


Hellmann-Feynman theorem in non-Hermitian systems

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We revisit the celebrated Hellmann-Feynman theorem (HFT) in the parity-time (\mathcal{PT}) invariant non-Hermitian quantum physics framework. We derive a modified version of HFT by changing the definition of inner product and explicitly show that it holds good for both \mathcal{PT} broken and unbroken phases and even at the exceptional point of the theory. The derivation is extremely general and works for even the \mathcal{PT} noninvariant Hamiltonian. We consider several examples of discrete and continuum variable systems to test our results. We find that, if the eigenvalue goes through a real-to-complex transition as a function of the Hermiticity breaking parameter, both sides of the modified HFT expression diverge at that point. If that point turns out to be an EP of the \mathcal{PT} -invariant quantum theory, then one also sees the divergence at EP. Moreover, we have also demonstrated that using the modified HFT can give rise to a potential numerical advantage for computing the expectation value of many-body operators for interacting many-body Hamiltonian. Finally, we also derive a generalized virial theorem for non-Hermitian systems using the modified HFT, which potentially can be tested in experiments.

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I. INTRODUCTION

The so-called Hellmann-Feynman theorem (HFT) states that the derivative of the system's total energy with respect to a parameter is equal to the expectation value of the derivative of the Hamiltonian of the system with respect to the same parameter [1,2], which is mathematically written as

$$\frac{\partial E_\lambda}{\partial \lambda} = \left\langle \psi_\lambda \left| \frac{\partial \hat{H}_\lambda}{\partial \lambda} \right| \psi_\lambda \right\rangle, \quad (1)$$

where λ is some arbitrary parameter in the Hamiltonian and $|\psi_\lambda\rangle$ is an eigenstate of the system. The origin of this theorem is not very clear. Neither Feynman nor Hellmann was the first to use it. Paul Guttinger may have been the first to derive Eq. (1) in 1932 [3]. Hellmann first proved the theorem in 1937 [4]. Later in 1939, Feynman, who apparently did not know about the earlier works, derived the theorem in his undergraduate thesis and used it to calculate forces in molecules directly [1]. However, the usefulness of HFT in evaluating the expectation values of dynamical quantities in some potential problems have been well demonstrated by several groups [5]. Since its inception, this theorem is widely in use in various branches of physics and chemistry, including high-energy physics [6–20], condensed-matter physics [21–29], machine learning [30], and quantum chemistry [31]. Various issues and discussions regarding its validity for degenerate systems can be found in Refs. [32–34]. Our work aims to explore the hidden power of this theorem, particularly to study its applicability beyond the usual quantum framework.

During the past two and half decades, non-Hermitian physics has become very exciting and secured its position in frontier research in almost all branches of physics [35,36]. Non-Hermiticity can originate from exchanges of energy or particles with an environment and leads to rich properties in quantum dynamics [37–40], localization [41–43], and topology [44–47]. On the other hand, non-Hermitian Hamiltonians also play a very important role in understanding quantum measurement problems [48,49].

While in general non-Hermitian Hamiltonians have complex eigenvalues, by replacing the self-adjoint condition on the Hamiltonian with a much more physical and rather less constraining condition of space-time reflection symmetry known as parity-time (\mathcal{PT}) symmetry [50–52], can have real eigenvalues. Such systems described by \mathcal{PT} -invariant non-Hermitian Hamiltonians can typically be divided into two categories, one in which the eigenvectors respect \mathcal{PT} symmetry and the entire spectrum is real, known as the \mathcal{PT} -unbroken phase, and the system is in the \mathcal{PT} -broken phase when it has at least one complex eigenvalue in its spectrum, and the eigenvector(s) corresponding to those complex values do not respect the \mathcal{PT} symmetry [43–45,53–57]. The phase-transition point is known as the exceptional point (EP). It has been demonstrated that a consistent quantum theory with an entirely real spectrum, a complete set of orthonormal eigenfunctions having positive-definite norms and unitary time evolution in the unbroken phase, can be constructed in a modified Hilbert space equipped with an appropriate positive-definite inner product [58,59]. This field of \mathcal{PT} -symmetric non-Hermitian physics received a huge boost when the consequence of \mathcal{PT} transition was observed experimentally in various analogous systems [35,60–64].

In this work, our main goal is to derive a Hellmann-Feynman-type theorem for non-Hermitian systems. It is to

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be noted that HFT has been used for non-Hermitian systems earlier as well [65–67], however, we aim to obtain an equation for the HFT in the non-Hermitian regime in a detailed manner which was not provided in the earlier works. Given that HFT for Hermitian systems has huge applications in different branches of physics, a similar theorem for non-Hermitian systems can also be extremely useful, especially in the context of open quantum systems. HFT can be used to derive a generalized virial theorem for quantum particles with zero-range or finite-range interactions in an arbitrary external potential [68]. In the case of unitary gas in a harmonic trap, this theorem provides us with a relation between the energy of the system and the trapping energy. Virial theorem for such systems has been verified experimentally in cold atom experiments [69,70]. We construct the generalized virial theorem for non-Hermitian systems, which we believe can be tested in experiments.

The paper is organized as follows. First, we derive the modified HFT in Sec. II. Next, we show the validation of it for discrete models and continuum models in Secs. III and IV, respectively. In Sec. V, we prove the generalized virial theorem for the non-Hermitian system, and, finally, we conclude in Sec. VI.

II. HELLMANN FEYNMAN THEOREM FOR NON-HERMITIAN SYSTEM

First, let us consider a general \mathcal{PT} -invariant, non-Hermitian $\widehat{\mathcal{H}}^\dagger \neq \widehat{\mathcal{H}}$, $[\mathcal{PT}, \widehat{\mathcal{H}}] = 0$ system. Such systems are characterized by right eigenvectors $|R_i\rangle$ and left eigenvectors $\langle L_i|$ as defined by

$$\widehat{\mathcal{H}}|R_i\rangle = E_i|R_i\rangle \quad \widehat{\mathcal{H}}^\dagger\langle L_i| = E_i^*\langle L_i|.$$

These eigenvectors form a complete biorthogonal set [71,72] satisfying $\langle L_i|R_j\rangle = \delta_{ij}$ and $\sum_i |R_i\rangle\langle L_i| = I$. Alternatively, we can introduce a Hermitian metric operator G such that $\langle L_i| = \langle R_i|G$ and use it to define a more general inner product or G -inner product [58,73]. The orthonormality and completeness relations then are expressed in terms of the G -inner product as

$$\langle R_i|R_j\rangle_G = \langle R_i|G|R_j\rangle = \langle L_i|R_j\rangle = \delta_{ij}. \quad (2)$$

The G operator can be calculated for the theory as

$$G = \sum_i |L_i\rangle\langle L_i| = \left[\sum_i |R_i\rangle\langle R_i| \right]^{-1}. \quad (3)$$

The expectation value of an observable O will now be defined with respect to the G -inner product as

$$\langle O\rangle_G = \langle R_i|GO|R_i\rangle = \langle L_i|O|R_i\rangle. \quad (4)$$

It has been demonstrated explicitly in Refs. [58,59,74,75] that $\langle O\rangle_G$ is a real number for any state in the Hilbert space if and only if O satisfies the following condition i.e.,

$$O^\dagger G = GO.$$

The observables which obey the above condition are called “good observables.”

Now we are in a position to obtain HFT for \mathcal{PT} -invariant non-Hermitian quantum mechanics. We consider our Hamiltonian depends on a real parameter λ and E_λ is the energy

eigenvalue of an arbitrary right eigenstate $|R\rangle$ [note that we drop the suffix i from Eq. (2) to simplify the notation]. Differentiating the equation $\langle L|\widehat{\mathcal{H}}|R\rangle = E_\lambda$ with respect to λ , we obtain

$$\begin{aligned} \frac{\partial E_\lambda}{\partial \lambda} &= \left(\frac{\partial \langle L|}{\partial \lambda} \right) \widehat{\mathcal{H}}|R\rangle + \left\langle L \left| \frac{\partial \widehat{\mathcal{H}}}{\partial \lambda} \right| R \right\rangle + \langle L|\widehat{\mathcal{H}} \left(\frac{\partial |R\rangle}{\partial \lambda} \right) \\ &= E_\lambda \left(\frac{\partial \langle L|}{\partial \lambda} \right) |R\rangle + \left\langle L \left| \frac{\partial \widehat{\mathcal{H}}}{\partial \lambda} \right| R \right\rangle + \langle \widehat{\mathcal{H}}^\dagger GR | \left(\frac{\partial |R\rangle}{\partial \lambda} \right). \end{aligned} \quad (5)$$

On the other hand, $\widehat{\mathcal{H}}^\dagger\langle L| = E_\lambda^*\langle L|$ can be written as $\langle \widehat{\mathcal{H}}^\dagger GR | = E_\lambda \langle R|G$. Using this in the last term of the above equation we obtain

$$\frac{\partial E_\lambda}{\partial \lambda} = E_\lambda \frac{\partial \langle L|R\rangle}{\partial \lambda} + \left\langle L \left| \frac{\partial \widehat{\mathcal{H}}}{\partial \lambda} \right| R \right\rangle. \quad (6)$$

$$\boxed{\frac{\partial E_\lambda}{\partial \lambda} = \left\langle L \left| \frac{\partial \widehat{\mathcal{H}}}{\partial \lambda} \right| R \right\rangle = \left\langle R \left| G \frac{\partial \widehat{\mathcal{H}}}{\partial \lambda} \right| R \right\rangle.} \quad (7)$$

Remarkably, this proof is extremely general and should work for any non-Hermitian Hamiltonian even if the Hamiltonian is not \mathcal{PT} invariant, i.e., $[\widehat{\mathcal{H}}, \mathcal{PT}] \neq 0$. We can explicitly obtain this relation for the unbroken case of a \mathcal{PT} -invariant Hamiltonian using the good observable condition $\widehat{\mathcal{H}}^\dagger G = G\widehat{\mathcal{H}}$ as well.

Next, we consider explicit examples of non-Hermitian Hamiltonian, discrete and continuum to verify our claim.

III. DISCRETE MODELS

First, we consider a \mathcal{PT} -symmetric non-Hermitian two-level system [53] described by the following Hamiltonian:

$$H_{2 \times 2} = \begin{pmatrix} i\lambda & -1 \\ -1 & -i\lambda \end{pmatrix}.$$

This system undergoes a \mathcal{PT} phase transition at $\lambda_c = 1$ The eigenvalues are $E_\pm = \pm(1 - \lambda^2)^{1/2}$ and corresponding right eigenvectors in the unbroken phase i.e., $\lambda < 1$ are given by,

$$|R_+\rangle = \frac{i}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{-\frac{i\alpha}{2}} \\ -e^{\frac{i\alpha}{2}} \end{pmatrix},$$

$$|R_-\rangle = \frac{1}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{\frac{i\alpha}{2}} \\ e^{-\frac{i\alpha}{2}} \end{pmatrix},$$

where $\sin \alpha = -\lambda$. The G operator in the unbroken phase reads

$$G^u = \frac{1}{\sqrt{1 - \lambda^2}} \begin{bmatrix} 1 & i\lambda \\ -i\lambda & 1 \end{bmatrix}. \quad (8)$$

Now it is straightforward to check that, for $|R_+\rangle$ in the unbroken phase,

$$\left\langle R_+ \left| G^u \frac{\partial H_{2 \times 2}}{\partial \lambda} \right| R_+ \right\rangle = -\frac{\lambda}{\sqrt{1 - \lambda^2}} = \frac{\partial E_+}{\partial \lambda}. \quad (9)$$

Even in the broken phase, one obtains

$$\left\langle R_+ \left| G^b \frac{\partial H_{2 \times 2}}{\partial \lambda} \right| R_+ \right\rangle = i \frac{\lambda}{\sqrt{\lambda^2 - 1}} = \frac{\partial E_+}{\partial \lambda}, \quad (10)$$

where G^b is the G matrix in the broken phase. $|R_-\rangle$ also satisfies Eq. (7) for both broken and unbroken phases. This confirms the validity of the modified HFT for this model. We have explicitly verified the validity of modified HFT even for 4×4 \mathcal{PT} -symmetric non-Hermitian system (see Appendix A for details).

Noninteracting discrete system. Next, we study an $L \times L$ version of the above 2×2 ; such a Hamiltonian can be interpreted as a model of noninteracting fermions in a one-dimensional (1d) lattice with an open boundary and described by the following Hamiltonian:

$$H_0 = - \sum_{j=1}^{L-1} (\hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.}), \quad (11)$$

where \hat{c}_j^\dagger (\hat{c}_j) is the fermionic creation (annihilation) operator at site j , which satisfies standard anticommutation relations. L is the size of the system, which we set to be an even number for all our calculations (we choose the lattice spacing as unity).

To make the Hamiltonian \mathcal{PT} symmetric and non-Hermitian, we add a local term at site $L/2$ and $L/2 + 1$. The \mathcal{PT} -symmetric Hamiltonian reads

$$H_{L \times L} = H_0 + i\lambda(\hat{n}_{L/2} - \hat{n}_{L/2+1}), \quad (12)$$

where, $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ is the number operator and λ is identified as the Hermiticity-breaking parameter. While under parity transformation $c_j \rightarrow c_{L-j+1}$, the time-reversal symmetry operation changes $i \rightarrow -i$. Hence, $H_{L \times L}$ remains invariant under \mathcal{PT} transformation, which implies $[H_{L \times L}, \mathcal{PT}] = 0$. For nonzero values of λ , $H_{L \times L}$ is non-Hermitian. For $L = 2$, this model is identical to the two-level system we have studied previously. For any finite and even L , the Hamiltonian (12) shows a \mathcal{PT} transition at $\lambda = 1$ [53]. Like a two-level system, all eigenvalues are completely complex for $\lambda > 1$. Note that it is not necessary to have all eigenvalues be complex in the \mathcal{PT} -broken phase; in contrast, we only need two of them to be complex. Figure 1 shows excellent agreement between left-hand side (LHS) and right-hand side (RHS) of Eq. (7) [which we refer to as $f(\lambda)$]. Interestingly, while Eq. (7) remains valid even when we approach the EP, i.e., $\lambda = 1$, the numerical value seems to diverge at the EP. This is already clear for two-level systems from Eqs. (9) and (10), which diverge in the $\lambda \rightarrow 1$ limit. While this result tempts us to conclude that, near the EP, the LHS and RHS of Eq. (7) always diverge, it turns out to be not always true.

Next, we study another model that is described by the Hamiltonian

$$\tilde{H}_{L \times L} = H_0 + i\lambda \sum_{j=L/2-r}^{L/2+r} (-1)^j \hat{n}_j, \quad (13)$$

where we chose $r = 2$. Hamiltonian (13) is interesting in the sense that in the \mathcal{PT} broken phase of this model, not all eigenvalues are completely complex. A parameter regime exists when some eigenvalues are completely real, even in

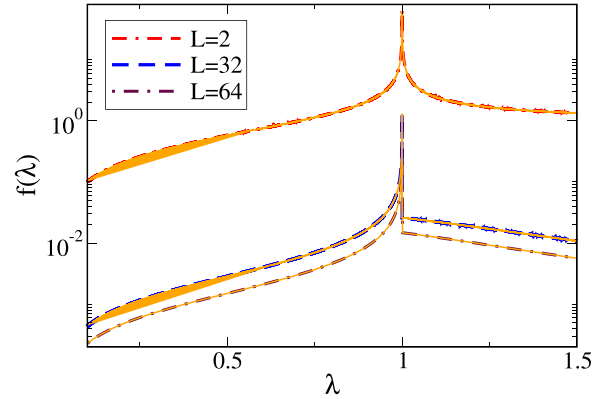


FIG. 1. Comparison between the absolute values of RHS and LHS of the Eq. (7) for Hamiltonian Eq. (12) in solid lines and dashed and dashed-dot lines, respectively, for different values of L .

the broken phase. We find that while all eigenvalues and eigenstates of modified HFT are valid, the divergence of the LHS and RHS of Eq. (7) near the EP occurs only for those eigenstates that show a real-to-complex transition at the EP. We refer to a point EP as soon as any two eigenvalues of the entire spectrum become complex from real. Eigenstates correspond to eigenvalues that remain real even after the EP, for which no divergence has been observed at the EP (see Fig. 2). We focus on three eigenstates of the Hamiltonian (13) for $L = 64$ in Fig. 2 and also plot the imaginary part of those eigenvalues as a function of λ . Note that while the EP of this model corresponds to $\lambda_c \simeq 0.48$ [53,59], some states show no signature of divergence in $f(\lambda)$ at the EP. However, it seems that $f(\lambda)$ tends to diverge when that eigenvalue also shows a real-to-complex transition. Hence, we conjecture the divergence of Eq. (7) is because of the real-to-complex transition of eigenvalues, and it explicitly has nothing to do with the EP. Also, we believe that a variant of our lattice models with gain and loss is experimentally realizable in an ultracold fermionic

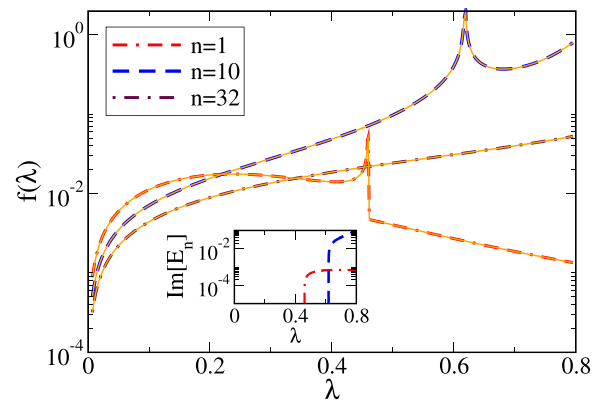


FIG. 2. Comparison between the absolute value of RHS and LHS of the Eq. (7) for Hamiltonian Eq. (13) in solid lines and dashed and dashed-dot lines, respectively, for $L = 64$ and different eigenstates. Inset shows the imaginary part of those eigenvalues as a function of λ . Note that the $n = 32$ plot is missing from the inset, that is because imaginary part of that eigenvalue is zero for $\lambda \leq 0.8$.

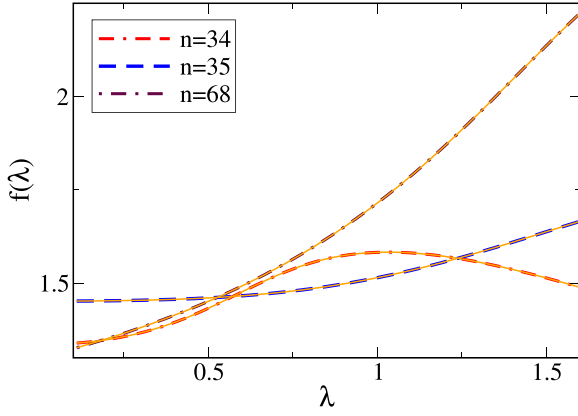


FIG. 3. Comparison between the absolute value of the RHS and LHS of Eq. (7) for Hamiltonian (14) ($g = 0.1$) in solid lines and dashed and dashed-dot lines, respectively, for $L = 8$ and different eigenstates.

system, and the modified HFT can be verified within the weak measurement framework [64,76].

Many-body interacting discrete system. So far, we have focused on noninteracting systems. Next, we turn our attention to interacting many-body systems. We consider a system that is governed by the following Hamiltonian:

$$H_I = - \sum_{j=1}^{L-1} (\hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.}) + ig(\hat{n}_{L/2} - \hat{n}_{L/2+1}) + \lambda \sum_{j=1}^{L-1} \hat{n}_j \hat{n}_{j+1}, \quad (14)$$

where λ is the nearest-neighbor interaction strength. Figure 3 clearly shows that the modified HFT gets satisfied for the interacting Hamiltonian as well. These results also suggest that, in order to calculate the expectation value of $\langle \sum_{j=1}^{L-1} \hat{n}_j \hat{n}_{j+1} \rangle$ with respect to eigenstates of the Hamiltonian H_I , one does not necessarily need to compute the eigenstates of $H_I(\lambda)$, but instead simply calculating the energy eigenvalues E_n is sufficient, given $\langle L_n | dH_I/d\lambda | R_n \rangle = \langle L_n | \sum_{j=1}^{L-1} \hat{n}_j \hat{n}_{j+1} | R_n \rangle = dE_n/d\lambda$. Computation-wise, calculating eigenvalues is much less costly compared with calculating eigenstates of $N \times N$ matrices; while computation costs in both cases are $O(N^3)$, the prefactor is much smaller for eigenvalue computation. Given the Hilbert-space dimension N scales exponentially with system size for many-body systems, computation using the modified HFT could be a significant advantage in evaluating the expectation value of certain many-body operators for such systems.

IV. MODELS OF CONTINUUM VARIABLES

Now we consider models of continuum variables as an example; we take a two-dimensional (2d) anharmonic oscillator with a non-Hermitian interaction term [57], which is described by

$$H_{2d} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2 + i\lambda xy, \quad (15)$$

where λ is real and $\omega_x \neq \omega_y$. This system can be solved exactly. The energy eigenvalues and the right eigenvectors are given by

$$R_{n_1, n_2} = N e^{-\frac{m}{2\hbar} [(C_1 X^2 + C_2 Y^2)]} H_{n_1}(\alpha_1 X) H_{n_2}(\alpha_2 Y),$$

$$E_{n_1, n_2} = \left(n_1 + \frac{1}{2}\right) \hbar C_1 + \left(n_2 + \frac{1}{2}\right) \hbar C_2, \quad (16)$$

where

$$X = \sqrt{\frac{k+1}{2}} x - i\sqrt{\frac{k-1}{2}} y, \quad Y = i\sqrt{\frac{k-1}{2}} x + \sqrt{\frac{k+1}{2}} y,$$

$$C_1 = \sqrt{\frac{1}{2} \left(\omega_+^2 - \frac{\omega_-^2}{k} \right)}, \quad C_2 = \sqrt{\frac{1}{2} \left(\omega_+^2 + \frac{\omega_-^2}{k} \right)},$$

and

$$\alpha_1 = \sqrt{m C_1 / \hbar}, \quad \alpha_2 = \sqrt{m C_2 / \hbar},$$

where

$$\omega_+^2 = \omega_y^2 + \omega_x^2, \quad \omega_-^2 = \omega_y^2 - \omega_x^2,$$

$$\frac{1}{k} = \sqrt{1 - \frac{\lambda^2}{\lambda_c^2}}, \quad \lambda_c = \frac{m\omega_-^2}{2}.$$

The left eigenvectors are given by

$$L_{n_1, n_2} = N e^{-\frac{m}{2\hbar} [(C_1^* X^{*2} + C_2^* Y^{*2})]} H_{n_1}(\alpha_1^* X^*) H_{n_2}(\alpha_2^* Y^*), \quad (17)$$

where $\alpha_1^* = (\frac{m C_1^*}{\hbar})^{1/2}$ and $\alpha_2^* = (\frac{m C_2^*}{\hbar})^{1/2}$.

The modified HFT in the case of continuum models is written in the integral form as

$$\frac{\int (L_{n_1, n_2}^*) \frac{\partial H_{2d}}{\partial \lambda} (R_{n_1, n_2}) dx dy}{\int (L_{n_1, n_2}^*) (R_{n_1, n_2}) dx dy} = \frac{\partial E_{n_1, n_2}}{\partial \lambda}. \quad (18)$$

It is straightforward to show that, when $n_1 = n_2$, the energy eigenvalues are real, and the eigenvectors are \mathcal{PT} symmetric over all values of λ . We have explicitly shown that the LHS and RHS of Eq. (19) are the same for ground state ($n_1 = n_2 = 0$) (see Appendix B for details).

Next we consider some of the low-lying excited states. The energy eigenvalues can be real or complex depending on the value of λ . We have plotted the absolute value of LHS and RHS of the modified HFT for all these states in Fig. 4 to check the validity of the theorem. Note that we have also checked explicitly for (1,0), (2,0), the real and imaginary parts of the LHS and RHS of the Eq. (19) separately (see Appendix B). We also find that $f(\lambda)$ for the first excited state diverges near $\lambda = 4$ and at the same value of λ the eigenvalue of the first excited state also shows a real-to-complex transition. This result strengthens our previous claim, i.e., the divergence of $f(\lambda)$ corresponds to the real-to-complex transition of the eigenvalues.

V. VIRIAL THEOREM FOR NON-HERMITIAN SYSTEM

A generalized virial theorem has been derived for N particles quantum system [68], with arbitrary statistics and dispersion relations. One can consider a general Hamiltonian,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}' + U(r_1, \dots, r_N), \quad (19)$$

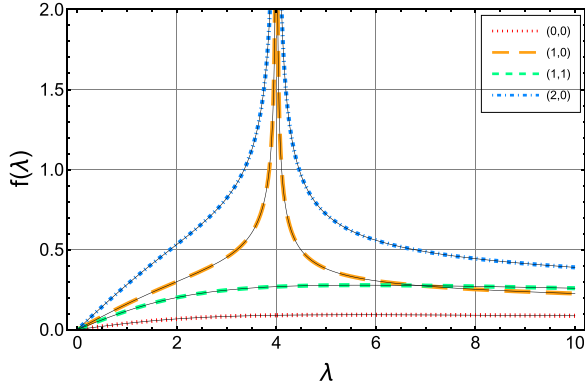


FIG. 4. Comparison between the absolute value of $\langle \partial \widehat{\mathcal{H}} / \partial \lambda \rangle_G$ and $\partial E_{n_1, n_2} / \partial \lambda$ for both broken and unbroken regions for the states $(n_1, n_2) = (0, 0)$, $(1, 0)$, $(1, 1)$, and $(2, 0)$. The dotted, dashed lines indicate the LHS and solid black lines indicate the RHS of Eq. (19).

where $\widehat{\mathcal{H}}$ and its domain depend on p parameters l_1, \dots, l_p which have the dimension of a length, and $U(r_1, \dots, r_N)$ is an arbitrary function, where r_i is the position of particle i . Using HFT for the Hermitian system, it has been shown in Ref. [68] that, for any stationary state energy E , the following relation holds:

$$E = \left\langle U + \frac{1}{2} \sum_{i=1}^N r_i \cdot \nabla U(r_i) \right\rangle - \frac{1}{2} \sum_{q=1}^p l_q \frac{\partial E}{\partial l_q}. \quad (20)$$

If $\widehat{\mathcal{H}}$ is non-Hermitian, it is straightforward to derive a generalized version of the virial theorem using the modified HFT. It just reads

$$E = \left\langle U + \frac{1}{2} \sum_{i=1}^N r_i \cdot \nabla U(r_i) \right\rangle_G - \frac{1}{2} \sum_{q=1}^p l_q \frac{\partial E}{\partial l_q}. \quad (21)$$

Next, we take a concrete example of 1d non-Hermitian harmonic oscillator with complex angular frequency; the Hamiltonian reads

$$H_{1d} = \frac{p^2}{2} + \frac{1}{2} \Omega^2 x^2, \quad (22)$$

where $\Omega = \omega_1 + i\omega_2$ and $\omega_1 \neq 0$. Note that this Hamiltonian is not \mathcal{PT} invariant. However, given that our modified HFT holds even for the Hamiltonian, which is not \mathcal{PT} invariant, one can still use the modified HFT to derive the generalized virial theorem (22).

In ultracold experiments, if one only has the lattice without trapping potential, the atoms can wander around and will not stay together. If one is interested in understanding the role of many-body interaction or even increasing the time of experiments by reducing the kinetic energy, the atoms need to be kept together using some trapping potential. The trapping energy for such a non-Hermitian system is given by

$$\tilde{E}_{\text{tr}} = \frac{1}{2} \langle U(x) + \frac{1}{2} x \cdot \nabla_x U(x) \rangle_G. \quad (23)$$

We have

$$U = \frac{1}{2} \Omega^2 x^2. \quad (24)$$

Therefore, Eq. (24) implies

$$\tilde{E}_{\text{tr}} = \frac{1}{2} \langle \frac{1}{2} \Omega^2 x^2 + \frac{1}{2} x \cdot \nabla (\frac{1}{2} \Omega^2 x^2) \rangle_G = \frac{1}{2} \langle \Omega^2 x^2 \rangle_G. \quad (25)$$

Using the definition of the G -inner product given in Eq. (4), we now deduce Eq. (26) for the ground state and all the excited states.

For ground state, the left eigenvector of H_{1d} is given by

$$L_0 = \left(\frac{\omega_1 - i\omega_2}{\pi} \right)^{\frac{1}{4}} e^{-\frac{\omega_1 x^2}{2}} e^{\frac{i\omega_2 x^2}{2}}, \quad (26)$$

and right eigenvector of H_{1d} is given by

$$R_0 = \left(\frac{\omega_1 + i\omega_2}{\pi} \right)^{\frac{1}{4}} e^{-\frac{\omega_1 x^2}{2}} e^{-\frac{i\omega_2 x^2}{2}}. \quad (27)$$

Therefore, Eq. (26) implies

$$\begin{aligned} \tilde{E}_{\text{tr}0} &= \frac{\int (L_0^*) \frac{1}{2} \Omega^2 x^2 (R_0) dx}{\int (L_0^*) (R_0) dx} \\ &= \frac{\int e^{-\omega_1 x^2} e^{-i\omega_2 x^2} \frac{1}{2} \Omega^2 x^2 dx}{\int e^{-\omega_1 x^2} e^{-i\omega_2 x^2} dx} \\ &= \frac{1}{4} \Omega = \frac{1}{2} E_0, \end{aligned} \quad (28)$$

where E_0 is the ground-state energy of the Hamiltonian (23).

One can also compute trapping energy for the n th eigenstate. We have

$$x = \frac{1}{\sqrt{2\Omega}} (a^\dagger + a) \quad (29)$$

and

$$p = i\sqrt{\frac{\Omega}{2}} (a^\dagger - a), \quad (30)$$

such that

$$a|n\rangle = \sqrt{n}|n-1\rangle \text{ and } a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad (31)$$

where $|n\rangle$ is the n th state of H_{1d} , also, the right eigenvector $|R_n\rangle$ of H_{1d} (i.e., $|R_n\rangle = |n\rangle$).

Similarly,

$$H_{1d}^\dagger = \frac{p^2}{2} + \frac{1}{2} \Omega^{*2} x^2, \quad (32)$$

and we have

$$x = \frac{1}{\sqrt{2\Omega^*}} (b^\dagger + b) \quad (33)$$

and

$$p = i\sqrt{\frac{\Omega^*}{2}} (b^\dagger - b), \quad (34)$$

such that

$$b|\bar{n}\rangle = \sqrt{\bar{n}}|\bar{n}-1\rangle \text{ and } b^\dagger|\bar{n}\rangle = \sqrt{\bar{n}+1}|\bar{n}+1\rangle, \quad (35)$$

where $|\bar{n}\rangle$ is the \bar{n} th state of H_{1d}^\dagger , also, the left eigenvector $|L_n\rangle$ of H_{1d} (i.e., $|L_n\rangle = |\bar{n}\rangle$).

Therefore, by using Eq. (4), we can derive the trapping energy for n th-eigenstate as

$$\begin{aligned}\tilde{E}_{tr,n} &= \langle L_n | \frac{1}{2} \Omega^2 x^2 | R_n \rangle = \langle \bar{n} | \frac{1}{2} \Omega^2 x^2 | n \rangle \\ &= \frac{1}{2} \Omega^2 \left(\frac{1}{2\Omega} \right) \langle \bar{n} | a^{\dagger 2} + a^2 + a^\dagger a + a a^\dagger | n \rangle \\ &= \frac{\Omega}{4} \langle \bar{n} | 2n + 1 | n \rangle \\ &= \frac{1}{2} \left(n + \frac{1}{2} \right) \Omega = \frac{1}{2} E_n,\end{aligned}\quad (36)$$

where E_n corresponds to eigenenergy of the n th state. The relation between the energy eigenvalue and the trapping energy is the same even for the Hermitian harmonic oscillator.

VI. CONCLUSIONS

In this work, we derive the modified HFT for the non-Hermitian system. Our modified HFT works for both \mathcal{PT} -invariant and noninvariant systems. The derivation is extremely general. However, given that the Hamiltonian is a good observable in the \mathcal{PT} -symmetric phase of the \mathcal{PT} -invariant system, only in that phase is the LHS and RHS of the modified HFT in Eq. (7) guaranteed to be completely real. Moreover, if the eigenvalue goes through a real-to-complex transition as a function of the Hermiticity-breaking parameter, the LHS and RHS of the modified HFT diverge at that point. If that point is an EP of the \mathcal{PT} -invariant quantum theory, then one sees the divergence at EP as well; otherwise, both sides of Eq. (7) can be finite at EP as well. We test our results for different discrete and continuum models; some of those models have already been experimentally realized and have a huge technological application as a quantum sensor [64]. We also have demonstrated the validity of the modified

HFT for many-body interacting systems and moreover, show that the modified HFT allows one to compute the expectation of a many-body operator only from the eigenvalue spectrum (eigenvectors are not required). This gives rise to a significant numerical advantage in solving many-body interacting problems, given that eigenvector computation is much more numerically costly than calculating the eigenvalues for a non-Hermitian matrix.

Finally, we also derive a generalized virial theorem for non-Hermitian systems and show that, for a harmonic oscillator with complex frequency, the system's energy is twice the trapping energy, precisely what one observes for a Hermitian harmonic oscillator. For the Hermitian system, the trapping potential energy E_{tr} has been computed from the density profile [77,78] and the released energy $E - E_{tr}$ from a time-of-flight experiment [79]. Note that, recently, there has been an experimental proposal to compute the G -inner product for a non-Hermitian system using weak measurement [76]. We believe the same strategy can be used to compute both energy and trapping energy of the non-Hermitian system, hence the experimental verification of the virial theorem for the non-Hermitian system should be possible. Moreover, given that DNA-unzipping transition can be effectively described by a non-Hermitian Hatano-Nelson model [43,80], it will be interesting in the future to compute the critical force for the DNA-unzipping transition using the modified HFT.

ACKNOWLEDGMENTS

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APPENDIX A: FOUR-LEVEL SYSTEM

We consider a particular 4×4 non-Hermitian Hamiltonian [53]:

$$H_{4 \times 4} = \begin{pmatrix} i\lambda & -1 & 0 & 0 \\ -1 & -i\lambda & -1 & 0 \\ 0 & -1 & i\lambda & -1 \\ 0 & 0 & -1 & -i\lambda \end{pmatrix}.$$

The eigenvalues and right eigenfunctions for this system are calculated as

$$E_1 = -\sqrt{\frac{3 - \sqrt{5} - 2\lambda^2}{2}}, \quad E_2 = \sqrt{\frac{3 - \sqrt{5} - 2\lambda^2}{2}}, \quad E_3 = -\sqrt{\frac{3 + \sqrt{5} - 2\lambda^2}{2}}, \quad E_4 = \sqrt{\frac{3 + \sqrt{5} - 2\lambda^2}{2}},$$

and

$$|R_1\rangle = \begin{pmatrix} u_{1-} \\ v_1 \\ w_{1+} \\ 1 \end{pmatrix}, \quad |R_2\rangle = \begin{pmatrix} u_{1+} \\ v_1 \\ w_{1-} \\ 1 \end{pmatrix}, \quad |R_3\rangle = \begin{pmatrix} u_{2-} \\ v_2 \\ w_{2+} \\ 1 \end{pmatrix}, \quad |R_4\rangle = \begin{pmatrix} u_{2+} \\ v_2 \\ w_{2-} \\ 1 \end{pmatrix},$$

where

$$\begin{aligned} u_{1\pm} &= \frac{1}{4}[2i\lambda(1 + \sqrt{5}) \pm (\sqrt{2} + \sqrt{10})\sqrt{3 - \sqrt{5} - 2\lambda^2}], \\ u_{2\pm} &= \frac{1}{4}[2i\lambda(1 - \sqrt{5}) \pm (\sqrt{2} - \sqrt{10})\sqrt{3 + \sqrt{5} - 2\lambda^2}], \quad v_1 = \frac{(1 - \sqrt{5})}{2}, \quad v_2 = \frac{(1 + \sqrt{5})}{2}, \\ w_{1\pm} &= -i\lambda \pm \sqrt{\frac{3 - \sqrt{5} - 2\lambda^2}{2}}, \quad w_{2\pm} = -i\lambda \pm \sqrt{\frac{3 + \sqrt{5} - 2\lambda^2}{2}}. \end{aligned} \quad (\text{A1})$$

We observe that if $\lambda < \lambda_{C_1} = [(3 - \sqrt{5})/2]^{1/2}$, then all eigenvalues are real and if $\lambda_{C_1} < \lambda < \lambda_{C_2} = [(3 + \sqrt{5})/2]^{1/2}$, then two of the eigenvalues are real and two are a complex-conjugate pair. For $\lambda > \lambda_{C_2}$, all four eigenvalues are complex. It can be shown that the system is in the unbroken phase for $\lambda < \lambda_{C_1}$.

We calculate the G metric in the unbroken phase using Eq. (3) as

$$G^u = \frac{1}{10(1 - 3\lambda^2 + \lambda^4)} \begin{bmatrix} 3 - 2\lambda^2 & i\lambda(3 - 2\lambda^2) & -(\lambda^2 + 1) & i\lambda(\lambda^2 - 4) \\ i\lambda(2\lambda^2 - 3) & 2 - 3\lambda^2 & i(\lambda^3 + \lambda) & -(\lambda^2 + 1) \\ -(\lambda^2 + 1) & -i(\lambda^3 + \lambda) & 2 - 3\lambda^2 & i\lambda(3 - 2\lambda^2) \\ -i\lambda(\lambda^2 - 4) & -(\lambda^2 + 1) & i\lambda(2\lambda^2 - 3) & 3 - 2\lambda^2 \end{bmatrix}.$$

We explicitly check that $|R_1\rangle$ satisfies the modified HFT relation in Eq. (7):

$$\frac{\partial E_1}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(-\sqrt{\frac{3 - \sqrt{5} - 2\lambda^2}{2}} \right) = \frac{\sqrt{2}\lambda}{\sqrt{3 - \sqrt{5} - 2\lambda^2}}. \quad (\text{A2})$$

We further calculate

$$\left\langle R_1 \left| G^u \frac{\partial H_{4 \times 4}}{\partial \lambda} \right| R_1 \right\rangle = \frac{\sqrt{2}\lambda}{\sqrt{3 - \sqrt{5} - 2\lambda^2}}, \quad (\text{A3})$$

to establish the modified HFT for the state $|R_1\rangle$,

$$\left\langle R_1 \left| G^u \frac{\partial H_{4 \times 4}}{\partial \lambda} \right| R_1 \right\rangle = \frac{\partial E_1}{\partial \lambda}.$$

In the similar way, it can be shown that other states also satisfy the modified HFT.

Now we consider the system in the broken phase, when $\lambda_{C_1} < \lambda < \lambda_{C_2}$. The eigenvalues in this region are

$$\begin{aligned} E'_1 &= -i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}}, \quad E'_2 = i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}}, \\ E'_3 &= -\sqrt{\frac{3 + \sqrt{5} - 2\lambda^2}{2}}, \quad E'_4 = \sqrt{\frac{3 + \sqrt{5} - 2\lambda^2}{2}}. \end{aligned}$$

The G metric in this region of coupling λ is calculated as

$$G^b = \frac{1}{10(1 - 3\lambda^2 + \lambda^4)} \begin{bmatrix} -\sqrt{5} & -i\lambda\sqrt{5} & -\sqrt{5}(\lambda^2 - 1) & -i\lambda\sqrt{5}(\lambda^2 - 2) \\ i\lambda\sqrt{5} & 2 - (6 + \sqrt{5})\lambda^2 + 2\lambda^4 & i\lambda(\lambda^2 - 1) & g_{2,4} \\ -\sqrt{5}(\lambda^2 - 1) & -i\lambda(\lambda^2 - 1) & -\sqrt{5}\lambda^2 & -i\lambda\sqrt{5} \\ i\lambda\sqrt{5}(\lambda^2 - 2) & g_{4,2} & i\lambda\sqrt{5} & g_{4,4} \end{bmatrix},$$

where $g_{4,2} = g_{2,4} = -1 + (3 + 2\sqrt{5})\lambda^2 - (1 + \sqrt{5})\lambda^4$ and $g_{4,4} = 3 + (3 + \sqrt{5})\lambda^2(-3 + \lambda^2)$.

We find that the states in this broken region also satisfy the modified HFT relation [Eq. (7)]:

$$\frac{\partial E'_1}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(-i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}} \right) = -\frac{i\sqrt{2}\lambda}{\sqrt{-3 + \sqrt{5} + 2\lambda^2}}, \quad (\text{A4})$$

and

$$\left\langle R_1 \left| G^b \frac{\partial H_{4 \times 4}}{\partial \lambda} \right| R_1 \right\rangle = -\frac{i\sqrt{2}\lambda}{\sqrt{-3 + \sqrt{5} + 2\lambda^2}} = \frac{\partial E'_1}{\partial \lambda}, \quad (\text{A5})$$

implying that

$$\left\langle R_1 \left| G_1^b \frac{\partial H_{4 \times 4}}{\partial \lambda} \right| R_1 \right\rangle = \frac{\partial E_1'}{\partial \lambda}.$$

In the similar straightforward manner other states can be shown to satisfy the modified HFT in this broken region. Finally, we consider the region $\lambda > \lambda_{c_2}$, where all eigenvalues are complex. The eigenvalues in this region are calculated as

$$E_1'' = -i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}}, \quad E_2'' = i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}},$$

$$E_3'' = -i\sqrt{\frac{-3 - \sqrt{5} + 2\lambda^2}{2}}, \quad E_4'' = i\sqrt{\frac{-3 - \sqrt{5} + 2\lambda^2}{2}}.$$

The G metric is constructed as

$$G_2^b = \frac{1}{10(1 - 3\lambda^2 + \lambda^4)} \begin{bmatrix} -3 + 2\lambda^2 & i\lambda(-3 + 2\lambda^2) & (\lambda^2 + 1) & -i\lambda(\lambda^2 - 4) \\ i\lambda(-2\lambda^2 + 3) & 2 - 9\lambda^2 + 4\lambda^4 & -i(\lambda^3 + \lambda) & -1 + 7\lambda^2 - 2\lambda^4 \\ (\lambda^2 + 1) & i(\lambda^3 + \lambda) & -2 + 3\lambda^2 & i\lambda(-3 + 2\lambda^2) \\ i\lambda(\lambda^2 - 4) & -1 + 7\lambda^2 - 2\lambda^4 & i\lambda(-2\lambda^2 + 3) & 3 - 16\lambda^2 + 6\lambda^4 \end{bmatrix}.$$

We now check below that $|R_1\rangle$ still satisfies the modified HFT relation as given in Eq. (7). The LHS of the modified HFT is

$$\frac{\partial E_1''}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(-i\sqrt{\frac{-3 + \sqrt{5} + 2\lambda^2}{2}} \right) = -\frac{i\sqrt{2}\lambda}{\sqrt{-3 + \sqrt{5} + 2\lambda^2}}, \quad (\text{A6})$$

which is exactly equal to the RHS of the modified HFT,

$$\left\langle R_1 \left| G_2^b \frac{\partial H_{4 \times 4}}{\partial \lambda} \right| R_1 \right\rangle = -\frac{i\sqrt{2}\lambda}{\sqrt{-3 + \sqrt{5} + 2\lambda^2}} = \frac{\partial E_1''}{\partial \lambda}. \quad (\text{A7})$$

The same is true for all other states. This establishes the verification of the modified HFT for 4×4 system in broken and unbroken phases.

APPENDIX B: HELLMANN-FEYNMAN THEOREM FOR 2D ANHARMONIC OSCILLATOR WITH NON-HERMITIAN INTERACTION

We consider the 2d anharmonic oscillator as described in Eq. (15). We choose the following numerical values for different parameters, $\omega_x = 1$, $\omega_y = 3$, $\hbar = 1$, $m = 1$ for the numerical computations. The critical coupling $\lambda_c = m\omega_-^2/2$ becomes four.

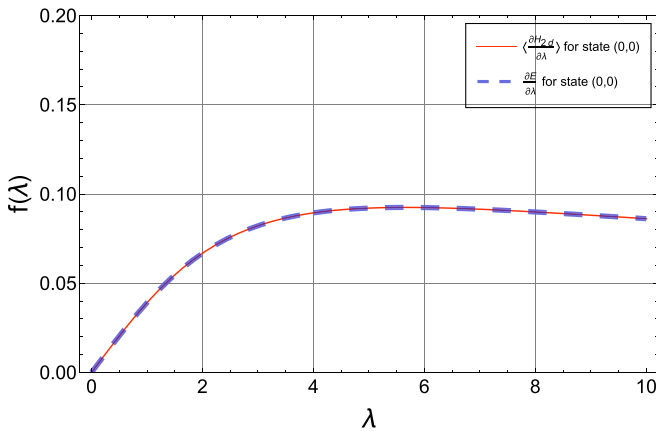


FIG. 5. Comparison between $\langle \partial H_{2d} / \partial \lambda \rangle_{G,(0,0)}$ and $\partial E_{0,0} / \partial \lambda$, represented by the solid and the dashed lines, respectively.

(1) For the unbroken region ($\lambda < \lambda_c$),

$$k^* = k, \quad C_1^* = C_1, \quad C_2^* = C_2; \quad \alpha_1^* = \alpha_1, \quad \alpha_2^* = \alpha_2, \quad (\text{B1})$$

$$X^* = \sqrt{\frac{k+1}{2}}x + i\sqrt{\frac{k-1}{2}}y, \quad (\text{B2})$$

$$Y^* = -i\sqrt{\frac{k-1}{2}}x + \sqrt{\frac{k+1}{2}}y. \quad (\text{B3})$$

(2) For the broken region ($\lambda > \lambda_c$),

$$k^* = -k, \quad C_1^* = C_2 = A + iB; \quad \alpha_1^* = \alpha_2, \quad \alpha_2^* = \alpha_1, \quad (\text{B4})$$

$$X^* = i\sqrt{\frac{k-1}{2}}x - \sqrt{\frac{k+1}{2}}y, \quad (\text{B5})$$

$$Y^* = \sqrt{\frac{k+1}{2}}x + i\sqrt{\frac{k-1}{2}}y, \quad (\text{B6})$$

with

$$A = \frac{1}{2}\sqrt{\frac{\omega_+^4}{k_1^2} + \omega_+^4 + \omega_+^2},$$

$$B = \frac{1}{2}\sqrt{\frac{\omega_+^4}{k_1^2} + \omega_+^4 - \omega_+^2}, \quad \text{and } k_1 = ik. \quad (\text{B7})$$

(1) Now for the ground state $n_1 = 0, n_2 = 0$, the energy eigenvalues $E_{0,0}$ are always real for all values of λ , suggesting that there is no broken phase. We have calculated LHS and RHS of modified HFT analytically to show the equivalence. Using Eqs. (B1) to (B3), Eqs. (16) and (18) are rewritten as

$$R_{0,0} = N \exp \left(-\frac{1}{4} \left\{ (C_1 + C_2)(x^2 + y^2) + (C_2 - C_1) \left[\frac{2i\lambda kxy}{\lambda_c} - k(x^2 - y^2) \right] \right\} \right), \quad (\text{B8})$$

$$L_{0,0} = N \exp \left(-\frac{1}{4} \left\{ (C_1 + C_2)(x^2 + y^2) + (C_1 - C_2) \left[\frac{2i\lambda kxy}{\lambda_c} + k(x^2 - y^2) \right] \right\} \right). \quad (\text{B9})$$

Now, we proceed to verify the modified HFT. Using Eqs. (B8) and (B9), the LHS of Eq. (19) implies

$$\begin{aligned} \left\langle \frac{\partial H_{2d}}{\partial \lambda} \right\rangle_{G,(0,0)} &= \frac{\int (L_{0,0}^*) \frac{\partial H_{2d}}{\partial \lambda} (R_{0,0}) dx dy}{\int (L_{0,0}^*) (R_{0,0}) dx dy} \\ &= \frac{|N|^2 \int ixy e^{-\frac{m}{2\hbar} [(C_1+C_2)(x^2+y^2)+(C_2-C_1)\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy}{|N|^2 \int e^{-\frac{m}{2\hbar} [(C_1+C_2)(x^2+y^2)+(C_2-C_1)\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy} \\ &= -\frac{\lambda(\lambda^2 - 4\sqrt{\lambda^2 + 9} + 4)\sqrt{5 - \sqrt{16 - \lambda^2}}}{(16 - \lambda^2)(\lambda^2 + 8)\sqrt{\lambda^2 + 9}} \\ &\quad - \frac{\lambda(\lambda^2 - 4\sqrt{\lambda^2 + 9} + 4)\sqrt{5 - \sqrt{16 - \lambda^2}}}{4\sqrt{16 - \lambda^2}(\lambda^2 + 8)\sqrt{\lambda^2 + 9}} \\ &\quad + \frac{\lambda(\lambda^2 - 4\sqrt{\lambda^2 + 9} + 4)\sqrt{\sqrt{16 - \lambda^2} + 5}}{4\sqrt{16 - \lambda^2}(\lambda^2 + 8)\sqrt{\lambda^2 + 9}} \\ &\quad - \frac{\lambda(\lambda^2 - 4\sqrt{\lambda^2 + 9} + 4)\sqrt{\sqrt{16 - \lambda^2} + 5}}{(16 - \lambda^2)(\lambda^2 + 8)\sqrt{\lambda^2 + 9}}. \end{aligned} \quad (\text{B10})$$

The RHS of Eq. (19) for the (0,0) state is

$$\frac{\partial E_{0,0}}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(\frac{1}{2} C_1 + \frac{1}{2} C_2 \right) = \frac{\lambda \sqrt{\sqrt{\lambda^2 + 9} - 5}}{2\sqrt{2}\sqrt{\lambda^2 - 16}\sqrt{\lambda^2 + 9}}. \quad (\text{B11})$$

The RHS of Eqs. (B10) and (B11) are same for all values of λ , as shown in Fig. 5, indicating that the modified HFT is valid for the ground state $n_1 = n_2 = 0$ for all values of λ .

(2) First-excited state: $n_1 = 1, n_2 = 0$.

(a) Unbroken phase: $\lambda < \lambda_c$

Using the relations in Eqs. (B1) to (B3), the right and the left eigenvectors are derived as

$$R_{1,0} = N e^{-\frac{1}{4} [(C_1+C_2)(x^2+y^2)+(C_2-C_1)\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} 2\alpha_1 \left(\sqrt{\frac{k+1}{2}} x - i\sqrt{\frac{k-1}{2}} y \right), \quad (\text{B12})$$

$$L_{1,0} = N e^{-\frac{1}{4} [(C_1+C_2)(x^2+y^2)+(C_1-C_2)\{\frac{2i\lambda kxy}{\lambda_c}+k(x^2-y^2)\}]} 2\alpha_1 \left(\sqrt{\frac{k+1}{2}} x + i\sqrt{\frac{k-1}{2}} y \right), \quad (\text{B13})$$

with the common eigenvalue $E_{1,0}^* = E_{1,0} = (\frac{3}{2})C_1 + (\frac{1}{2})C_2$. Hence, the LHS of the modified HFT is

$$\left\langle \frac{\partial H_{2d}}{\partial \lambda} \right\rangle_{G,(1,0)} = \frac{\int (L_{1,0}^*) \frac{\partial H_{2d}}{\partial \lambda} (R_{1,0}) dx dy}{\int (L_{1,0}^*) (R_{1,0}) dx dy} = \frac{|N|^2 \int ixy c_1 \left(\sqrt{\frac{k+1}{2}} x - i\sqrt{\frac{k-1}{2}} y \right)^2 e^{-\frac{1}{2} [(C_1+C_2)(x^2+y^2)+(C_2-C_1)\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy}{|N|^2 \int c_1 \left(\sqrt{\frac{k+1}{2}} x - i\sqrt{\frac{k-1}{2}} y \right)^2 e^{-\frac{1}{2} [(C_1+C_2)(x^2+y^2)+(C_2-C_1)\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy}. \quad (\text{B14})$$

The RHS of the modified HFT is

$$\frac{\partial E_{1,0}}{\partial \lambda} = \frac{\partial}{\partial \lambda} \left(\frac{3}{2} C_1 + \frac{1}{2} C_2 \right) = \frac{3\lambda}{8\sqrt{2(1 - \frac{\lambda^2}{16})} \left(10 - 8\sqrt{1 - \frac{\lambda^2}{16}} \right)} - \frac{\lambda}{8\sqrt{2(1 - \frac{\lambda^2}{16})} \left(10 + 8\sqrt{1 - \frac{\lambda^2}{16}} \right)}. \quad (\text{B15})$$

The expressions on the RHSs of Eqs. (B14) and (B15) in the domain $\lambda < \lambda_c$ ($=4$) are equal, as shown in Fig. 4, indicating that the modified HFT is valid for the state ($n_1 = 1, n_2 = 0$) in the unbroken case.

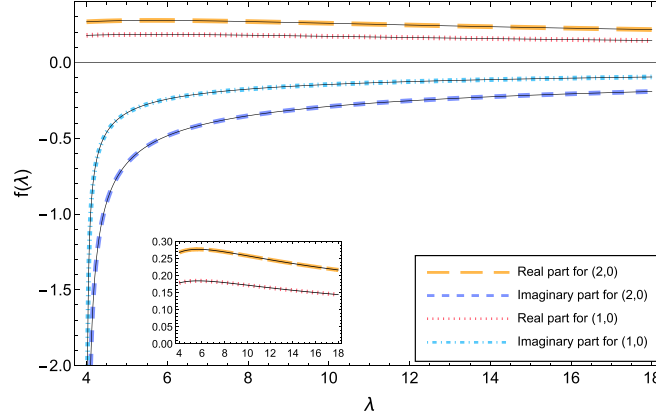


FIG. 6. Comparison between real and imaginary parts of $\langle \partial H_{2d} / \partial \lambda \rangle_{G,(1,0)}$ and $\langle \partial H_{2d} / \partial \lambda \rangle_{G,(2,0)}$ with that of $\partial E_{1,0} / \partial \lambda$ and $\partial E_{2,0} / \partial \lambda$ in the broken region. The dotted and dashed lines represent the LHS and solid lines represent the RHS of the modified HFT, respectively.

(b) Broken phase: $\lambda > \lambda_c$

Using the relations in Eqs. (B4) to (B6), the right and left eigenvectors are calculated along with their eigenvalues as

$$R_{1,0} = N e^{-\frac{1}{4}[2A(x^2+y^2)+2iB\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} 2\alpha_1 \left(\sqrt{\frac{k+1}{2}}x - i\sqrt{\frac{k-1}{2}}y \right), \quad (\text{B16})$$

$$E_{1,0} = \frac{3}{2}C_1 + \frac{1}{2}C_2 = \frac{3}{2}(A - iB) + \frac{1}{2}(A + iB) = 2A - iB, \quad (\text{B17})$$

$$L_{1,0} = N e^{-\frac{1}{4}[2A(x^2+y^2)-2iB\{\frac{2i\lambda kxy}{\lambda_c}+k(x^2-y^2)\}]} 2\alpha_1^* \left(i\sqrt{\frac{k-1}{2}}x - \sqrt{\frac{k+1}{2}}y \right), \quad (\text{B18})$$

with eigenvalue $E_{1,0}^*$. The LHS of the modified HFT is calculated as

$$\left\langle \frac{\partial H_{2d}}{\partial \lambda} \right\rangle_{G,(1,0)} = \frac{\int (L_{1,0}^*) \frac{\partial H_{2d}}{\partial \lambda} (R_{1,0}) dx dy}{\int (L_{1,0}^*) (R_{1,0}) dx dy} = \frac{|N|^2 \int i x y c_1 \left(\sqrt{\frac{k+1}{2}}x - i\sqrt{\frac{k-1}{2}}y \right)^2 e^{-\frac{1}{2}[2A(x^2+y^2)+2iB\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy}{|N|^2 \int c_1 \left(\sqrt{\frac{k+1}{2}}x - i\sqrt{\frac{k-1}{2}}y \right)^2 e^{-\frac{1}{2}[2A(x^2+y^2)+2iB\{\frac{2i\lambda kxy}{\lambda_c}-k(x^2-y^2)\}]} dx dy}. \quad (\text{B19})$$

The RHS of the modified HFT is

$$\frac{\partial E_{1,0}}{\partial \lambda} = \frac{\partial}{\partial \lambda} (2A - iB) = \frac{2\lambda}{\sqrt{64(\frac{\lambda^2}{16} - 1) + 100} \sqrt{\sqrt{64(\frac{\lambda^2}{16} - 1) + 100} + 10}} - \frac{i\lambda}{\sqrt{64(\frac{\lambda^2}{16} - 1) + 100} \sqrt{\sqrt{64(\frac{\lambda^2}{16} - 1) + 100} - 10}}. \quad (\text{B20})$$

The imaginary and the real parts of the relations given by Eqs. (B19) and (B20) over the broken region are shown in Fig. 6. We have also shown the real and imaginary parts of Eq. (19) for (2,0) state in the same figure in order to compare it with the (1,0) state. We find that the curves representing the LHS and RHS of Eq. (19) completely overlap each other for both (1,0) and (2,0) states, indicating the validity of the modified HFT for these states as well.

APPENDIX C: HELLMANN-FEYNMAN THEOREM FOR NON- \mathcal{PT} -INVARIANT NON-HERMITIAN SYSTEM

We consider here a simple 1d Hamiltonian [Eq. (23)] representing a non- \mathcal{PT} -symmetric non-Hermitian system,

$$H_{1d} = \frac{p^2}{2} + \frac{1}{2}\Omega^2 x^2, \quad (\text{C1})$$

where $\Omega = \omega_1 + i\omega_2$ and $\omega_{1,2}$ are real and $\omega_{1,2} \neq 0$.

We intend to verify the modified HFT,

$$\left\langle \frac{\partial H_{1d}}{\partial \lambda} \right\rangle_{G,(n)} = \frac{\partial E_n}{\partial \lambda}, \quad (\text{C2})$$

for the above system for an arbitrary n th state with three different choices of λ :

(1) First choice, $\lambda = \omega_1$: Considering the relations in equations from Eqs. (30) to (32), we can write

$$\begin{aligned} \left\langle \frac{\partial H_{1d}}{\partial \omega_1} \right\rangle_{G,(n)} &= \langle \bar{n} | \Omega x^2 | n \rangle = \frac{1}{2} \langle \bar{n} | a^{+2} + a^2 + a^+ a + a a^+ | n \rangle \\ &= \frac{1}{2} \langle \bar{n} | 2n + 1 | n \rangle = \left(n + \frac{1}{2} \right). \end{aligned} \quad (\text{C3})$$

And it is straightforward to check that

$$\frac{\partial E_n}{\partial \omega_1} = \left(n + \frac{1}{2} \right) = \left\langle \frac{\partial H_{1d}}{\partial \omega_1} \right\rangle_{G,(n)}. \quad (\text{C4})$$

(2) Second choice, $\lambda = \omega_2$: Here too it is straightforward to check:

$$\begin{aligned} \left\langle \frac{\partial H_{1d}}{\partial \omega_2} \right\rangle_{G,(n)} &= \langle \bar{n} | i\Omega x^2 | n \rangle \\ &= \frac{i}{2} \langle \bar{n} | a^{+2} + a^2 + a^+ a + a a^+ | n \rangle \\ &= \frac{i}{2} \langle \bar{n} | 2n + 1 | n \rangle = i \left(n + \frac{1}{2} \right). \end{aligned} \quad (\text{C5})$$

Again,

$$\boxed{\frac{\partial E_n}{\partial \omega_2} = i \left(n + \frac{1}{2} \right) = \left\langle \frac{\partial H_{1d}}{\partial \omega_2} \right\rangle_{G,(n)}}. \quad (\text{C6})$$

(3) Third choice, $\lambda = \Omega$: Similarly for this choice,

$$\begin{aligned} \left\langle \frac{\partial H_{1d}}{\partial \Omega} \right\rangle_{G,(n)} &= \langle \bar{n} | \Omega x^2 | n \rangle \\ &= \frac{1}{2} \langle \bar{n} | a^{+2} + a^2 + a^+ a + a a^+ | n \rangle \\ &= \frac{1}{2} \langle \bar{n} | 2n + 1 | n \rangle = \left(n + \frac{1}{2} \right). \end{aligned} \quad (\text{C7})$$

Again,

$$\boxed{\frac{\partial E_n}{\partial \Omega} = \left(n + \frac{1}{2} \right) = \left\langle \frac{\partial H_{1d}}{\partial \Omega} \right\rangle_{G,(n)}}. \quad (\text{C8})$$

From Eqs. (C4), (C6), and (C8), we see that the modified HFT is valid in case of a non- \mathcal{PT} -invariant, non-Hermitian system as well.

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