the usual definition of scalar product $\langle f|g\rangle$. The general definition of the inner product deals with possibilities of having an incomplete spectrum for non-Hermitian Hamiltonians (see, for example, Ref. [5] about the different possible definitions of a general inner product and Ref. [6] about the incomplete spectrum of non-Hermitian Hamiltonians which are represented by complex symmetric matrices).

An incomplete spectrum of a given non-Hermitian Hamiltonian implies that the eigenfunctions of $\hat{\mathcal{H}}$ do not form a complete set and that at least one of the eigenfunctions is ''orthogonal'' to itself in the sense that $(f|f)=0$. When $\hat{\mathcal{H}}$ is represented by a complex symmetric matrix, then $(f|g) \equiv \langle f^*|g\rangle$. The incompleteness of the spectrum of $\hat{\mathcal{H}}$ leads to numerical instabilities when Eqs. (1),(2) are solved numerically.

As we will show here, Eqs. (1),(2) can be solved without the need to solve a non-Hermitian time-dependent Schrödinger-like equation and without the need to introduce a super-Hermitian matrix which has twice the dimension of $\hat{\mathcal{H}}$. When the super-Hermitian matrix is introduced, the complex frequency of $\hat{\mathcal{H}}$ is a parameter in the super-Hamiltonian and not an eigenvalue as in the usual cases. See, for example, Ref. [7] where this technique has been used for calculating the spectra of the non-Hermitian Fokker-Plank operator and Ref. [8] where the complex scaling method for the calculation of the complex resonance eigenvalues is reviewed.

We will show that the solution of Eq. (1), $\psi(\mathbf{x},t)$, can be associated with the solutions of an eigenvalue problem of Hermitian Hamiltonians and all numerical operations involve only multiplications of *Hermitian* matrices.

The solution $\psi(\mathbf{x},t)$ can be given by

$$\psi(\mathbf{x},t) = \exp(-t\mathbf{v}\cdot\boldsymbol{\nabla})\,\phi(\mathbf{x},t), \tag{3}$$

where,

$$\psi(\mathbf{x},0) = \psi_0(\mathbf{x}) \tag{4}$$

and $\phi(\mathbf{x},t)$ is in $\mathcal{L}_2$ (i.e., a square-integrable function) in any given time t. In contrast to the imaginary gauge transformation which has been used before [1–3], the transformation we use here, $\exp(-t\mathbf{v}\cdot\boldsymbol{\nabla})$, is a unitary transformation and has a physical interpretation.

By substituting Eqs. (3) and (2) into Eq. (1), one obtains

$$[-D\boldsymbol{\nabla}^2 + V(\mathbf{x}+\mathbf{v}t)]\,\phi(\mathbf{x},t) = -\frac{\partial}{\partial t}\phi(\mathbf{x},t). \tag{5}$$

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Here we used the fact that $\exp(-t\mathbf{v}\cdot\boldsymbol{\nabla})$ is a translation operator which commutes with the kinetic operator $-D\nabla^2$. Specifically,

$$V(\mathbf{x})\exp(-t\mathbf{v}\cdot\boldsymbol{\nabla})\phi(\mathbf{x})=V(\mathbf{x})\phi(\mathbf{x}-\mathbf{v}t) \tag{6}$$

and, therefore,

$$\exp(+t\mathbf{v}\cdot\boldsymbol{\nabla})V(\mathbf{x})\exp(-t\mathbf{v}\cdot\boldsymbol{\nabla})\phi(\mathbf{x})=V(\mathbf{x}+\mathbf{v}t)\phi(\mathbf{x}). \tag{7}$$

The solutions of Eq. (5) can be described as

$$\phi(\mathbf{x},t)=\sum_{n=0}^{\infty} e^{-\varepsilon_n t}\chi_n(t)\varphi_n(\mathbf{x}+\mathbf{v}t). \tag{8}$$

By substituting Eq. (8) into Eq. (3), the desired solution of Eq. (1) is given by

$$\psi(\mathbf{x},t)=\sum_{n=0}^{\infty} e^{-\varepsilon_n t}\chi_n(t)\varphi_n(\mathbf{x}). \tag{9}$$

The functions φ_n and the decay constants ε_n are, respectively, the eigenfunctions and eigenvalues of the time-independent Schrödinger equation,

$$\hat{H}_0\varphi_n=\varepsilon_n\varphi_n, \tag{10}$$

where $\hat{H}_0$ is a *Hermitian time-independent Hamiltonian*,

$$\hat{H}_0=-D\nabla^2+V(\mathbf{x}). \tag{11}$$

The oscillating time-dependent functions $\chi_n(t)$ are the components of the vector solution of the following linear matrix problem:

$$\mathbf{B}(t)\boldsymbol{\chi}(t)=i\frac{\partial}{\partial t}\boldsymbol{\chi}(t), \tag{12}$$

where

$$B_{m,n}(t)=-ie^{-(\varepsilon_n-\varepsilon_m)t}\langle\varphi_m|\mathbf{v}\cdot\boldsymbol{\nabla}|\varphi_n\rangle \tag{13}$$

and

$$\chi_n(0)=\langle\varphi_n|\psi_0\rangle,\quad n=1,2,\ldots. \tag{14}$$

The proof of Eqs. (12) and (13) is simple. By substituting Eq. (8) into Eq. (5), one obtains

$$-\sum_{n=0}^{\infty} e^{-\varepsilon_n t}\frac{\partial\chi_n(t)}{\partial t}\varphi_n(\mathbf{z})=\sum_{n=0}^{\infty} e^{-\varepsilon_n t}\chi_n(t)\frac{\partial\varphi_n(\mathbf{z},t)}{\partial t}, \tag{15}$$

where

$$\mathbf{z}=\mathbf{x}+\mathbf{v}t. \tag{16}$$

Let us multiply Eq. (15) from the left with $\varphi_m^*(\mathbf{z})$ and carry out the integration over $\mathbf{x}$. Since

$$\langle\varphi_m(\mathbf{x}+\mathbf{v}t)|\varphi_n(\mathbf{x}+\mathbf{v}t)\rangle=\langle\varphi_n|\mathbf{x}|\varphi_m(\mathbf{x})\rangle=\delta_{m,n}, \tag{17}$$

we obtain that

$$-e^{-\varepsilon_m t}\frac{\partial\chi_m(t)}{\partial t}\delta_{m,n}=\sum_n e^{-\varepsilon_n t}\chi_n(t)\times\left\langle\varphi_m(\mathbf{x}+\mathbf{v}t)\left|\frac{\partial}{\partial t}\right|\varphi_n(\mathbf{x}+\mathbf{v}t)\right\rangle. \tag{18}$$

Using the fact that

$$\frac{\partial\mathbf{z}}{\partial t}=\mathbf{v}, \tag{19}$$

we get

$$\left\langle\varphi_m(\mathbf{x}+\mathbf{v}t)\left|\frac{\partial}{\partial t}\right|\varphi_n(\mathbf{x}+\mathbf{v}t)\right\rangle=\langle\varphi_m(\mathbf{x})|\mathbf{v}\cdot\boldsymbol{\nabla}|\varphi_n(\mathbf{x})\rangle \tag{20}$$

and Eqs. (12) and (13) are immediately obtained.

Let us return now to the desired solution as given in Eq. (9). The unknown coefficients $\chi_n(t)$ are solutions of Eq. (12), which can be solved by realizing that

$$\mathbf{B}(t)=\mathbf{D}^{-1}(t)\mathbf{A}\mathbf{D}(t), \tag{21}$$

where $\mathbf{D}(t)=e^{-\mathbf{E}t}$ and $\mathbf{E}$ is the diagonal matrix $E_{m,n}=\varepsilon_n\delta_{m,n}$ which contains the eigenvalues ε_n of $\hat{H}_0$. The matrix $\mathbf{A}$ is a time-independent Hermitian matrix with the matrix elements $A_{m,n}=-i\langle\varphi_m|\mathbf{v}\cdot\boldsymbol{\nabla}|\varphi_n\rangle$. Using the commutator relation $\boldsymbol{\nabla}=-[\hat{H}_0,\mathbf{x}]/2D$, we can express $\mathbf{A}$ as $\mathbf{A}$ $\Sigma_\alpha v_\alpha(\mathbf{E}\mathbf{X}^{(\alpha)}-\mathbf{X}^{(\alpha)}\mathbf{E})/2D$, where $X_{m,n}^{(\alpha)}=\langle\varphi_m|x_\alpha|\varphi_n\rangle$, $\alpha=1,\ldots,3$. Since the eigenfunctions φ_n of $\hat{H}_0$ are real, $\mathbf{X}$ is real and $i\mathbf{A}$ is a real and antisymmetric matrix.

With the help of Eq. (21), we can rewrite Eq. (12) as

$$\left(-i\mathbf{D}(t)\frac{\partial}{\partial t}\mathbf{D}^{-1}(t)+\mathbf{A}\right)\mathbf{D}(t)\chi(t)=0 \tag{22}$$

and, consequently,

$$\left(-i\frac{\partial}{\partial t}+\mathbf{A}-i\mathbf{E}\right)\mathbf{D}(t)\chi(t)=0. \tag{23}$$

Since $\mathbf{A}-i\mathbf{E}$ is a time-independent matrix, the solution of Eq. (23) is given by

$$\boldsymbol{\chi}(t)=\mathbf{D}^{-1}(t)e^{-i(\mathbf{A}-i\mathbf{E})t}\boldsymbol{\chi}(0), \tag{24}$$

where $\chi(0)$ is obtained by projecting the initial state onto the eigenfunctions of the unperturbed Hamiltonian $\hat{H}_0$. The desired solution of Eq. (9),

$$\psi(\mathbf{x},t)=[\varphi(\mathbf{x})]^t\mathbf{D}(t)\boldsymbol{\chi}(t), \tag{25}$$

is immediately obtained by substituting Eq. (24) into Eq. (25),

$$\psi(\mathbf{x},t)=[\varphi(\mathbf{x})]^t e^{-(\mathbf{E}+i\mathbf{A})t}\boldsymbol{\chi}(0), \tag{26}$$

where $[\boldsymbol{\varphi}(\mathbf{x})]^t$ is the transposed vector of $\boldsymbol{\varphi}(\mathbf{x})$, i.e., a vector function with the eigenfunctions $\varphi_n(x)$ of the unperturbed Hamiltonian $\hat{H}_0$ as components.

Since $i\mathbf{A}$ is a real and antisymmetric, the matrix $\mathbf{E}+i\mathbf{A}$ appearing in the exponent in Eq. (26) is also a real matrix. *Its eigenvalues are the eigenvalues of the non-Hermitian Hamiltonian $\hat{H}$ given in Eq. (2)*. This approach enables us to study the delocalization in general systems in a rather simple way as follows.

(1) Calculate the eigenvalues and eigenfunctions of $\hat{H}_0$ [see Eq. (11)].

(2) Use these eigenfunctions as a basis set in the matrix representation of the operator $\mathbf{x}$; i.e., calculate the matrix $X_{m,n}=\langle\varphi_m|\mathbf{x}|\varphi_n\rangle$.

(3) Calculate the eigenvalues and eigenvectors of the real matrix $\mathbf{E}-\Sigma_{\alpha=1}^{3}v_\alpha(\mathbf{E}\mathbf{X}^{(\alpha)}-\mathbf{X}^{(\alpha)}\mathbf{E})/2D$ as a function of $\mathbf{v}$.

This approach allows a straightforward treatment of different type of model systems and also provides a method to analyze the problem on an abstract level with appropriately chosen matrices $\mathbf{E}$ and $\mathbf{X}$.

It is easy to get the conditions for the delocalization phenomenon from Eq. (26). For the sake of simplicity and without loss of generality, let us assume that the drift velocity is in one dimension only, i.e., $\mathbf{v}\cdot\boldsymbol{\nabla}=v\cdot\partial_x$. As an initial state, we take the ground state of the unperturbed Hamiltonian $\hat{H}_0$, i.e., $\psi(x,t=0)=\varphi_0(x)$. We carry out a small time-step propagation and expand Eq. (26) for sufficiently small time step τ in a Taylor series expansion. In such a case the solution is approximately given by

$$\psi(x,\tau)=\varphi_0(x)-\tau\left(\varepsilon_0\varphi_0-\frac{v}{2D}\sum_{n=0}^{\infty}(\varepsilon_n-\varepsilon_0)X_{n,0}\varphi_n(x)\right), \tag{27}$$

where $X_{n,0}=\langle\varphi_n|x|\varphi_0\rangle$. From Eq. (27) one can see immediately that delocalization is obtained when $vX_{n,0}(\varepsilon_n-\varepsilon_0)/2D>\varepsilon_0$. Namely, the perturbation strength parameter v should be large enough to couple ''all'' states. Approximating $X_{n,0}$ by the localization length ξ and skipping the factor $(\varepsilon_n-\varepsilon_0)/2\varepsilon_0$, we deduce the delocalization condition $\xi>D/v$ in agreement with the results of [2].

Our approach is equivalent to the time-independent approach using the eigenfunctions of the unperturbed Hamiltonian as a basis set. However, the Galilean transformation provides additional insight to the problem.

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