Optimal Fluctuations and Tail States of non-Hermitian Operators

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We develop a general variational approach to study the statistical properties of the tail states of a wide class of non-Hermitian operators. The utility of the method, which is a refinement of the instanton approach introduced by Zittartz and Langer, is illustrated in detail by reference to the problem of a quantum particle propagating in an imaginary scalar potential.

Over recent years considerable interest has been shown in the spectral properties of random Fokker-Planck operators, and their application to the dynamics of various classical systems. Of these, perhaps the best known example is the “Passive Scalar” problem which concerns the diffusion of a classical particle subjected to a random velocity field. Here, in contrast to quantum mechanical evolution, the random classical dynamics is typically specified by a linear non-Hermitian operator. Non-Hermitian operators also appear in a number of problems in statistical physics. For example, the statistical mechanics of a repulsive polymer chain can be described in terms of the classical diffusion of a particle subject to a random imaginary scalar potential. Similarly, the statistical mechanics of flux lines in a type II superconductor pinned by a background of impurities can be described as the quantum evolution of a particle in a disordered environment subject to an imaginary vector potential. While these connections have been known for a long time, the ramifications of non-Hermiticity on the nature of the dynamics is only now being fully explored. Beginning with early work on random matrix ensembles, a number of attempts have been made to analyze spectral properties of non-Hermitian operators, and to apply the results to the description of classical systems. For example, it has been found that the generic localization properties of non-Hermitian systems are drastically different from those of their Hermitian counterparts, a fact that can be attributed to an implicit chiral symmetry of non-Hermitian operators.

Previous studies of non-Hermitian operators have been largely based on perturbative schemes, such as the self-consistent Born approximation in the diagrammatic analysis (e.g. Ref. [13]), or the mean field approximation in the field-theoretic approach (e.g. Ref. [18]). However, there are indications that an important role can be played by those parts of the spectrum which are populated by exponentially rare, localized states. These “Lifshitz tail” states, first introduced in the context of semiconductor physics, cannot be treated perturbatively. Since the original works of Lifshitz [24], a number of sophisticated mathematical methods to deal with tail states have appeared, including the instanton technique in statistical field theory [27]. The aim of this letter is to propose a new non-perturbative scheme to investigate properties of the tail states of non-Hermitian operators.

Although our approach is quite general, for clarity, we choose to explain the main features of the method by applying it to possibly the simplest model system. Specifically, we study the Hamiltonian of a quantum particle subject to a random imaginary scalar potential

\[ \hat{H} = -\Delta + iV(\mathbf{r}), \]

where the potential \( V(\mathbf{r}) \) is drawn from a Gaussian \( \delta \)-correlated impurity distribution with zero average, and correlator given by \( \langle V(\mathbf{r})V(\mathbf{r}') \rangle = \gamma \delta(\mathbf{r} - \mathbf{r}') \). Previous studies have shown that, when averaged over realizations of \( V(\mathbf{r}) \), the Feynman propagator of the Hamiltonian above can be identified with the partition function of a self-repelling polymer chain with a contact interaction. Moreover, this model can be used to describe NMR in inhomogeneous materials, where the interplay of diffusion and local variations in the spin precession rate results in the dynamics of magnetization being specified by the operator. Indeed, in the case of the latter, the tails of the operator can be shown to provide a significant contribution to the relaxation of the NMR signal.

![FIG. 1. Support of the states in the complex plane (d = 1). The density of states outside the shaded region is zero if calculated in the self-consistent Born approximation.](image-url)

The Hamiltonian is non-Hermitian, and its eigenvalues \( \epsilon_k \) occupy some area in the complex plane. In the self-consistent Born approximation, the density of complex eigenvalues, defined as \( \rho = \langle \sum_k \delta(x-x_k)\delta(y-y_k) \rangle \), is given by...
\[ \rho(x, y) = \begin{cases} (4\pi\gamma)^{-1}, & |y| < \Delta(x), \\ 0, & |y| > \Delta(x), \end{cases} \]  

where \( x \) and \( y \) are the real and imaginary parts of the complex energy \( \epsilon = x + iy \), \( \Delta(x) = 2\pi\gamma\nu(x) \), and \( \nu(x) \) is the density of states of the clean (\( \gamma = 0 \)) system. The validity of this “mean field” result is restricted to values of \( x \) such that \( \Delta(x) \ll x \), which corresponds to large \( x \) in dimensions lower than four.

According to Eq. (3), there are no states outside the region \( |y| < \Delta(x) \). This can be understood if one recalls that the mean field approximation is essentially a way to determine the self-consistent contribution of typical fluctuations of the random potential. On the other hand, numerical simulations suggest the existence of rare states with \( |y| \gg \Delta(x) \), which are generated by atypically strong fluctuations of \( V(r) \). Such fluctuations occur with an exponentially small probability \( \exp[-W/\gamma] \), where

\[ W = \frac{1}{2} \int V^2(r) \, dr. \]  

For any given configuration \( V(r) \) of the random potential, we will describe \( W \) as the energy associated with the “energy” \( \epsilon \) of a quantum state, which by definition is the eigenvalue of \( \hat{H} \) corresponding to that state. Since strong fluctuations of the disorder potential are suppressed by an exponential factor, states with \( |y| \gg \Delta(x) \) are dominated by those configurations of \( V(r) \) that have the highest statistical weight \( \exp[-W/\gamma] \) or, equivalently, the lowest energy \( W \). Thus, we come to the idea of the optimal fluctuation method, whose rigorous formulation can be given as follows: Amongst all the configurations of \( V(r) \) such that \( \epsilon \) is an eigenvalue of the Hamiltonian \( \hat{H} \), we choose the one that minimizes the energy functional \( W[V(r)] \). The density of states is then given with exponential accuracy by the statistical weight \( \exp[-W/\gamma] \). This approach is similar to that employed in the seminal work by Zittartz and Langer in the treatment of the Hermitian model. There, a saddle-point technique was applied to estimate the functional integral over \( V(r) \). Although based on the same physical ideas, this technique leads to inconsistent results when formally applied to a non-Hermitian problem. Instead, we introduce below a more general variational formulation tailored to the consideration of non-Hermitian operators.

The arguments outlined above are not restricted to the particular form of the Hamiltonian \( \hat{H} \), and can be applied whenever one has to deal with tail states (i.e. localized states created by strong fluctuations of the disorder potential). Formally, the limitations of this scheme are set by the inequality \( W_{\text{min}}(x,y) \gg \gamma \), which defines a certain area in the complex plane of eigenvalues. Below we will show that the precise form of the optimal fluctuation potential can, in general, be determined by solving a system of coupled non-linear equations. For the particular case of the Hamiltonian \( \hat{H} \), we will obtain an explicit form of the solution in the limit \( y \ll x \).

With this preparation, we now turn to the derivation of the variational approach: Our aim is to minimize the functional \( W[V(r)] \) subject to the constraint \( \det(\hat{H} - \epsilon) = 0 \). Account for the latter can be made by introducing two Lagrange multipliers, \( \mu_1 \) and \( \mu_2 \), which in turn leads to the functional

\[ F[V(r)] = W - \mu_1 \Re \det(\hat{H} - \epsilon) - \mu_2 \Im \det(\hat{H} - \epsilon). \]  

If \( \epsilon \) is an eigenvalue of \( \hat{H} \) with left and right eigenfunctions \( \psi^L(r) \) and \( \psi^R(r) \), a spectral decomposition of the Hamiltonian \( \hat{H} \) obtains the identity

\[ \frac{\delta}{\delta V(r)} \det(\hat{H} - \epsilon) = i \psi^L(r) \psi^R(r) \prod_{k,\epsilon_k \neq \epsilon} (\epsilon_k - \epsilon), \]  

where \( \epsilon_k \) denote the remaining eigenvalues of \( \hat{H} \) (i.e. those different from \( \epsilon \)). Equating the functional derivative \( \delta F/\delta V(r) \) to zero, and applying Eq. (3) we obtain

\[ V(r) = \lambda_1 \Re \psi^L(r) \psi^R(r) + \lambda_2 \Im \psi^L(r) \psi^R(r), \]  

where \( \lambda_1 \) and \( \lambda_2 \) denote redefined Lagrangian multipliers. When combined with the eigenvalue equations

\[ \hat{H} \psi^R(r) = \epsilon \psi^R(r), \quad \hat{H} \psi^L(r) = \epsilon^* \psi^L(r), \]  

and with the binormality condition

\[ \int dr \psi^L(r) \psi^R(r) = 1, \]  

Eq. (4) defines a closed system of non-linear equations for \( \psi^R, \psi^L, \lambda_1, \lambda_2 \), which has to be solved in order to extract the optimal configuration \( V(r) \) of the disorder potential.

Note that Eq. (5) depends explicitly on the nature of the impurity distribution and on the structure of the operator at hand, whereas Eqs. (3) and (4) are universal. To treat other random non-Hermitian operators, one simply has to modify Eq. (3) accordingly. For example, in the case of the Passive Scalar problem, where the disorder has the form of a random velocity field, the analogue of Eq. (3) relates the optimal configuration of the random velocity field to spatial derivatives of the eigenfunctions \( \psi^R, \psi^L \).

For the Hamiltonian \( \hat{H} \), further progress can be made by exploiting symmetry properties. From the relation \( \hat{H}^\dagger = \hat{H}^* \) it follows that one can constrain the complex wavefunctions to obey the relation \( \psi^R(r) = \psi^L(r) \). In doing so, leaving aside the lengthy but straightforward analysis \( (\ref{30}) \), one can show that the following simplifications obtain: Firstly, Eq. (8) can be effectively disregarded; secondly, by performing a complex rotation...
of \( \psi(\mathbf{r}) \), one finds that arbitrary non-zero values can be assigned to the Lagrange multipliers \( \lambda_1 \) and \( \lambda_2 \). For convenience, we will set \( \lambda_1 = 1, \lambda_2 = 0 \). With these simplifications, focusing initially on the one-dimensional problem, one finds

\[
V = \text{Re} \psi^2, \quad (9)
\]

where the wavefunction \( \psi \) is obtained self-consistently by solving the Schrödinger equation in the potential \( V \),

\[
-\psi'' + iV \psi = \epsilon \psi. \quad (10)
\]

Eqs. (9) and (10), which represent the non-Hermitian analogue of the non-linear Schrödinger equation of Zit- tartz and Langer, are the main result of the program. To complete the program, one should find the localized solution \( \psi \) (which is assumed to be unique) of Eqs. (9) and (10) for each value of \( \epsilon \), and calculate the energy \( W(\epsilon) \) of the corresponding configuration \( V = \text{Re} \psi^2 \) of the potential. Note that, in the derivation of Eqs. (9) and (10), no approximation has been made. However, the applicability of the optimal fluctuation method itself is restricted by the condition \( W_{\text{min}}(\epsilon) \gg \gamma \).

As mentioned above, an analogous calculation can be carried out for other model systems including the Passive Scalar operator

\[
\hat{H}_{\text{ps}} = -\Delta + \mathbf{v}(\mathbf{r}) \cdot \nabla. \quad (11)
\]

Indeed, in the case of a Gaussian distributed incompressible \( (\nabla \cdot \mathbf{v} = 0) \) flow, the tail states of \( \hat{H}_{\text{ps}} \) are found to be governed by equations which have the same form as Eqs. (9) and (10).

In the analysis of Eqs. (9) and (10), it is convenient to interpret the one-dimensional spatial coordinate \( r \) as a time \( t \), and the complex wavefunction \( \psi(t) \) as the position of a fictitious classical particle in the two-dimensional plane. With this interpretation, one can recast Eqs. (9) and (10) in the Lagrangian form,

\[
L = \psi_1^\prime \psi_2^\prime - x \psi_1 \psi_2 - \frac{y}{2} (\psi_1^2 - \psi_2^2) + \frac{1}{4} (\psi_1^2 - \psi_2^2)^2, \quad (12)
\]

and \( \psi = \psi_1 + i \psi_2 \) has been separated into real and imaginary parts. The Lagrangian (12) has at least one invariant of the motion — the classical energy. Although we can not rule out the possibility of this system being integrable, we have been unable to find a second invariant of the motion. Therefore, integrability remains an open question, which deserves a separate investigation.

As follows from Eqs. (9) and (10), the wavefunction of a tail state is defined by the components of the energy, \( x \) and \( y \), which determine the position of the state in the complex plane of eigenvalues. In order to exploit the optimal fluctuation method to its fullest potential, one should analyze these equations over the entire complex plane. However, at present, we do not have a method of finding the exact analytical solution of Eqs. (9) and (10) for arbitrary values of \( x \) and \( y \). Therefore, we will focus on a specific domain, in which an approximate solution can be found.

As we will see later, the density of Lifshitz tails decays exponentially as a function of the distance from the boundary of the “mean field spectrum”, \( |y| = \Delta(x) \). Therefore, the most physically relevant states lie close to the boundary. For such states, the condition \( |y| \ll x \) is satisfied (recall that \( \Delta(x) \ll x \)) allowing the following separation of scales: Since the wavefunction of a tail state oscillates with a high frequency \( \sqrt{x} \), while the amplitude of these oscillations varies at a much lower rate \( |y|/\sqrt{x} \) (the ratio of the two time-scales being \( |y|/x \ll 1 \)), the solution of Eqs. (9) and (10) can be parameterized in the form of a wavepacket,

\[
\psi(t) = \sqrt{2|y|} \left[ \varphi_+ \left( \frac{|y|t}{2\sqrt{x}} \right) e^{i\sqrt{x}t} + \varphi_- \left( \frac{|y|t}{2\sqrt{x}} \right) e^{-i\sqrt{x}t} \right]. \quad (13)
\]

Substituting the parameterization (13) into Eqs. (9) and (10), one obtains an equation for the envelope. Following a standard procedure [34], we neglect the second derivatives of \( \varphi_{\pm} \), and perform the averaging over the intermediate scales. As a result, one obtains a system of parameter-free first-order differential equations for \( \varphi_{\pm}(\tau) \):

\[
\begin{align*}
\varphi_+ & = -\varphi_+ + 5\varphi_+^2 \varphi_- + \varphi_-^3, \\
\varphi_- & = \varphi_- - 5\varphi_+ \varphi_-^2 - \varphi_+^3.
\end{align*} \quad (14)
\]

In general, the solution of equations of this kind, which can easily be computed numerically, yields a universal dimensionless constant in the final result for the density of states. Surprisingly, for the problem at hand, Eqs. (14) can be represented in the form of Hamilton’s equations, wherein \( \varphi_{\pm} \) play the role of the canonical variables, \( \varphi_{\pm} = \pm \partial \mathcal{H}/\partial \varphi_{\pm} \), with the Hamiltonian

\[
\mathcal{H} = -\varphi_+ \varphi_- + \frac{5}{2} \varphi_+^2 \varphi_-^2 + \frac{1}{4} (\varphi_+^4 + \varphi_-^4). \quad (15)
\]

Of the infinite set of solutions, defined by values of \( \mathcal{H} \), we are interested in the localized solution, which corresponds to \( \mathcal{H} = 0 \). Integrating Eqs. (14) along the line \( \mathcal{H} = 0 \), we obtain

\[
\varphi_{\pm}(\tau) = \frac{2e^{\pm \tau}}{\sqrt{e^{4\tau} + e^{-4\tau} + 10}}. \quad (16)
\]

Now, with the help of Eq. (13), we can restore the wavefunction \( \psi(t) \). It has a rather unusual shape shown in Fig. 2(a). The combination of an oscillatory wavefunction modulated by a localized envelope is characteristic of the tail states of non-Hermitian operators. The optimal configuration of \( \mathcal{V}(t) \), which is expressed through
ψ(t) according to Eq. (3), also has the form of localized oscillations (see Fig. 2(b)), and its energy can be straightforwardly determined:

\[ W_{\text{min}}(\epsilon) = \alpha |y| \sqrt{x}, \quad \alpha = \frac{4}{\sqrt{6}} \log(5 + 2\sqrt{6}) \approx 3.744. \]

(17)

Recalling that, in one dimension, \( \nu(x) = 1/(2\pi \sqrt{x}) \), we arrive at the expression for the density of tail states,

\[ \rho(\epsilon) \sim \exp \left[ -\alpha \frac{|y|}{\Delta(x)} \right], \quad \Delta(x) \ll |y| \ll x. \]

(18)

We remark that, in higher dimensions, the spherical symmetry of the optimal potential reduces the problem to being effectively one-dimensional. In this case, one obtains the general result:

\[ \rho(\epsilon) \sim \begin{cases} 
\exp \left[ -\alpha \frac{|y|}{\Delta(x)} \right], & \Delta(x) \ll |y| \ll x, \\
\exp \left[ -\beta \frac{|y|}{\gamma \Delta(x)} \right], & |y| \gg x,
\end{cases} \]

(19)

where the values of the numerical factors \( \alpha \) and \( \beta \) depend on the dimensionality, and \( \Delta(x) = 2\pi \gamma \nu(x) \sim \gamma x^{(d-2)/2} \).

![Fig. 2. Solution of the non-linear Schrödinger equation (9) and (14) for \( x = 8.0, y = 1.0 \). (a) shows the square modulus \(|\psi|^2\) of the complex wavefunction. The optimal fluctuation of the disorder potential \( V = \text{Re}\psi^* \) is shown in (b).](mat/9906279)

For completeness, one should add that in addition to the tail states depicted in Fig. 1 and studied here, the random imaginary scalar potential exhibits another class of exponentially rare states which inhabit the region of very small \( x \to 0 \) [3]. The origin of the latter seems to be associated with large areas in real space which are almost free of disorder. Such states are inaccessible within the present framework.

To summarize, in this paper we have developed a general variational approach to study spectral properties of non-Hermitian operators. Applied to the problem of a particle propagating in a random imaginary scalar potential, one finds that properties of the strongly localized (tail) states are governed by a system of coupled nonlinear dynamical equations. These equations show that tail states associated with the non-Hermitian Hamiltonian exhibit oscillations on scales much shorter than the localization length. Employing a procedure of scale separation, both the density of tail states as well as the corresponding wavefunctions have been determined.

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