Friedel formula and Krein's theorem in complex potential scattering theory

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In this work, the generalization of the Friedel formula and Krein's theorem in complex potential scattering theory is presented. The consequences of various symmetry constraints on dynamical systems are discussed. In addition, the Muskhelishvili-Omnès representation of Krein's theorem is also given and discussed.

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I. INTRODUCTION

A remarkable relation that connects the integrated density of states of a system and the energy derivative of scattering phase shifts was given by Friedel in Refs. [1,2], which is referred to as the Friedel formula and finds wide applications in solid states, multiple-scattering theory, etc. A similar relation was also derived and found uses in statistical mechanics [3,4]. The Friedel formula was originally used to describe the change of density of states due to the perturbation of impurity placed in the metal. Integrating both sides of the Friedel formula over the energy up to the Fermi energy, it leads to the well-known Friedel sum rule [2], which relates the total charge of screening conduction electrons around a charged impurity to the scattering phase shifts. The generalization of the Friedel formula into multiple-scattering theory in the calculation of electronic band structure results in another well-known relation: the Lloyd formula [5]. Other important modern applications of the Friedel formula include the development of the concept of time delay in collision theory; see Refs. [6–8], where the integrated density of states is interpreted as the lifetime of scattering states tunneling through potential barriers and usually referred as the Wigner time delay. Later on, it was recognized by Faulkner in Ref. [9] that the Friedel formula can be derived from Krein's theorem [10] in spectral theory.

The aim of the present work is to explore the possibility of generalization of the Friedel formula and Krein's theorem when the interaction potential is complex, and also to study what other new features the complex potential scattering theory may bring in. All the discussions are currently confined only in one-dimensional space. We will show later on that even with complex potentials in general, relations similar to the Friedel formula and Krein's theorem in real potential theory can be obtained; see Eq. (39) and Eqs. (48)–(50). However, the physical interpretation of such relations in complex potential scattering theory may be drastically different from that in real potential scattering theory. In real potential scattering theory, the conservation of the norm of states plays the central role in interpreting the absorptive part of the Green's function as density of states of the system. On the contrary, in complex potential scattering theory, because of the absorbing or emissive nature of the complex potential, the norm of states is no longer conserved. However, for dual systems with two subsystems, one absorbing with loss and another emissive with gain, when the gain and loss of dual systems are balanced in dynamic equilibrium, the biorthogonal relation between the eigenstates of dual systems can be established. Due to the resemblance of the biorthogonal basis in non-Hermitian theory and the orthogonal basis in Hermitian theory, the Friedel formula and Krein's theorem type of relations in complex potential scattering theory maintain similar mathematical forms, but the absorptive part of the Green's function is no longer related to the density of states, and it is a complex function in general. Similar mathematical forms of Friedel formula and Krein's theorem types of relations in complex potential scattering theory are the consequence of the balanced gain and loss in dual systems. Only in special cases, such as $\mathcal{PT}$-symmetric systems, the absorptive part of the Green's function may still be real, though the positive-definite norm is not guaranteed. Therefore, in collision theory, the absorptive part of the $\mathcal{PT}$-symmetric Green's function may be interpreted as the generalized time delay of particle scattering off $\mathcal{PT}$-symmetric complex barriers. The positivity and negativity of generalized time delay simply reflect the nature of potential barriers that either tend to keep a particle in or force it out.

Such a study is primarily motivated by recent advances in both experimental and theoretical developments in the study of $\mathcal{PT}$-symmetric systems; see Refs. [11–18]. Especially the experimental realization of $\mathcal{PT}$-symmetric systems in optics [16–18], atomic gases [19,20], plasmonic waveguides [21,22], acoustics [23], etc., may make it feasible for the study of some interesting subjects, such as the tunneling time of a particle through complex barriers, multiple-scattering theory in $\mathcal{PT}$-symmetric systems, etc. Many intriguing processes take place in photonic systems with unbroken

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$\mathcal{PT}$ symmetry or in the $\mathcal{PT}$-symmetry-breaking phase. For instance, in $\mathcal{PT}$-symmetric crystals, the violation of the normal conservation of the photon flux leads to anisotropic transmission resonances [24]. In the $\mathcal{PT}$-symmetry-breaking phase, the optical reciprocity yields the unity of the product of the two eigenvalues of the scattering matrix [25]; consequently double refraction and unidirectional invisibility become possible. This may have a significant impact on the dwell time of a particle tunneling through barriers, which is conventionally defined as a weighted average between both transmission and reflection times.

The paper is organized as follows. A brief summary of the Friedel formula and Krein's theorem in real potential scattering theory is provided in Sec. II. The derivations of the Friedel formula and Krein's theorem in complex potential scattering theory are presented in Sec. III and Sec. IV, respectively, followed by our discussion and summary in Sec. V. A short introduction of complex potential scattering theory and a discussion of symmetry constraints are provided in Appendix A and Appendix B, respectively, for readers who may not be familiar with complex potential scattering theory.

II. SUMMARY OF FRIEDEL FORMULA AND KREIN'S THEOREM IN A REAL POTENTIAL SCATTERING THEORY

In the real potential scattering theory, the local density of states of a system, $n_E(x)$, is related to the imaginary part of the Green's function by

$$n_E(x) = -\frac{1}{\pi}\mathrm{Im}[\langle x|\hat{G}(E+i0)|x\rangle], \tag{1}$$

where

$$\hat{G}(E) = \frac{1}{E-\hat{H}}$$

refers to the full Green's function operator of an interacting system, and $\hat{H}$ stands for the Hamiltonian operator of the system. The spectral representation of the Green's function has the form of

$$\hat{G}(E) = \sum_{\epsilon}\frac{|\Psi_\epsilon\rangle\langle\Psi_\epsilon|}{E-\epsilon}, \tag{2}$$

where $|\Psi_\epsilon\rangle$ are eigenstates of Hamiltonian $\hat{H}$, $\hat{H}|\Psi_\epsilon\rangle = \epsilon|\Psi_\epsilon\rangle$, and the spectrum sum in Eq. (2) includes the sum of both discrete bound states and continuous scattering states. The normalization and completeness of eigenstates,

$$\sum_{\epsilon}|\Psi_\epsilon\rangle\langle\Psi_\epsilon| = \mathbb{I},$$

warrants the interpretation of the imaginary part of the Green's function as the density of state

$$n_E(x) = |\langle x|\Psi_{E+i0}\rangle|^2. \tag{3}$$

In Refs. [1,2], Friedel showed that the difference between the integrated density of states of the interacting system and free-particle system, $n_E^{(0)}(x)$, is related to the scattering phase shifts by

$$\int_{-\infty}^{\infty}dx\big[n_E(x) - n_E^{(0)}(x)\big] = \frac{1}{\pi}\frac{d}{dE}\mathrm{Tr}[\delta(k)], \tag{4}$$

where $\delta(k)$ stands for the diagonal matrix of scattering phase shifts, and k is related to the mass and energy of the scattering particle, m and E, respectively, by

$$k^2 = 2mE.$$

We remark that both k and E are used to label the energy dependence of a physical quantity throughout the entire presentation; the purpose is solely for the convenience of presentation. The relation given in Eq. (4) sometime is referred as the Friedel formula, and it is usually also given in terms of the S matrix,

$$S(k) = e^{2i\delta(k)},$$

by

$$-\frac{i}{2\pi}\frac{d}{dE}\ln\det[S(k)] = \mathrm{Im}\left[\int_{-\infty}^{\infty}dx\langle x|\hat{G}(E+i0) - \hat{G}_0(E+i0)|x\rangle\right], \tag{5}$$

where

$$\hat{G}_0(E) = \frac{1}{E-\hat{H}_0}$$

denotes the free particle's Green's function operator.

Given the fact that the Green's function has a physical branch cut along the positive real axis in the complex E plane, $E\in[0,\infty]$, the physical observables, such as density of states, phase shifts, the S matrix, etc., are all defined right above the physical branch cut. In addition, the Green's function may also have an unphysical branch cut sitting along the negative real axis: $E\in[-\infty,-E_L]$, where $-E_L$ represents the branch point of the unphysical cut. In the unphysical region, though Eq. (5) is still formally valid, the S matrix and scattering amplitudes are usually not well constrained and largely model dependent. The imaginary part (absorptive part) of the Green's function is identical to the discontinuity of the Green's function across the physical and unphysical branch cuts, which is given in Eq. (5). The real part (principal part) of the Green's function can be constructed through the imaginary part by Cauchy's integral theorem (also referred as the dispersion integral relation in nuclear/particle physics); hence,

$$\int_{-\infty}^{\infty}dx\langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = \frac{d}{dE}\frac{i}{2\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right]d\epsilon\frac{\ln\det[S(\sqrt{2m\epsilon})]}{\epsilon - E}. \tag{6}$$

The equivalence of relation given in Eq. (6) and Krein's theorem [10,26] in spectral theory is recognized by Faulkner [9], where $\frac{i}{2\pi}\ln\det[S(k)]$ is exactly the Krein's spectral shift function; see Ref. [10]. In the collision theory, $-i\frac{d}{dE}\ln\det[S(k)]$ is also used to describe the time delay of a scattered particle off potential barriers.

In Sec. III and Sec. IV, we will show that even in complex potential scattering, the Friedel formula and Krein's theorem remain forms similar to those in Eq. (5) and Eq. (6) in real potential scattering theory. However, the imaginary part of the Green's function must be replaced by the absorptive part of

the Green's function. In complex potential scattering theory, the spectral representation of the Green's function is given in terms of the biorthogonal basis of dual systems with balanced gain and loss: one is absorbing with loss and another is emissive with gain. Hence the absorptive part of the Green's function in complex potential scattering is no longer related to the density of states of a single system.

III. FRIEDEL FORMULA IN COMPLEX POTENTIAL SCATTERING THEORY

In this section, we show in great detail the derivation of generalizing the Friedel formula in Eq. (5) in the complex potential scattering theory. The derivation can be made in a rather more general but intuitive way following the discussion and approach presented in Ref. [3].

First of all, considering that a nonrelativistic spinless particle of mass m is scattered off a complex absorbing potential, the dynamics is thus described by the Schrödinger equation,

$$\hat{H}|\Psi_E\rangle = E|\Psi_E\rangle, \quad \hat{H} = \hat{H}_0 + \hat{V}, \tag{7}$$

where $\hat{H}_0 = -\frac{1}{2m}\frac{d^2}{dx^2}$ and $\hat{V}$ stand for the free Hamiltonian and complex absorbing potential operators of the system, respectively. Its dual system with an adjoint Hamiltonian $\hat{H}^\dagger$ thus describes a particle that scatters off an emissive complex potential of $\hat{V}^\dagger$; thus the dynamics of the emissive system is given by the Schrödinger equation,

$$\hat{H}^\dagger|\widetilde{\Psi}_E\rangle = E|\widetilde{\Psi}_E\rangle. \tag{8}$$

The emissive system with gain can be considered as the time-reversed version of the absorbing system with equal but opposite loss, and vice versa. Hence dual systems have no net gain or loss. The wave function of an absorbing system and its dual are defined in Hilbert space $\mathcal{H}$ and its dual space $\mathcal{H}^*$, respectively, and they are related by

$$|\Psi_E\rangle \leftrightarrow \langle\widetilde{\Psi}_{E^*}|. \tag{9}$$

The eigenstates of neither an absorbing nor an emissive system alone form an orthogonal basis; however, the eigenstates of dual systems together are biorthogonal and normalized as, see Refs. [27–29],

$$\sum_E |\Psi_E\rangle\langle\widetilde{\Psi}_E| = \mathbb{I}. \tag{10}$$

The expectation value of an observable $\hat{\mathcal{O}}$ is defined by

$$\langle\hat{\mathcal{O}}\rangle = \langle\widetilde{\Psi}_E|\hat{\mathcal{O}}|\Psi_E\rangle. \tag{11}$$

A. S matrix and Møller operators in complex potential scattering theory

The S-matrix operators for dual systems are defined by, see Refs. [27,28],

$$\hat{S}(E) = \hat{\tilde{\Omega}}^\dagger_{E-i0}\hat{\Omega}_{E+i0}, \quad \hat{\tilde{S}}(E) = \hat{\Omega}^\dagger_{E-i0}\hat{\tilde{\Omega}}_{E+i0}, \tag{12}$$

where Møller operators are defined through wave functions by

$$|\Psi_E\rangle = \hat{\Omega}_E|\Psi_E^{(0)}\rangle \tag{13}$$

for an absorbing system with loss, and

$$\langle\widetilde{\Psi}_E| = \langle\Psi_E^{(0)}|\hat{\tilde{\Omega}}^\dagger_E \tag{14}$$

for an emissive system with gain, respectively. $|\Psi_E^{(0)}\rangle$ stands for the eigenstate of free Hamiltonian,

$$\hat{H}_0|\Psi_E^{(0)}\rangle = E|\Psi_E^{(0)}\rangle. \tag{15}$$

Møller operators, $\hat{\Omega}_{E+i0}$ and $\hat{\tilde{\Omega}}_{E-i0}$, hence describe systems that evolve forward in time with $\hat{H}$ and backward in time with $\hat{H}^\dagger$, respectively. As the consequence of balanced gain and loss in dual systems, biorthogonal eigenstates of dual systems are normalized according to

$$\langle\widetilde{\Psi}_E|\Psi_E\rangle = \mathbb{I}; \tag{16}$$

hence it yields

$$\hat{\tilde{\Omega}}^\dagger_E\hat{\Omega}_E = \mathbb{I}. \tag{17}$$

The unitarity relation of the S-matrix operator is also warranted:

$$\hat{\tilde{S}}^\dagger(E)\hat{S}(E) = \hat{\tilde{\Omega}}^\dagger_{E+i0}\hat{\Omega}_{E-i0}\hat{\tilde{\Omega}}^\dagger_{E-i0}\hat{\Omega}_{E+i0} = \mathbb{I}. \tag{18}$$

Using Eq. (12), we also find

$$\begin{aligned}\mathrm{Tr}\left[\hat{\tilde{S}}^\dagger(E)\frac{d}{dE}\hat{S}(E) - \hat{S}(E)\frac{d}{dE}\hat{\tilde{S}}^\dagger(E)\right] &= \mathrm{Tr}\left[\hat{\Omega}_{E-i0}\frac{d}{dE}\hat{\tilde{\Omega}}^\dagger_{E-i0} - \hat{\tilde{\Omega}}^\dagger_{E-i0}\frac{d}{dE}\hat{\Omega}_{E-i0}\right] \\ &+ \mathrm{Tr}\left[\hat{\tilde{\Omega}}^\dagger_{E+i0}\frac{d}{dE}\hat{\Omega}_{E+i0} - \hat{\Omega}_{E+i0}\frac{d}{dE}\hat{\tilde{\Omega}}^\dagger_{E+i0}\right].\end{aligned} \tag{19}$$

Next, before we start simplifying Eq. (19), let us make a list of some useful equations for complex scattering systems. The Lippmann-Schwinger (LS) equation for an absorbing system

$$|\Psi_E\rangle = |\Psi_E^{(0)}\rangle + \hat{G}_0(E)\hat{V}|\Psi_E\rangle \tag{20}$$

yields

$$\hat{\Omega}_E = \mathbb{I} - \hat{G}_0(E)\hat{T}(E), \tag{21}$$

where $\hat{T}(E)$ stands for the scattering amplitude operator and is defined by

$$\hat{T}(E) = -\hat{V}\hat{\Omega}_E. \tag{22}$$

Also using the relation between the wave function and full Green's function of an absorbing system,

$$|\Psi_E\rangle = |\Psi_E^{(0)}\rangle + \hat{G}(E)\hat{V}|\Psi_E^{(0)}\rangle, \tag{23}$$

the Møller operator $\hat{\Omega}_E$ is hence also given by

$$\hat{\Omega}_E = \mathbb{I} + \hat{G}(E)\hat{V}. \tag{24}$$

The scattering amplitude operator, $\hat{T}(E)$, is related to the Green's function by

$$\hat{T}(E) = -\hat{V} - \hat{V}\hat{G}(E)\hat{V}. \tag{25}$$

The normalization of Møller operators in dual systems in Eq. (17) and the Dyson equation,

$$\hat{G}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}(E), \tag{26}$$

suggest that

$$\hat{\tilde{\Omega}}^\dagger_E = \hat{\Omega}_E^{-1} = \mathbb{I} - \hat{G}_0(E)\hat{V}. \tag{27}$$

Now we are ready to simplify Eq. (19) and derive the Friedel formula for complex potential scattering systems. Using Eq. (22) and Eq. (27), we first find

$$\begin{aligned}&\mathrm{Tr}\left[\hat{\Omega}_E\frac{d}{dE}\hat{\tilde{\Omega}}_E^\dagger-\hat{\tilde{\Omega}}_E^\dagger\frac{d}{dE}\hat{\Omega}_E\right]\\&=\mathrm{Tr}\left[-\hat{\Omega}_E\frac{d}{dE}\hat{G}_0(E)\hat{V}-\frac{d}{dE}\hat{\Omega}_E+\hat{G}_0(E)\hat{V}\frac{d}{dE}\hat{\Omega}_E\right]\\&=\mathrm{Tr}\left[\hat{T}(E)\frac{d}{dE}\hat{G}_0(E)-\frac{d}{dE}\hat{\Omega}_E-\hat{G}_0(E)\frac{d}{dE}\hat{T}(E)\right].\end{aligned}\tag{28}$$

Next using Eq. (21), we can write it again to

$$\begin{aligned}&\mathrm{Tr}\left[\hat{\Omega}_E\frac{d}{dE}\hat{\tilde{\Omega}}_E^\dagger-\hat{\tilde{\Omega}}_E^\dagger\frac{d}{dE}\hat{\Omega}_E\right]\\&=2\,\mathrm{Tr}\left[\hat{T}(E)\frac{d}{dE}\hat{G}_0(E)\right]=-2\,\mathrm{Tr}[\hat{G}_0(E)\hat{T}(E)\hat{G}_0(E)].\end{aligned}\tag{29}$$

Finally Eq. (25) and the Dyson equation yield

$$-\hat{G}_0(E)\hat{T}(E)\hat{G}_0(E)=\hat{G}(E)\hat{V}\hat{G}_0(E);\tag{30}$$

hence Eq. (29) can be rewritten further to

$$\mathrm{Tr}\left[\hat{\Omega}_E\frac{d}{dE}\hat{\tilde{\Omega}}_E^\dagger-\hat{\tilde{\Omega}}_E^\dagger\frac{d}{dE}\hat{\Omega}_E\right]=2\mathrm{Tr}[\hat{G}(E)\hat{V}\hat{G}_0(E)].\tag{31}$$

In the end, Eq. (19) and Eq. (31) together lead to

$$\begin{aligned}&-\frac{1}{2}\mathrm{Tr}\left[\hat{\tilde{S}}^\dagger(E)\frac{d}{dE}\hat{S}(E)-\hat{S}(E)\frac{d}{dE}\hat{\tilde{S}}^\dagger(E)\right]\\&=\mathrm{Tr}[\hat{G}(E+i0)\hat{V}\hat{G}_0(E+i0)-\hat{G}(E-i0)\hat{V}\hat{G}_0(E-i0)].\end{aligned}\tag{32}$$

Equation (32) holds in general for an arbitrary complex potential without any symmetry consideration. However, in general

$$\hat{G}(E)\hat{V}\hat{G}_0(E)\neq\hat{G}_0(E)\hat{V}\hat{G}(E)=\hat{G}(E)-\hat{G}_0(E);$$

the Dyson equation in Eq. (26) for an arbitrary complex potential is in fact direction dependent. The transpose of the Dyson equation

$$\hat{G}(E)\hat{V}\hat{G}_0(E)=\hat{G}(E)-\hat{G}_0(E)$$

is valid only if

$$\hat{G}^T(E)=\hat{G}(E).$$

This is indeed the case when reciprocity symmetry is satisfied under the condition $\hat{V}^T=\hat{V}$; see Refs. [30–32].

B. Friedel formula under symmetry constraints

For the local complex potentials, the reciprocity symmetry is automatically satisfied:

$$\hat{V}^T=\hat{V}.$$

It can be easily shown [30–32] that the Green's function is reciprocal symmetric under the exchange of variables,

$$\langle x|\hat{G}(E)|x'\rangle=\langle x'|\hat{G}(E)|x\rangle.\tag{33}$$

Therefore, the Dyson equation is now also reciprocal symmetric:

$$\hat{G}(E)-\hat{G}_0(E)=\hat{G}(E)\hat{V}\hat{G}_0(E)=\hat{G}_0(E)\hat{V}\hat{G}(E).\tag{34}$$

Hence, under reciprocity, Eq. (31) is given by

$$\mathrm{Tr}\left[\hat{\Omega}_E\frac{d}{dE}\hat{\tilde{\Omega}}_E^\dagger-\hat{\tilde{\Omega}}_E^\dagger\frac{d}{dE}\hat{\Omega}_E\right]=2\,\mathrm{Tr}\big[\hat{G}(E)-\hat{G}_0(E)\big],\tag{35}$$

where the trace on the right-hand side of Eq. (35) in coordinate space is defined by

$$\mathrm{Tr}\big[\hat{G}(E)-\hat{G}_0(E)\big]=\int_{-\infty}^{\infty}dx\langle x|G(E)-\hat{G}_0(E)|x\rangle.\tag{36}$$

In the end, Eq. (32) results in a Friedel formula for complex local potential scattering systems:

$$\begin{aligned}&\frac{1}{4i}\mathrm{Tr}\left[\widetilde{S}^\dagger(k)\frac{d}{dE}S(k)-S(k)\frac{d}{dE}\widetilde{S}^\dagger(k)\right]\\&\quad=-\mathrm{Disc}_E\left[\int_{-\infty}^{\infty}dx\langle x|\hat{G}(E)-\hat{G}_0(E)|x\rangle\right],\end{aligned}\tag{37}$$

where the hat on the S-matrix operator in Eq. (32) has been dropped, and now $S(k)/\widetilde{S}(k)$ in Eq. (37) represents the reduced on-energy-shell S matrix. Hence the trace on the left-hand side of Eq. (37) is defined as the regular trace of a matrix. The discontinuity of the Green's function crossing branch cut in the complex E plane is defined by

$$\mathrm{Disc}_E\hat{G}(E)=\frac{1}{2i}[\hat{G}(E+i0)-\hat{G}(E-i0)].\tag{38}$$

We also remark that for a complex potential, the discontinuity of the Green's function is not equivalent to the imaginary part of the Green's function. This statement can be illustrated by considering the spectral representation of the Green's function in Appendix C.

Using the unitarity relation of dual systems

$$\widetilde{S}^\dagger(k)=S^{-1}(k)$$

and identity

$$\mathrm{Tr}[\ln S(k)]=\ln\det[S(k)],$$

the Friedel formula is thus also given in a more compact form:

$$\begin{aligned}&\frac{1}{2i}\frac{d}{dE}\ln\{\det[S(k)]\}\\&\quad=-\mathrm{Disc}_E\left[\int_{-\infty}^{\infty}dx\langle x|\hat{G}(E)-\hat{G}_0(E)|x\rangle\right].\end{aligned}\tag{39}$$

Therefore, the Friedel formula is invariant under unitary transform of the S matrix, and does not depend on a specific basis of eigensolutions.

In a real potential scattering, the left-hand side of the Friedel formula in Eq. (39) is real and positive, which is related to the scattering phase shift matrix by

$$\frac{1}{2i}\frac{d}{dE}\ln\{\det[S(k)]\}=\frac{d}{dE}\mathrm{Tr}[\delta(k)].\tag{40}$$

However, for a complex potential in general, it is a complex matrix. As presented in Appendix A and Appendix B, the S matrix of complex potential dual systems cannot be

parametrized by phase shifts without additional symmetry constraints.

1. Spatial inversion symmetry

For a local and spatial inversion ($\mathcal{P}$) symmetric potential,

$$V(x) = V(-x),$$

as presented in Appendix B 1 b, the S matrix can be parametrized by two real phase shifts, $\delta_\pm(k)$, and two real inelasticities, $\eta_\pm(k)$, see Eq. (B12),

$$S^{(+/-)}(k) = \begin{bmatrix} e^{2i\Delta_+(k)} & 0 \\ 0 & e^{2i\Delta_-(k)} \end{bmatrix}, \tag{41}$$

where

$$e^{2i\Delta_\pm(k)} = \eta_\pm(k) e^{2i\delta_\pm(k)}. \tag{42}$$

Hence, the Friedel formula under the $\mathcal{P}$ symmetry constraint is determined by the sum of two complex functions, $\Delta_\pm(k)$, that play the role of complex phase shifts,

$$\frac{1}{2i}\frac{d}{dE}\ln\{\det[S(k)]\} = \frac{d}{dE}[\Delta_+(k) + \Delta_-(k)]. \tag{43}$$

2. $\mathcal{PT}$ symmetry

For a local and $\mathcal{PT}$-symmetric potential,

$$V^*(x) = V(-x),$$

the S matrix in the parity basis can be parametrized by two real phase shifts and one real inelasticity; see Eq. (B28) and Eq. (B30). In the parity basis, the S matrix is no longer diagonal; however, because of

$$\det[S^{(+/-)}(k)] = e^{2i[\delta_+(k)+\delta_-(k)]}, \tag{44}$$

the Friedel formula with $\mathcal{PT}$ symmetry constraints does not depend on inelasticity, and is given by the sum of two real phase shifts,

$$\frac{1}{2i}\frac{d}{dE}\ln\{\det[S(k)]\} = \frac{d}{dE}[\delta_+(k) + \delta_-(k)]. \tag{45}$$

Using the expression of discontinuity of the Green's function in Eq. (C12), the Friedel formula under $\mathcal{PT}$ symmetry thus yields a real equation,

$$\frac{d}{dk}[\delta_+(k) + \delta_-(k)] = \sum_{p=\pm k} \mathrm{Re}\left[\int_{-\infty}^{\infty} dx \Psi_k(x,p)\Psi_k^*(-x,-p)\right]. \tag{46}$$

IV. KREIN'S THEOREM IN COMPLEX POTENTIAL SCATTERING THEORY

A. Krein's theorem in complex potential scattering theory and symmetry constraints

For a complex potential, using the Friedel formula in Eq. (39), assuming both the Green's function and S matrix having the branch cuts along the real axis in the complex E plane, the Green's function is thus constructed by Cauchy's integral through the discontinuity of the Green's function across both physical and unphysical cuts. Hence even with a complex potential, the expression of Krein's theorem given in Eq. (6) is still valid and remains the same. We would also point out that the integration of the Green's function over x may bring down an extra singularity factor, such as $1/k$. Hence in addition to the branch cut that is inherited from the unintegrated Green's function itself, the integrated Green's function may have extra singularities, such as a pole contribution at the physical threshold because of the extra $1/k$ factor brought down by integration. A simple example of the singularity structure of the integrated Green's function for the scattering with a complex contact interaction can be found in Sec. V A. Therefore, when extra singularity factors show up in the integrated Green's function, though the unintegrated Green's function still satisfies Cauchy's integral relation

$$\langle x|\hat{G}(E)|x\rangle = \frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\mathrm{Disc}_\epsilon \langle x|\hat{G}(\epsilon)|x\rangle}{\epsilon - E}, \tag{47}$$

Cauchy's integral of the integrated Green's function in terms of the discontinuity of the integrated Green's function must be modified and pick up the contribution of extra singularities. The extra singularity contribution in the integrated Green's function can also be understood by Krein's theorem in Eq. (6). Let us rewrite the right-hand side of Eq. (6) by integration by parts, and also using the Friedel formula in Eq. (39), we thus find

$$\int_{-\infty}^{\infty} dx \langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = -\frac{i}{2\pi}\frac{\ln\{\det[S(0)]\}}{E} + \frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\mathrm{Disc}_\epsilon\left[\int_{-\infty}^{\infty} dx \langle x|\hat{G}(\epsilon) - \hat{G}_0(\epsilon)|x\rangle\right]}{\epsilon - E}, \tag{48}$$

where the surface term on the right-hand side of the above equation reflects the extra pole contribution of the integrated Green's function; other surface terms are assumed vanishing and have been dropped. The nontrivial value of $\ln\{\det[S(0)]\}$ at physical threshold thus determines the presence of an extra pole singularity of the integrated Green's function.

Using Eq. (43) and Eq. (45) for $\mathcal{P}$- and $\mathcal{PT}$-symmetric systems, respectively, the integrated Green's functions are related to phase shifts explicitly by

$$\int_{-\infty}^{\infty} dx \langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = -\frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\Delta_+(\sqrt{2m\epsilon}) + \Delta_-(\sqrt{2m\epsilon})}{(\epsilon - E)^2}, \tag{49}$$

for $\mathcal{P}$-symmetric systems, and

$$\int_{-\infty}^{\infty} dx \langle x|\hat{G}(E) - \hat{G}_0(E)|x\rangle = -\frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\delta_+(\sqrt{2m\epsilon}) + \delta_-(\sqrt{2m\epsilon})}{(\epsilon - E)^2}, \tag{50}$$

for $\mathcal{PT}$-symmetric systems.

B. Muskhelishvili-Omnès representation of Krein's theorem

1. Muskhelishvili-Omnès function

In the nuclear/particle physics community, the dispersion theoretical approach by considering the analytical properties of reaction amplitude has been widely used in solving particle-scattering, decaying, and production problems; see, e.g., Refs. [33–37]. The Muskhelishvili-Omnès (MO) representation [38,39] that is sometimes also referred to as the N/D method [40,41] provides an elegant way of expressing the reaction amplitude as the product of two analytic functions: (1) an MO function that possesses only a right-hand branch cut running along the positive real E axis, and the logarithm of the MO function is given by the Cauchy integral of the phase shift, and (2) an analytic function that may possess other singularities but a right-hand branch cut, such as a left-hand branch cut, etc. The MO function is constrained by a unitarity relation that warrants the conservation of the total probability of reactions.

Even in the complex potential scattering theory, the MO dispersive approach still applies. However, we need to be aware that in general, especially with a complex potential, the discontinuity of a reaction amplitude is no longer the same as the imaginary part of the reaction amplitude, and the phase shift function may become a complex function, etc.

Next, we will give a brief and concise introduction to the MO dispersive approach, so later on we can apply and cite the main result directly. Let us consider a reaction amplitude, $F(E)$, which is analytic in the complex E plane and the property of $F(E)$ along the right-hand branch cut is constrained by the unitarity relation,

$$e^{2i\Phi(E+i0)}F(E-i0)=F(E+i0),\quad E\geqslant 0, \tag{51}$$

where the functions $\Phi(E\pm i0)$ that are defined above/below the right-hand branch cut are related by

$$\Phi(E-i0)=-\Phi(E+i0). \tag{52}$$

Equation (51) defines the discontinuity of $F(E)$ across the right-hand branch cut,

$$\mathrm{Disc}_E F(E)=\left[\frac{e^{2i\Phi^*(E+i0)}-1}{2i}\right]^* F(E+i0),\quad E\geqslant 0. \tag{53}$$

In the real potential scattering theory, the $\Phi(E)$ function is real and related directly to the elastic scattering phase shift; see, e.g., Refs. [38,39]. Later on we will show that in $\mathcal{P}$- and $\mathcal{PT}$-symmetric systems, $\Phi(E)$ is given by the sum of $\Delta_\pm(k)$ and $\delta_\pm(k)$, respectively, where the condition of the $\Phi(E)$ function in Eq. (52) is indeed satisfied. Equation (51) suggests that the solution of $F(E)$ has the form of

$$F(E)=N(E)e^{\lambda(E)}, \tag{54}$$

where $N(E)$ has no right-hand branch cut singularity,

$$N(E+i0)=N(E-i0),\quad E\geqslant 0. \tag{55}$$

The $e^{\lambda(E)}$ is usually referred to as the MO function or $D^{-1}(E)$ function. The $\lambda(E)$ has only the right-hand branch cut singularity, and using Eq. (51), we find

$$\mathrm{Disc}_E\lambda(E)=\Phi(E+i0),\quad E\geqslant 0; \tag{56}$$

hence the Cauchy integral theorem yields

$$\lambda(E)=\frac{1}{\pi}\int_0^\infty d\epsilon\frac{\Phi(\epsilon)}{\epsilon-E}, \tag{57}$$

and

$$F(E)=N(E)e^{\frac{1}{\pi}\int_0^\infty d\epsilon\frac{\Phi(\epsilon)}{\epsilon-E}}. \tag{58}$$

The $N(E)$ usually describes the virtual physical processes, such as contributions from t- and u-channel virtual particle exchange processes in a relativistic theory that produce a left-hand cut contribution below the elastic threshold; see, e.g., Ref. [42]. The elastic scattering phase shift is a physical observable; hence the unitarity relation imposes a strong constraint on reaction amplitudes along the right-hand branch cut. Unlike the unitarity relation above the elastic threshold, the discontinuity of reaction amplitude across the left-hand cut below the elastic threshold in the unphysical region is normally less constrained and heavily model dependent. When the left-hand cut is far away from the physical region, the $N(E)$ may be parametrized by approximate methods, such as conformal expansion [43], or simply treated as a constant [36,37]. In nonrelativistic potential scattering theory, for some short-range local potentials in 1D, such as contact interaction or nonsingular potential, it can be shown that $N(E)$ is indeed an energy-independent constant; see the example in Sec. V A.

The argument of the right-hand cut solution can be extended into a left-hand singularity as well. Assume that the $\Phi(E)$ function is defined in both the physical region, $E\in[0,\infty]$, and unphysical region, $E\in[-\infty,-E_L]$, so that Eq. (51) is now valid for both right-hand and left-hand singularities. Both physical and unphysical branch cuts are now described by the $\Phi(E)$ function. In the unphysical region, $E\in[-\infty,-E_L]$, the discontinuity of the MO function vanishes,

$$e^{\lambda(E+i0)}=e^{\lambda(E-i0)},$$

and the solution of $N(E)$ also has the form of

$$N(E)=N_0e^{\chi(E)}, \tag{59}$$

where N_0 is a normalization constant, and

$$\mathrm{Disc}_E\chi(E)=\Phi(E+i0),\quad E\in[-\infty,-E_L]. \tag{60}$$

Therefore the Cauchy integral theorem yields

$$\chi(E)=\frac{1}{\pi}\int_{-\infty}^{-E_L}d\epsilon\frac{\Phi(\epsilon)}{\epsilon-E}. \tag{61}$$

With both left-hand and right-hand singularities described by the $\Phi(E)$ function, thus, we finally get

$$F(E)=N_0e^{\frac{1}{\pi}\left[\int_{-\infty}^{-E_L}+\int_0^\infty\right]d\epsilon\frac{\Phi(\epsilon)}{\epsilon-E}}. \tag{62}$$

2. Muskhelishvili-Omnès representation of Krein's theorem in $\mathcal{P}$-symmetric systems

For a $\mathcal{P}$-symmetric system, using the unitary transform relation in Eq. (A22), the transmission amplitude $t(k)$ is related to $\Delta_\pm(k)$ by

$$t(k)=\frac{e^{2i\Delta_+(k)}+e^{2i\Delta_-(k)}}{2}. \tag{63}$$

The unitarity relation constraint in Eq. (B13) yields

$$\Delta_{\pm}(-k) = -\Delta_{\pm}(k); \tag{64}$$

hence we find

$$e^{2i[\Delta_+(k)+\Delta_-(k)]}t(-k) = t(k). \tag{65}$$

Equations (65) and (64) are the exact MO representation type in Eq. (51) and Eq. (52):

$$t(\pm k) = F(E \pm i0), \quad \Delta_+(\pm k) + \Delta_-(\pm k) = \Phi(E \pm i0). \tag{66}$$

Therefore, the MO representation of transmission amplitude, $t(k)$, is given by

$$\ln\left[\frac{t(k)}{N_0}\right] = \frac{1}{\pi}\left[\int_{-\infty}^{-E_L} + \int_0^{\infty}\right] d\epsilon \frac{\Delta_+(\sqrt{2m\epsilon}) + \Delta_-(\sqrt{2m\epsilon})}{\epsilon - E - i0}, \tag{67}$$

and Krein's theorem can also be written as

$$-\frac{d}{dE}\ln t(k) = \int_{-\infty}^{\infty} dx \langle x|\hat{G}(E+i0) - \hat{G}_0(E+i0)|x\rangle. \tag{68}$$

3. Muskhelishvili-Omnès representation of Krein's theorem in $\mathcal{PT}$-symmetric systems

Similarly, in a $\mathcal{PT}$-symmetric system, using the expression of the transmission amplitude $t(k)$ in Eq. (B32) and unitarity constraint in Eq. (B33), $t(-k) = t^*(k)$, we find

$$\eta(-k) = \eta(k), \quad \delta_{\pm}(-k) = -\delta_{\pm}(k), \tag{69}$$

and

$$e^{2i[\delta_+(k)+\delta_-(k)]}t(-k) = t(k). \tag{70}$$

Hence, in the $\mathcal{PT}$-symmetric system,

$$t(\pm k) = F(E \pm i0), \quad \delta_+(\pm k) + \delta_-(\pm k) = \Phi(E \pm i0), \tag{71}$$

and the MO representation of Krein's theorem has the same form as in Eq. (68).

V. DISCUSSION AND SUMMARY

Before we summarize the results of our finding, a simple and exactly solvable example of a particle scattering with a contact interaction is presented below, which is sufficient to demonstrate a number of unique features of complex scattering theory, such as spectral singularities, etc.

A. A simple example of particle scattering with a complex contact potential

1. Scattering solutions

Let us consider a simple but intuitive example of scattering solutions with a complex contact potential,

$$V(x) = V\delta(x), \quad V = |V|e^{i\theta}. \tag{72}$$

The scattering solutions can be obtained rather straightforwardly by considering Eq. (A2) and Eq. (A9); hence for an absorbing system, we find

$$\Psi_k(x,p) = e^{ipx} + if_k e^{ik|x|}, \tag{73}$$

where the on-shell amplitude depends only on k as the result of contact interaction,

$$f_k = -\frac{mV}{k + imV}. \tag{74}$$

For an emissive system, we thus have

$$\widetilde{\Psi}_k(x,p) = e^{ipx} + i\widetilde{f}_k e^{ik|x|}, \tag{75}$$

where

$$\widetilde{f}_k = -\frac{mV^*}{k + imV^*} = -f^*_{-k}. \tag{76}$$

As a symmetric potential, only one transmission and one reflection amplitude are needed,

$$t(k) = 1 + if_k, \quad r(k) = if_k; \tag{77}$$

the S matrix in the parity basis is thus given by

$$S^{(+/-)}(k) = \begin{bmatrix} 1+2if_k & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{k-imV}{k+imV} & 0 \\ 0 & 1 \end{bmatrix}. \tag{78}$$

For a contact interaction, only the positive parity solution survives. Similarly for an emissive system, we obtain

$$\widetilde{S}^{(+/-)}(k) = \begin{bmatrix} 1+2i\widetilde{f}_k & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{k-imV^*}{k+imV^*} & 0 \\ 0 & 1 \end{bmatrix}. \tag{79}$$

Hence, the unitarity is indeed given by

$$\widetilde{S}^{(+/-)\dagger}(k)S^{(+/-)}(k) = \begin{bmatrix} \frac{k+imV}{k-imV} & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} \frac{k-imV}{k+imV} & 0 \\ 0 & 1 \end{bmatrix} = \mathbb{I}. \tag{80}$$

The complex functions, $\Delta_{\pm}(k)$, are given by

$$\Delta_+(k) = -\cot^{-1}\left(\frac{k}{mV}\right), \quad \Delta_-(k) = 0, \tag{81}$$

and

$$\frac{d}{dE}\Delta_+(k) = \frac{m}{k}\frac{mV}{k^2 + (mV)^2}. \tag{82}$$

2. Green's function solution

The Dyson equation for a contact potential is given by an algebra equation,

$$G(x,x';E) = G_0(x-x';E) + G_0(x;E)VG(0,x';E), \tag{83}$$

where $G_0(x;E)$ is defined in Eq. (A3). The solution of the Green's function is thus given analytically by

$$G(x,x';E+i0) = -\frac{im}{k}\left[e^{ik|x-x'|} - \frac{imV}{k+imV}e^{ik(|x|+|x'|)}\right]. \tag{84}$$

3. Friedel formula check

The Green's functions that are defined below the real E axis, $E - i0$, are simply obtained by replacing k by $-k$ in the above expressions. Thus we find

$$-\mathrm{Disc}_E \int_{-\infty}^{\infty} dx[G(x,x;E) - G_0(0;E)] = \frac{m}{k}\frac{mV}{k^2 + (mV)^2}. \tag{85}$$

The discontinuity of the integrated Green's function difference is hence a complex function as well and indeed equal

to $\frac{d}{dE}\Delta_+(k)$. The left-hand branch cut is absent for a contact interaction. The Friedel formula is satisfied.

4. Krein's theorem check

Using the analytic expression given in Eq. (84) and Eq. (81), thus we can show easily that Krein's theorem is indeed also satisfied for a contact interaction,

$$\int_{-\infty}^{\infty} dx[G(x,x;E+i0)-G_0(0;E+i0)] = -\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\Delta_+(\sqrt{2m\epsilon})}{(\epsilon-E-i0)^2} = -\frac{m}{k^2}\frac{imV}{k+imV}. \quad (86)$$

From the above expression, we can see clearly the presence of a pole contribution $1/k^2$ in addition to the branch cut singularity, and $\Delta_+(0) = -\frac{\pi}{2}$ is indeed nonzero. For $\theta \in [0, \frac{\pi}{2}]$, the interaction is repulsive-like; we find

$$\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\mathrm{Disc}_\epsilon \int_{-\infty}^{\infty} dx[G(x,x;\epsilon)-G_0(0;\epsilon)]}{\epsilon-E-i0} = \frac{m}{k}\frac{1}{k+imV}; \quad (87)$$

hence we can verify that the Cauchy integral equation for the integrated Green's function is indeed Eq. (48) type,

$$-\frac{m}{k^2}+\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\mathrm{Disc}_\epsilon \int_{-\infty}^{\infty} dx[G(x,x;\epsilon)-G_0(0;\epsilon)]}{\epsilon-E-i0} = \int_{-\infty}^{\infty} dx[G(x,x;E+i0)-G_0(0;E+i0)]. \quad (88)$$

For the contact interaction, the MO representation of transmission amplitude, $t(k)$, only has a physical branch cut singularity,

$$t(k) = \frac{k}{k+imV} = N_0 e^{\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\Delta_+(\sqrt{2m\epsilon})}{\epsilon-E-i0}}, \quad (89)$$

where N_0 is a constant and simply plays the role of integral subtraction to ensure the fast convergence of the dispersive integral,

$$N_0 = t(i\kappa_0) e^{-\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\Delta_+(\sqrt{2m\epsilon})}{\epsilon+\frac{\kappa_0^2}{2m}}}, \quad (90)$$

and κ_0 can be chosen arbitrarily. Hence, the MO representation of Krein's theorem is indeed given by Eq. (68).

5. Spectral singularity and bound state above physical threshold

It has been well known that in non-Hermitian complex potential scattering theory, the bound state may appear above a physical threshold, which is usually referred to spectral singularities [44–46]. It was shown in Ref. [44] that spectral singularities of a non-Hermitian Hamiltonian yield divergences of reflection and transmission coefficients of scattered states, and are interpreted as resonance states with vanishing spectral width. The origin of zero-width resonances and bound states are nevertheless the same; both are the results of pole solutions in dynamical related amplitudes and quantities, such as scattering amplitudes and Green's functions, etc. Conventionally the pole solutions below the physical threshold are referred to as bound states, in contrast to the spectral singularity related zero-width resonances in non-Hermitian scattering theory that appear in the physical continuous spectrum. This can be easily understood by the simple example of contact interaction scattering: the pole singularity of the dynamical system is proportional to $\frac{1}{k+imV}$; hence for the real potential scattering, the pole solution, $k_{\mathrm{pole}} = -imV$, corresponds to a bound state for attractive potential ($V < 0$) or a virtual bound state if the potential is repulsive ($V > 0$). On the complex E plane, the bound state solution is located on the first Riemann sheet below the physical threshold, $2mE_B = -(mV)^2$, and the virtual bound state however is on the second Riemann sheet (unphysical sheet). In the complex potential scattering, $V = |V|e^{i\theta}$ has access to the entire complex plane; hence when θ is rotated from 0 to π, now the pole solution can move from below the physical threshold on the first Riemann sheet into the second Riemann sheet by crossing the positive real E axis from below. Therefore the spectral singularity of zero-width resonance occurs, $2mE_{\mathrm{pole}} = (m|V|)^2$, at $\theta = \frac{\pi}{2}$.

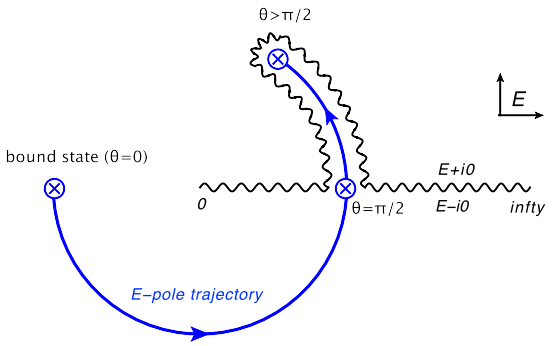

FIG. 1. The plot of motion of pole singularity on the first Riemann sheet of the complex E plane; the pole position is given by $E_{\mathrm{pole}} = -(m|V|)^2 e^{2i\theta}$ as θ increases from 0 up to the $[\frac{\pi}{2}, \pi]$ region. The trajectory of motion of the pole is represented by the solid blue curve.

The motion of pole singularities in the complex plane also affects the Cauchy integral representation of the Green's function. Equation (47) is valid only when $\theta \in [0, \frac{\pi}{2}]$, and the pole is located right below the contour of integration over the positive real E axis on the physical sheet. When the value of θ is further increased into the $[\frac{\pi}{2}, \pi]$ region, the pole starts moving across the integral contour into the second Riemann sheet. The motion of the pole hence drags the contour of integration moving with it to keep the Cauchy integral well defined on the physical sheet; see Fig. 1. In the end, the extra term as the residue of the deformed contour of integration must be added into the Cauchy integral representation of the Green's function. The same is true for the Cauchy integral representation of the integrated Green's function in Eq. (87) and Eq. (88); it is sufficient to demonstrate spectral singularity by considering the expression in Eq. (87),

$$\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{\mathrm{Disc}_\epsilon \int_{-\infty}^{\infty} dx[G(x,x;\epsilon)-G_0(0;\epsilon)]}{\epsilon-E} = -\frac{1}{\pi}\int_0^{\infty} d\epsilon \frac{1}{\epsilon-E}\frac{m}{\sqrt{2m\epsilon}}\frac{mV}{2m\epsilon+(mV)^2}. \quad (91)$$

For $\theta \in [0, \frac{\pi}{2}]$, we already know the result of integration is

$$-\frac{1}{\pi}\int_0^\infty d\epsilon \frac{1}{\epsilon - E - i0}\frac{m}{\sqrt{2m\epsilon}}\frac{mV}{2m\epsilon + (mV)^2} = \frac{m}{k}\frac{1}{k + imV}. \tag{92}$$

The pole singularity that is determined by the condition

$$2m\epsilon + (mV)^2 = 0$$

is now well illustrated on the left-hand side of the above equation. When the θ value is increased from $\theta \in [0, \frac{\pi}{2}]$ into $\theta \in [\frac{\pi}{2}, \pi]$, the pole moves from below the contour of the integral to above; hence the contour of the integral must be deformed to follow the motion of the pole, see Fig. 1, so that the residue contribution due to the deformation of the integration contour must be added. We find

$$\frac{1}{\pi}\int_0^\infty d\epsilon \frac{\mathrm{Disc}_\epsilon \int_{-\infty}^{\infty} dx[G(x,x;\epsilon) - G_0(0;\epsilon)]}{\epsilon - E - i0} + \frac{2m}{k^2 + (mV)^2} = \frac{m}{k}\frac{1}{k + imV}, \quad \theta \in \left[\frac{\pi}{2}, \pi\right]. \tag{93}$$

B. Summary and outlook

In summary, as the consequence of the balanced gain and loss dual systems, the biorthogonal relation can be established between eigenstates of dual systems. Hence the Friedel formula in complex potential scattering theory is still given in the same form,

$$\frac{1}{2i}\frac{d}{dE}\ln\{\det[S(k)]\} = -\mathrm{Disc}_E\{\mathrm{Tr}\big[\hat{G}(E) - \hat{G}_0(E)\big]\};$$

the same is true for Krein's theorem given in Eq. (6). The same mathematical forms of the Friedel formula and Krein's theorem in both real and complex potential scattering theories suggest that the Friedel formula and Krein's theorem for real and complex potentials can be simply connected by analytical continuation. This argument may be also supported by the Muskhelishvili-Omnès representation of Krein's theorem in Eq. (68). Therefore, numbers of useful relations in real potential scattering theory may still apply to complex systems, such as $\mathcal{PT}$-symmetric systems.

One of these useful relations that is closely related to Eq. (68) is the formula given in Refs. [47,48],

$$-\frac{d\ln t(k)}{dE} - \frac{r^{(L)}(k) + r^{(R)}(k)}{4E}e^{2ikL} = \int_{-L}^{L} dx\langle x|\hat{G}(E + i0) - \hat{G}_0(E + i0)|x\rangle. \tag{94}$$

Equation (94) shows the relation between the partially integrated Green's function up to a range L and both transmission $t(k)$ and reflection $r^{(R/L)}(k)$ amplitudes for a finite-range potential scattering system. The potential regardless of the specific shape may be approximated by the sum of multiple layers of the square well potential. After some lengthy derivations, see Refs. [47,48], Eq. (94) can be obtained remarkably. As pointed out in Ref. [48], a calculation of the density of states without taking into account the extra oscillation term in Eq. (94) yields a wrong result. Such oscillations in density of states and the partial density of states influence the conduction properties of sufficiently small conductors [49]. At the limit of $L \gg 1/k$, or in cases such as the resonant scattering where reflection is negligible, the second oscillation term in Eq. (94) can be neglected, and Eq. (68) is recovered. The relations given in Eq. (94) and Eq. (68) may also be valid in describing the dynamics of other waves, such as acoustic or electromagnetic waves, as far as its propagation in the medium is a second-order Schrödinger-equation-like differential equation [50]. For an example, in Ref. [51], a similar result to relation in Eq. (94) is obtained for an electromagnetic wave propagating in a finite system with an arbitrary position-dependent refractive index that plays the role of the interaction potential. The partially integrated Green's function over the finite range of the scattering region naturally appears in the theory of calculating the expectation value of the spin components along or perpendicular to the direction of the external magnetic field. In addition, it also arises in the general analysis of the so-called Büttiker-Landauer tunneling time through a real potential. The question of how the average value of the spin or tunneling time components behave explicitly in the case of $\mathcal{PT}$-symmetric systems has not been properly studied. On top of the above-mentioned cases, a similar expression also arises for the "Cooperon" in the theory of weak localization and weak antilocalization in semiconductor films.

One of the important features of the Friedel formula in complex potential scattering theory is that the absorptive part of the Green's function is in general a complex function and no longer related to the conventional definition of density of states of Hermitian quantum theory. In the case of $\mathcal{PT}$-symmetric systems, the absorptive part of the Green's function is real; hence, the integrated absorptive part of the Green's function may still be interpreted as a time delay function for dual systems with balanced gain and loss. The imaginary part of the Green's function in $\mathcal{PT}$-symmetric systems may be considered as a generalized density of states; it is still a conserved quantity but no longer positive-definite. Hence it is also referred to as a pseudonorm in Refs. [52,53]. An alternative view of the physical interpretation of biorthogonal quantum theory is given in Ref. [29]: the dual Hilbert spaces where the dual systems are defined are replaced by a single Hilbert space with a nontrivial metric that connects eigenstates of dual systems, and hence the physical observable is thus evaluated as the expectation value in the Hilbert space endowed with a nontrivial metric. Similarly, the absorptive part of the Green's function in complex potential scattering theory now may be interpreted as the density of states in the Hilbert space with a nontrivial metric that describes the absorbing/emissive nature of the complex system.

There are a number of problems in $\mathcal{PT}$-symmetric systems that are worth studying in detail—for instance, finite-size effects and related Tamm states. These Tamm states arising at the boundary of any finite semiconductor are practically independent of the distribution of defects and external perturbations. Another problem that is less discussed in the literature for a $\mathcal{PT}$ system is the field dependence of the anomalous magnetoresistance for a sample with a thickness at the order of the external magnetic length. In such a case, the interference effects associated with the boundary become very important, affect the charge's quantum transport, and may lead to interesting oscillations of the magnetoresistance.

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APPENDIX A: SCATTERING THEORY FOR A COMPLEX POTENTIAL

In this Appendix, we give a brief description of scattering theory for a complex potential in general in one-dimensional space; good references can be found in Refs. [27–29].

1. Scattering solutions of an absorbing system

In terms of the Lippmann-Schwinger (LS) equation, the wave function of an absorbing system that is defined above the real axis in a complex E plane,

$$\Psi_k(x) = \langle x|\Psi_{E+i0}\rangle, \quad k = \sqrt{2m(E+i0)}, \tag{A1}$$

satisfies the integral equation

$$\Psi_k(x,p) = e^{ipx} + \int_{-\infty}^{\infty} dx' G_0(x-x';E+i0)V(x')\Psi_k(x',p), \tag{A2}$$

where the symbol

$$p = \pm k$$

is used to label two independent boundary conditions: the right (e^{ikx}) and left (e^{-ikx}) propagating incoming plane waves, respectively. The Green's function of a free propagating particle is given by

$$G_0(x;E+i0) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{ipx}}{E-\frac{p^2}{2m}+i0} = -\frac{im}{k} e^{ik|x|}. \tag{A3}$$

The on-shell scattering amplitudes for an absorbing system are thus defined through the asymptotic behavior of the wave function,

$$\Psi_k(x,p) \overset{|x|\gtrsim L}{\to} e^{ipx} + i f_k(p',p) e^{ik|x|}, \quad p' = k\frac{x}{|x|}, \tag{A4}$$

where L stands for the range of potential: $V(x) \overset{|x|\gtrsim L}{\to} 0$. The on-shell scattering amplitudes with right/left propagating waves are given by

$$f_k(p',p) = -\frac{m}{k}\int_{-\infty}^{\infty} dx' e^{-ip'x'} V(x')\Psi_k(x',p), \tag{A5}$$

where

$$(p',p) \in \pm k.$$

After removing the δ functions that preserve the energy conservation between initial and final scattering states, the reduced S matrix for an absorbing system in the right/left propagating plane wave basis is thus defined by

$$S^{(R/L)}(k) = \begin{bmatrix} t^{(R)}(k) & r^{(L)}(k) \\ r^{(R)}(k) & t^{(L)}(k) \end{bmatrix}, \tag{A6}$$

where $t^{(R/L)}$ and $r^{(R/L)}$ denote the transmission and reflection amplitudes; the superscripts (R/L) are adopted to label amplitudes with boundary condition of right/left propagating waves, respectively. The transmission and reflection amplitudes are related to scattering amplitudes by

$$\begin{bmatrix} t^{(R)}(k) & r^{(L)}(k) \\ r^{(R)}(k) & t^{(L)}(k) \end{bmatrix} = \begin{bmatrix} 1+if_k(k,k) & if_k(k,-k) \\ if_k(-k,k) & 1+if_k(-k,-k) \end{bmatrix}. \tag{A7}$$

2. Scattering solutions of an emissive system

Similarly, for an emissive system with a complex potential $V^*(x)$, the wave function solution that is defined above the real axis in a complex E plane,

$$\widetilde{\Psi}_k(x) = \langle x|\widetilde{\Psi}_{E+i0}\rangle, \tag{A8}$$

is also given by the LS equation,

$$\widetilde{\Psi}_k(x,p) = e^{ipx} + \int_{-\infty}^{\infty} dx' G_0(x-x';E+i0)V^*(x')\widetilde{\Psi}_k(x',p). \tag{A9}$$

Hence the on-shell scattering amplitudes for an emissive system are defined by

$$\widetilde{f}_k(p',p) = -\frac{m}{k}\int_{-\infty}^{\infty} dx' e^{-ip'x'} V^*(x')\widetilde{\Psi}_k(x',p), \tag{A10}$$

and

$$\widetilde{\Psi}_k(x,p) \overset{|x|\gtrsim b}{\to} e^{ipx} + i\widetilde{f}_k(p',p) e^{ik|x|}, \quad p' = k\frac{x}{|x|}. \tag{A11}$$

The S matrix for an emissive system in the right/left propagating plane wave basis is thus given by

$$\widetilde{S}^{(R/L)}(k) = \begin{bmatrix} \widetilde{t}^{(R)}(k) & \widetilde{r}^{(L)}(k) \\ \widetilde{r}^{(R)}(k) & \widetilde{t}^{(L)}(k) \end{bmatrix}, \tag{A12}$$

where $\widetilde{t}^{(R/L)}$ and $\widetilde{r}^{(R/L)}$ are the transmission and reflection amplitudes for an emissive system, and they are related to $\widetilde{f}_k(p',p)$ in a way similar to that in Eq. (A7).

3. The relations of wave functions and scattering amplitudes in dual systems

First of all, the complex conjugate of Eq. (A9) for an emissive system yields

$$\widetilde{\Psi}_k^*(x,p) = e^{i(-p)x} - \frac{im}{(-k)}\int_{-\infty}^{\infty} \times\, dx' e^{i(-k)|x-x'|} V(x')\widetilde{\Psi}_k^*(x',p), \tag{A13}$$

where

$$k = \sqrt{2m(E+i0)}$$

and $\widetilde{\Psi}_k^*(x,p)$ is defined above the real axis in the complex E plane. Compared with the LS equation of an absorbing system that is defined below the real axis in the complex E

plane,

$$\Psi_{-k}(x,-p) = e^{i(-p)x} - \frac{im}{(-k)}\int_{-\infty}^{\infty} dx' e^{i(-k)|x-x'|}V(x')\Psi_{-k}(x',-p), \tag{A14}$$

where

$$-k = \sqrt{2m(E-i0)},$$

we conclude that the wave functions of dual systems are related by

$$\widetilde{\Psi}_k^*(x,p) = \Psi_{-k}(x,-p), \quad p = \pm k. \tag{A15}$$

This relation in fact is the explicit expression of Eq. (9) after the projection of the state operator into position space and also taking into account the boundary conditions.

Next, using the definition of scattering amplitudes of dual systems in Eq. (A5) and Eq. (A10), combined with the relation of wave functions in Eq. (A15), we find that the on-shell scattering amplitudes of dual systems are related by

$$\widetilde{f}_k^*(p',p) = -f_{-k}(-p',-p), \quad (p',p) \in \pm k. \tag{A16}$$

4. Unitarity relation of S matrix of dual systems

a. Unitarity relation of dual systems

The unitarity relation of dual systems is given by

$$\widetilde{S}^{(R/L)\dagger}(k)S^{(R/L)}(k) = \mathbb{I}. \tag{A17}$$

As shown in Eq. (A6) and Eq. (A12), in general the S matrix for both an absorbing system and an emissive system depends on four independent complex functions. Superficially eight complex functions are required to describe the dynamics of dual systems; the unitarity relation provides four complex constraint equations on eight dynamical functions. Hence, the S matrix of an emissive system is determined completely by the S matrix of the absorbing system,

$$\widetilde{S}^{(R/L)\dagger}(k) = [S^{(R/L)}(k)]^{-1}. \tag{A18}$$

In the end, for a general nonsymmetric complex potential, four independent complex dynamical functions are required. Using Eq. (A16), we also find

$$\widetilde{S}^{(R/L)\dagger}(k) = [S^{(R/L)}(-k)]^{T}. \tag{A19}$$

We remark that though in the present work, the terminology "unitarity relation" is constantly used to describe the relation in Eq. (A17), we must be aware that in complex potential theory, Eq. (A17) only refers to balanced gain and loss between dual systems instead of probability preserving unitary time evolution in Hermitian scattering theory.

b. S matrix in parity basis

For many occasions, especially in the cases that the potential displays spatial reflection symmetries, it is more convenient to use the scattering solutions with boundary conditions of positive parity ($\cos kx$) and negative parity ($i\sin kx$) propagating incoming waves. The wave function and scattering amplitude solutions with different boundary conditions are related simply by the linear superposition:

$$\Psi_k^{(+/-)}(x) = \frac{\Psi_k(x,k) \pm \Psi_k(x,-k)}{2}, \tag{A20}$$

and

$$f_k^{(+/-)}(p') = \frac{f_k(p',k) \pm f_k(p',-k)}{2}, \quad p' = \pm k, \tag{A21}$$

where the superscripts $(+/-)$ are used to label solutions that correspond respectively to positive/negative parity propagating incoming waves: $\cos kx/i\sin kx$. The symbol $p = \pm k$ that is used to label solutions that correspond to right/left propagating incoming waves is hence dropped and replaced by labels: $(+/-)$.

The S matrices in different bases are related by a unitary transformation,

$$S^{(+/-)}(k) = U^\dagger S^{(R/L)}(k)U, \tag{A22}$$

where $S^{(+/-)}(k)$ stands for the S matrix in the parity basis, and the U matrix is given by

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}. \tag{A23}$$

APPENDIX B: SYMMETRY CONSTRAINTS IN COMPLEX POTENTIAL SCATTERING THEORY

1. Reciprocity and spatial inversion symmetry

In addition to the unitarity constraints, the symmetries of potential also impose extra constraints on dynamical systems and further reduce the number of independent complex functions in describing dynamical systems. Most commonly considered symmetries are time reversal ($\mathcal{T}$), spatial inversion ($\mathcal{P}$), reciprocity ($\mathcal{R}$), and combined $\mathcal{PT}$ symmetry. The time reversal symmetry holds when $\hat{V} = \hat{V}^*$ is satisfied; hence for systems with complex potentials, time reversal symmetry alone is broken. The spatial inversion symmetry is related to potentials that display relations such as $V(x) = V(-x)$. The spatial inversion symmetry of systems yields the constraints on both transmission and reflection amplitudes: $t^{(R)}(k) = t^{(L)}(k)$ and $r^{(R)}(k) = r^{(L)}(k)$, which hold regardless of whether the potential is real or complex. The concept of reciprocity is distinct from time reversal symmetry; usually it refers to the equality in the signal received when the source and detector are reversed; see Refs. [30–32]. In terms of potential operator, the reciprocity holds if

$$\hat{V} = \hat{V}^T \tag{B1}$$

is satisfied. For a local potential

$$\langle x'|\hat{V}|x\rangle = \delta(x-x')V(x)$$

regardless real or complex, Eq. (B1) is guaranteed. The reciprocity symmetry leads to the constraint only on transmission amplitudes: $t^{(R)}(k) = t^{(L)}(k)$. In this subsection, we will give a brief discussion on the reciprocity and spatial inversion symmetry for local complex potentials. The discussion on combined $\mathcal{PT}$ symmetry will be given separately in Sec. B 2.

a. Reciprocity

For a local complex potential, reciprocity symmetry is automatically satisfied:

$$\langle x'|\hat{V}|x\rangle = \langle x|\hat{V}|x'\rangle = \delta(x-x')V(x). \tag{B2}$$

One of the important consequences of reciprocity is that the transmission amplitudes for the right/left incident particles are identical, see Refs. [30,54,55],

$$t^{(R)}(k) = t^{(L)}(k). \tag{B3}$$

Equality of right/left transmission amplitudes can be illustrated in a rather straightforward way. Using the Schrödinger equation, Eq. (7), we obtain

$$\frac{d}{dx}W(\Psi_k(x,k),\Psi_k(x,-k)) = 0, \tag{B4}$$

where $W(f,g) = fg' - gf'$ refers to the Wronskian of two functions. Hence, we first conclude that the Wronskian of right/left propagating solutions of the Schrödinger equation, $\Psi_k(x,\pm k)$, does not depend on position x. Next using asymptotic behavior of wave functions in Eq. (A4), we also find

$$W(\Psi_k(x,k),\Psi_k(x,-k)) = \begin{cases} -2ikt^{(R)}(k), & x\to+\infty, \\ -2ikt^{(L)}(k), & x\to-\infty. \end{cases} \tag{B5}$$

Together with the fact that the Wronskian of right/left propagating solutions of the Schrödinger equation, $\Psi_k(x,\pm k)$, does not depend on position x, this therefore yields the equality of right/left transmission amplitudes in Eq. (B3).

b. Spatial inversion

Next, let us consider a local complex potential that displays the spatial inversion symmetry,

$$V(x) = V(-x). \tag{B6}$$

For an absorbing system, using LS Eq. (A2) and symmetry of potential, we find

$$\Psi_k(-x,-p) = e^{ipx} - \frac{im}{k}\int_{-\infty}^{\infty} dx' e^{ik|x-x'|}V(x')\Psi_k(-x',-p), \tag{B7}$$

compared with Eq. (A2); hence we get

$$\Psi_k(-x,-p) = \Psi_k(x,p). \tag{B8}$$

Next, using the definition of scattering amplitude in Eq. (A5) combined with the symmetry relation of wave function given in Eq. (B8), we also find

$$f_k(-p',-p) = f_k(p',p). \tag{B9}$$

Similar relations also hold for an emissive system as well.

Therefore, the spatial inversion symmetric potential yields

$$t^{(R)}(k) = t^{(L)}(k) = t(k), \quad r^{(R)}(k) = r^{(L)}(k) = r(k), \tag{B10}$$

and the S matrix in the parity basis becomes diagonal and requires only two independent complex functions,

$$S^{(+/-)}(k) = \begin{bmatrix} t(k)+r(k) & 0 \\ 0 & t(k)-r(k) \end{bmatrix}. \tag{B11}$$

Hence it is now possible to use two real inelasticities and two real phase shifts to parametrize the S matrix,

$$S^{(+/-)}(k) = \begin{bmatrix} \eta_+(k)e^{2i\delta_+(k)} & 0 \\ 0 & \eta_-(k)e^{2i\delta_-(k)} \end{bmatrix}. \tag{B12}$$

The unitarity relation

$$[S^{(+/-)}(-k)]^T = [S^{(+/-)}(k)]^{-1}$$

adds extra constraints for the elements of the S matrix defined below and above the real E axis,

$$\eta_\pm(-k)e^{2i\delta_\pm(-k)} = \eta_\pm^{-1}(k)e^{-2i\delta_\pm(k)}. \tag{B13}$$

As $\mathrm{Im}\hat{V}\to 0$, dual systems become elastic and

$$\eta_\pm \overset{\mathrm{Im}\hat{V}\to 0}{\to} 1;$$

extra constraints in Eq. (B13) yield

$$\delta_\pm(-k) \overset{\mathrm{Im}\hat{V}\to 0}{\to} -\delta_\pm(k), \tag{B14}$$

and

$$\widetilde{S}^{(+/-)\dagger}(k) \overset{\mathrm{Im}\hat{V}\to 0}{\to} S^{(+/-)\dagger}(k) = \begin{bmatrix} e^{-2i\delta_+(k)} & 0 \\ 0 & e^{-2i\delta_-(k)} \end{bmatrix}. \tag{B15}$$

The unitarity relation is hence reduced to familiar form,

$$S^{(+/-)\dagger}(k)S^{(+/-)}(k) = \mathbb{I}. \tag{B16}$$

2. $\mathcal{PT}$ symmetry

For a local complex potential that displays the combined $\mathcal{PT}$ symmetry,

$$V^*(x) = V(-x), \tag{B17}$$

the most intriguing part is that the $\mathcal{PT}$-symmetric potential imposes the symmetry constraints between both an absorbing system and its dual system, which is different from the symmetry relations imposed by symmetric potentials such as one in Eq. (B6). In the case of symmetric potential in Eq. (B6), the symmetry constraints are only imposed on an absorbing and its dual system separately; see, e.g., Eq. (B8) and Eq. (B9). In addition to $\mathcal{PT}$ symmetry, since only local potential is considered in present work, the reciprocity symmetry is also satisfied automatically for dual systems; hence, for an absorbing system, we find

$$f_k(k,k) = f_k(-k,-k), \quad t^{(R)}(k) = t^{(L)}(k) = t(k). \tag{B18}$$

Similar relations hold for an emissive system as well.

a. $\mathcal{PT}$ symmetry constraints on wave functions and scattering amplitudes of dual systems

Using LS equation Eq. (A9) combined with the $\mathcal{PT}$-symmetric potential, for an emissive system, we thus get

$$\widetilde{\Psi}_k(-x,-p) = e^{ipx} - \frac{im}{k}\int_{-\infty}^{\infty} dx' e^{ik|x-x'|}V(x')\widetilde{\Psi}_k(-x',-p); \tag{B19}$$

compared with LS equation of the absorbing system in Eq. (A2), we find

$$\widetilde{\Psi}_k(x,p) = \Psi_k(-x,-p), \quad p = \pm k. \tag{B20}$$

Equation (B20) displays the explicit symmetry relation between an absorbing system and its dual system imposed by $\mathcal{PT}$ symmetry. Next, using the definition of scattering amplitudes of dual systems in Eq. (A5) and Eq. (A10) combined with Eq. (B20), we also find

$$\widetilde{f}_k(p',p) = f_k(-p',-p), \quad (p',p) \in \pm k. \tag{B21}$$

Putting all together, for $\mathcal{PT}$-symmetric dual systems, the plane wave basis wave functions in dual systems are related by

$$\widetilde{\Psi}^*_k(x,p) = \Psi^*_k(-x,-p) = \Psi_{-k}(x,-p), \tag{B22}$$

and the scattering amplitudes are related by

$$\widetilde{f}^*_k(p',p) = f^*_k(-p',-p) = -f_{-k}(-p',-p). \tag{B23}$$

In the parity basis, the relations are given by

$$\widetilde{\Psi}^{(+/-)*}_k(x) = \pm\Psi^{(+/-)*}_k(-x) = \Psi^{(+/-)}_{-k}(x), \tag{B24}$$

and

$$\widetilde{f}^{(+/-)*}_k(p') = \pm f^{(+/-)*}_k(-p') = -f^{(+/-)}_{-k}(-p'), \quad p' = \pm k. \tag{B25}$$

b. Parametrization of $\mathcal{PT}$-symmetric S matrix

With the constraints of $\mathcal{R}$ symmetry for a local potential, now the S matrix for an absorbing system only depends on three complex functions: $t(k)$ and $r^{(R/L)}(k)$. The $\mathcal{PT}$ symmetry puts further constraints on its dual; using Eq. (B21), we find

$$\widetilde{S}^{(R/L)}(k) = \left[S^{(R/L)}(k)\right]^T = \begin{bmatrix} t(k) & r^{(R)}(k) \\ r^{(L)}(k) & t(k) \end{bmatrix}. \tag{B26}$$

Hence the unitarity relation for $\mathcal{PT}$-symmetric dual systems now is given by

$$\widetilde{S}^{(R/L)\dagger}(k) S^{(R/L)}(k) = S^{(R/L)*}(k) S^{(R/L)}(k) = \mathbb{I}. \tag{B27}$$

Next, let us illustrate the consequence of $\mathcal{PT}$ symmetry on the S matrix. Working in the parity basis, the S matrix has the form of

$$S^{(+/-)}(k) = \begin{bmatrix} A_+(k) & B(k) \\ -B(k) & A_-(k) \end{bmatrix}, \tag{B28}$$

where

$$A_\pm(k) = t(k) \pm \frac{r^{(R)}(k) + r^{(L)}(k)}{2},$$
$$B(k) = \frac{r^{(R)}(k) - r^{(L)}(k)}{2}. \tag{B29}$$

The unitarity relation yields three independent equations

$$|A_\pm(k)|^2 - |B(k)|^2 = 1,$$
$$A_+(k)^* B(k) + B^*(k) A_-(k) = 0. \tag{B30}$$

With three constraints in Eq. (B30), the independent functions in the S matrix are now reduced to three real functions. Hence the $\mathcal{PT}$-symmetric S matrix can be parametrized by two phase shifts, $\delta_\pm(k)$, and one inelasticity, $\eta(k)$. The solutions of Eq. (B30) are

$$A_\pm(k) = \eta(k) e^{2i\delta_\pm(k)},$$
$$B(k) = i\sqrt{\eta^2(k) - 1} e^{i(\delta^{(+)}(k) + \delta^{(-)}(k))}, \quad \eta(k) \geqslant 1. \tag{B31}$$

In terms of phase shifts and inelasticity, the transmission and reflection amplitudes are given by

$$t(k) = \eta(k) \frac{e^{2i\delta_+(k)} + e^{2i\delta_-(k)}}{2},$$
$$r^{(R/L)}(k) = \eta(k) \frac{e^{2i\delta_+(k)} - e^{2i\delta_-(k)}}{2}$$
$$\pm i\sqrt{\eta^2(k) - 1} e^{i(\delta^{(+)}(k) + \delta^{(-)}(k))}. \tag{B32}$$

The unitarity relation

$$[S^{(R/L)}(-k)]^T = S^{(R/L)*}(k)$$

adds extra constraints for the elements of the S matrix defined below and above the real E axis,

$$t(-k) = t^*(k), \quad r^{(L)}(-k) = r^{(R)*}(k). \tag{B33}$$

The parametrization of the $\mathcal{PT}$-symmetric S matrix in Eq. (B28) and Eq. (B31) resembles the parametrization of the S matrix for a coupled-channel system of real potential scattering; see, e.g., Refs. [56,57]. However, in real potential scattering theory, the S matrix of a two-channel system for a single partial wave, e.g., an S wave, has the symmetric form of

$$S = \begin{bmatrix} A_1 & B \\ B & A_2 \end{bmatrix} = [S]^T. \tag{B34}$$

The constraints along the diagonal direction of a symmetric S matrix become

$$|A_{1/2}|^2 + |B|^2 = 1. \tag{B35}$$

Hence in terms of phase shifts and inelasticity, the S matrix of a two-channel system for a real potential scattering is parametrized by

$$S = \begin{bmatrix} \eta e^{2i\delta_1} & i\sqrt{1-\eta^2} e^{i(\delta_1+\delta_2)} \\ i\sqrt{1-\eta^2} e^{i(\delta_1+\delta_2)} & \eta e^{2i\delta_2} \end{bmatrix}, \tag{B36}$$

where the constraint equation in Eq. (B35) results that the value of inelasticity is in the range of $\eta \in [0,1]$. On the contrary, in $\mathcal{PT}$-symmetric systems, the antisymmetric form of the S matrix along the off-diagonal direction ultimately leads to $\eta \geqslant 1$. Since spatial inversion alone is not a good symmetry in $\mathcal{PT}$-symmetric systems, the mixing effect between parity basis solutions also contributes. The inelasticity in $\mathcal{PT}$-symmetric systems hence describes the transition between parity basis solutions, which resembles the inelasticity in two-coupled real potential scattering systems that is used to describe the transition between two channels.

APPENDIX C: SPECTRAL REPRESENTATION OF GREEN'S FUNCTION IN COMPLEX POTENTIAL SCATTERING THEORY

1. Spectral representation of Green's function

The biorthogonality of eigenstates of dual systems in Eq. (10) suggests that the spectral representation of the Green's function for an absorbing system is defined by

$$\hat{G}(E) = \sum_{\epsilon} \frac{|\Psi_\epsilon\rangle\langle\widetilde{\Psi}_\epsilon|}{E-\epsilon}, \tag{C1}$$

and $\hat{G}(E)$ satisfies differential equation

$$(E-\hat{H})\hat{G}(E) = \mathbb{I}. \tag{C2}$$

Similarly for an emissive system, we have

$$\hat{\tilde{G}}(E) = \sum_{\epsilon} \frac{|\widetilde{\Psi}_\epsilon\rangle\langle\Psi_\epsilon|}{E-\epsilon}, \tag{C3}$$

and $\hat{\tilde{G}}(E)$ satisfies the differential equation

$$(E-\hat{H}^\dagger)\hat{\tilde{G}}(E) = \mathbb{I}, \tag{C4}$$

and also the Dyson equation

$$\hat{\tilde{G}}(E) = \hat{G}_0(E) + \hat{G}_0(E)\hat{V}^\dagger\hat{\tilde{G}}(E). \tag{C5}$$

In general, the Dyson equations for both absorbing and emissive systems in Eq. (26) and Eq. (C5) respectively are direction dependent and nonreciprocal: the transpose of the Green's function is not identical to the Green's function itself. However, for the local potentials, reciprocity symmetry is guaranteed:

$$\hat{H}^T = \hat{H},$$

and using Eq. (C2) and Eq. (C4), we can easily show that Green's functions are indeed reciprocity symmetric:

$$\hat{G}(E) = \hat{G}^T(E), \quad \hat{\tilde{G}}(E) = \hat{\tilde{G}}^T(E). \tag{C6}$$

Therefore taking into consideration reciprocity symmetry, now $\hat{G}(E)$ and $\hat{\tilde{G}}(E)$ are related by

$$\hat{G}(E) = \hat{\tilde{G}}^*(E^*). \tag{C7}$$

From spectral representation of $\hat{G}(E)$ in Eq. (C1), we find

$$\langle x|\hat{G}(E)|x\rangle = \sum_{\epsilon} \frac{\langle x|\Psi_\epsilon\rangle\langle\widetilde{\Psi}_\epsilon|x\rangle}{E-\epsilon}; \tag{C8}$$

hence the absorptive part of the Green's function is given by discontinuity of the Green's function across the branch cut in the complex E plane,

$$-\mathrm{Disc}_E\langle x|\hat{G}(E)|x\rangle = \pi\sum_{\epsilon}\delta(E-\epsilon)\langle x|\Psi_\epsilon\rangle\langle\widetilde{\Psi}_\epsilon|x\rangle. \tag{C9}$$

Therefore we can conclude that in complex potential scattering theory, the following hold: (1) The imaginary part of the Green's function is not the same as the absorptive part of the Green's function; the absorptive part of the Green's function in general could be a complex function. However, with constraints under $\mathcal{PT}$ symmetry, the absorptive part of the Green's function is indeed real; this will be demonstrated below in Sec. C 2. (2) The absorptive part of the Green's function can no longer be interpreted as density of states in complex potential scattering theory.

2. Absorptive part of Green's function under $\mathcal{PT}$ symmetry

The spectral representation of the Green's function is explicitly given by

$$\langle x|\hat{G}(E)|x'\rangle = \int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{\sum_{p=\pm q}\Psi_q(x,p)\widetilde{\Psi}^*_q(x',p)}{E-\frac{q^2}{2m}}, \tag{C10}$$

where the wave functions are eigensolutions of LS equations in Eq. (A2) and Eq. (A9). The discontinuity of diagonal elements of the Green's function is thus

$$\mathrm{Disc}_E\langle x|\hat{G}(E)|x\rangle = -\frac{m}{2k}\sum_{p=\pm k}[\Psi_k(x,p)\widetilde{\Psi}^*_k(x,p) + \Psi_{-k}(x,p)\widetilde{\Psi}^*_{-k}(x,p)]. \tag{C11}$$

Using $\mathcal{PT}$-symmetric relations on wave functions in Eq. (B22), we thus find

$$\mathrm{Disc}_E\langle x|\hat{G}(E)|x\rangle = -\frac{m}{k}\sum_{p=\pm k}\mathrm{Re}[\Psi_k(x,p)\Psi^*_k(-x,-p)]. \tag{C12}$$

Therefore, under the constraints of $\mathcal{PT}$ symmetry, the absorptive part of the diagonal elements of the Green's function is a real function; however, the positivity is not guaranteed.

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