On spectral properties of the resonances for selected potential scattering systems

Hellmut Baumgärtel,[1,a)] Hani Kaldass,[2,b)] and Soliman Komy[3]
[1]*Mathematical Institute, University of Potsdam, D-14415 Potsdam, Germany*
[2]*Arab Academy of Science and Technology, P.O. Box 2033, Cairo, Egypt*
[3]*Department of Mathematics, Helwan University, Cairo, Egypt*

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The resonances (poles of the scattering matrix) of quantum mechanical scattering by central-symmetric potentials with compact support and zero angular momentum are spectrally characterized directly in terms of the Hamiltonian by a (generalized) eigenvalue problem distinguished by an additional condition (called boundary condition). The connection between the (generalized) eigenspace of a resonance and corresponding Gamov vectors is pointed out. A condition is presented such that a relation between special transition probabilities and infinite sums of residual terms for all complex-conjugated pairs of resonances can be proved. In the case of the square well potential the condition is satisfied. © *2009 American Institute of Physics.* [DOI: 10.1063/1.3072675]

I. INTRODUCTION

The rigorous spectral characterization of the resonances of scattering systems is a well-known old problem. Even if one has knowledge on the analytical properties of the scattering matrix (which is difficult to obtain in general) it is not *a priori* obvious how *characteristic* spectral properties of the resonances in terms of the Hamiltonian H itself could be derived.

A well-known approach to this spectral characterization problem—for potential scattering, applicable for potentials with analyticity properties—starts with the investigation of the resolvent of H, the meromorphic continuation of its matrix elements and their poles which are candidates for resonances. Then the problem is shifted to an eigenvalue problem of a related non-self-adjoint operator, i.e., these poles are associated with the eigenvalues of this operator. The so-called Aguilar–Balslev–Combes–Simon (ABCS) theory is representative for this approach (see Refs. 1–3).

In this note it is pointed out that for real-valued central-symmetric potentials with compact support and zero angular momentum a simple solution of the spectral characterization problem can be given using only spectral terms of H.

It is shown that exactly the resonances are solutions of an (generalized) eigenvalue problem for H, whose (generalized) eigenvectors are subjected to a distinguished *boundary condition*. Further the connection of these eigenvectors with so-called Gamov vectors (in the sense of Ref. 4) is pointed out.

This ansatz was suggested by a similar approach to the same problem for the Friedrichs model on the positive half line, where the decisive step is to require such a boundary condition for the (generalized) eigenvalue problem (see Refs. 5 and 6).

Second, a result on the relation between special transition probabilities and *infinite* residual

[a)]Electronic mail: baumg@rz.uni-potsdam.de.
[b)]Electronic mail: hani@physics.utexas.edu.
[c)]Electronic mail: sol_komy@yahoo.com

sums of all complex-conjugated pairs ζ, $\bar{\zeta}$ of resonance terms is included. As an example, the case of the square well potential is considered. In this case the assumption for the validity of this relation is satisfied (in this case the resonances ζ_n in the lower half plane appear as two-point clusters, where the distance between the cluster points vanishes in the limit $n \to \infty$). Results in the general context are known (see, e.g., Refs. 7–9). In Ref. 9 only the case of a finite number of resonances is considered, in Ref. 8 the case of infinitely many ones is taken into account but the residual sum refers only to the lower half plane. Concrete calculations for examples are missing there.

II. PRELIMINARIES

The resonances of these models were already investigated since 1950s. Therefore in this section for convenience of the reader the well-known basic material of the model is presented [see, e.g., Newton (Ref. 10, Chap. 12)].

A. The basic differential expression

Let $\mathbb{R}_+ \ni r \to V(r)$ be a real-valued function with compact support, i.e., $V(r)=0$ for $r>R$, where R is a positive constant and $\mathbb{R}_+ := (0,\infty)$. For simplicity we assume $V(\cdot)$ piecewise continuous. The so-called regular solution of the differential equation

$$-y''(r) + V(r)y(r) = Ey(r), \quad E \in \mathbb{C} \tag{1}$$

is denoted by $r \to \varphi(r,E)$, then $\varphi(0,E)=0$, $(d\varphi/dr)(0,E)=1$ and $\mathbb{C} \ni E \to \varphi(r_0,E)$ is an entire function for each fixed $r_0>0$. Note that $\overline{\phi(r,E)}=\phi(r,\bar{E})$, i.e., ϕ is real for real E. By $r \to \psi_\pm(r,E)$ we denote the solution of (1) satisfying

$$\psi_\pm(r,E) = e^{\pm i\sqrt{E}r}, \quad r > R. \tag{2}$$

Note that in this case the parameter $E \neq 0$ varies on the Riemann surface of $\sqrt{E}$. Sometimes we use instead of E the parameter k where $k := \sqrt{E}$. Then the first sheet corresponds to $\mathrm{Im}\, k>0$ and the second sheet to $\mathrm{Im}\, k<0$. If E is considered as a point of the first or second sheet we write sometimes for clarity E_+ or E_-. We use the cut $\mathbb{R}_+$. This means approaching $E \in \mathbb{R}_+$ as $(E+i0)_+$ or $(E-i0)_-$ means $\sqrt{E}=k>0$, as $(E-i0)_+$ or $(E+i0)_-$ means $\sqrt{E}=k<0$. For brevity we use also the notation $\psi_\pm(r,k)$ instead of $\psi_\pm(r,E)$. Then one has

$$\varphi(r,k^2) = \frac{1}{2ik}(F(-k)\psi_+(r,k) - F(k)\psi_-(r,k)), \quad k \in \mathbb{C}, \tag{3}$$

where $k \to F(k)$ is the so-called Jost function which is an entire function of k satisfying the symmetry relation

$$\overline{F(k)} = F(-\bar{k}), \quad k \in \mathbb{C}, \tag{4}$$

in particular, one has

$$F(-k) = \overline{F(k)}, \quad k \in \mathbb{R}. \tag{5}$$

Since $F(k)$ and $F(-k)$ cannot vanish simultaneously for $k \neq 0$ this implies $F(k) \neq 0$ for $k \in \mathbb{R}\setminus\{0\}$. Note that $F(0)=0$ is possible. The initial value of $\psi_+(\cdot,k)$ at $r=0$ coincides with $F(k)$, i.e., one has

$$\psi_\pm(0,k) = F(\pm k).$$

Using the regular solution the Jost function is explicitly given by

$$F(k) = 1 + \int_0^R e^{ikr}V(r)\varphi(r,k^2)dr. \tag{6}$$

Using the asymptotic expression

$$\varphi(r,k^2) = \frac{\sin kr}{k} + O(|k|^{-2}\exp(r|\mathrm{Im}\, k|)), \quad |k| \to \infty \tag{7}$$

(see, e.g., Newton[10]), one obtains asymptotic information for $F(\cdot)$ in the upper half plane,

$$|F(k) - 1| \le K|k|^{-1}, \quad \mathrm{Im}\, k \ge 0, \quad k \to \infty, \tag{8}$$

where K is a positive constant. Therefore $F(\cdot)$ cannot be bounded for $k \to \infty$ in the *lower* half plane. Its exact behavior at infinity depends mainly on the behavior of $V(\cdot)$ at $r := R$. For example, if $V(\cdot)$ is a *step function* (e.g., square well potential, constant repulsive potential or spherical shell potential), i.e.,

$$V(r) := \sum_{j=1}^{N} V_j \chi_{[a_{j-1},a_j]}(r),$$

where $a_0=0$ and $a_{N-1} < a_N = R$, then

$$F(k) = -\frac{V_N}{4k^2}e^{2ikR} + 1 + \frac{V_1}{4k^2} + \frac{1}{4k^2}\sum_{j=1}^{N-1} e^{2ika_j}(V_{j+1} - V_j) - \frac{1}{2ik}\int_0^R V(r)dr + O\left(\frac{e^{2R|\mathrm{Im}\, k|}}{|\mathrm{Im}\, k| \cdot |k|^2}\right),$$

$$\mathrm{Im}\, k < 0, \quad |k| \to \infty. \tag{9}$$

This implies

$$|F(k)| \ge \frac{|V_N|}{4|k|^2}e^{2R|\mathrm{Im}\, k|}(1 - \epsilon) - (1 + \epsilon)$$

for $0 < \epsilon < 1$ if $|\mathrm{Im}\, k|$ hence also $|k|$ is sufficiently large. Again this implies

$$|F(k)| \ge |V_N| e^{R\rho \sin \phi_0}, \quad k = \rho e^{-i\phi}, \quad 0 < \phi_0 < \phi < \pi - \phi_0, \quad \rho \ge \rho(\phi_0). \tag{10}$$

Obviously the smaller the ϕ_0, the larger the $\rho(\phi_0)$. In particular, this means that in the region $\{k = \rho e^{-i\phi} : \phi \in (\phi_0, \pi - \phi_0), \rho > \rho(\phi_0)\}$ there are no zeros of $F(\cdot)$; hence in the fourth quadrant $\mathrm{Re}\, k > 0$, $\mathrm{Im}\, k < 0$, almost all zeros of $F(\cdot)$ satisfy $|\mathrm{Im}\, k| < \beta\, \mathrm{Re}\, k$, where $\beta > 0$ is arbitrarily small.

B. The Hamiltonians H, H_0 and their spectral theory

The function $V(\cdot)$ represents a central-symmetric potential with compact support. We restrict the consideration to the angular momentum quantum number $l=0$. Then the corresponding Hamiltonian H is given on the Hilbert space $L^2(\mathbb{R}_+, dr)$ by the operator H defined as follows: its domain dom H consists of all functions $f \in L^2(\mathbb{R}_+, dr)$ such that f' is absolutely continuous, $f(0)=0$ and $f'' \in L^2(\mathbb{R}_+, dr)$. Then

$$Hf(r) := -f''(r) + V(r)f(r).$$

Note that for the corresponding "free" Hamiltonian H_0 the potential term vanishes. The operators H and H_0 are self-adjoint, unbounded and lower semibounded. The spectrum spec H of H is simple. There are at most finitely many eigenvalues $E_j < 0$, $j = 1, \ldots, N$. Note that there are no eigenvalues $E \ge 0$. The (finite-dimensional) projection onto the eigenspace $\mathcal{E}$ is denoted by P. The orthogonal complement of $\mathcal{E}$ is the absolutely continuous subspace of H, i.e., the projection P^{ac} onto the absolutely continuous subspace is given by $P^{\mathrm{ac}} = \mathbb{1} - P$. The absolutely continuous spectrum is $[0,\infty)$ and the spectral representation of H is given by P and by the partial isometry

$$(\Phi f)(E) := \frac{E^{1/4}}{\sqrt{\pi}|F(\sqrt{E})|}\int_0^\infty \varphi(r,E)f(r)dr, \quad E>0, \quad f\in L^2(\mathbb{R}_+,dr), \tag{11}$$

where

$$\Phi^*\Phi = P^{\mathrm{ac}}, \quad \Phi\Phi^* = \mathbb{1}_{L^2(\mathbb{R}_+,dE)},$$

i.e., Φ is isometric from $P^{\mathrm{ac}}L^2(\mathbb{R}_+,dr)$ onto $L^2(\mathbb{R}_+,dE)$ and vanishes on $\mathcal{E}$. This property is obvious because of the relation

$$(\Phi\psi_\pm(\cdot,k))(E) = \frac{E^{1/4}}{\sqrt{\pi}|F(\sqrt{E})|}\frac{F(\pm k)}{E-k^2}, \quad k\in\mathbb{C}_\pm \tag{12}$$

(see, e.g., Skibsted[11]). Note that there is no ambiguity in the notation $|F(\sqrt{E})|$ in (11) because of (5). The inverse transformation Φ^* is given by

$$(\Phi^* g)(r) := \frac{1}{\sqrt{\pi}}\int_0^\infty \varphi(r,E)\frac{E^{1/4}}{|F(\sqrt{E})|}g(E)dE, \quad g\in L^2(\mathbb{R}_+,dE). \tag{13}$$

The multiplication operator on $L^2(\mathbb{R}_+,dE)$ is denoted by M, i.e.,

$$Mg(E) := Eg(E), \quad g\in L^2(\mathbb{R}_+,dE).$$

Then one has

$$\Phi(\mathrm{dom}\, H \cap P^{\mathrm{ac}}L^2(\mathbb{R}_+,dr)) = \mathrm{dom}\, M$$

and

$$\Phi H f = M\Phi f, \quad f\in \mathrm{dom}\, H\cap P^{\mathrm{ac}}L^2(\mathbb{R}_+,dr). \tag{14}$$

The free Hamiltonian H_0 is absolutely continuous and spec $H_0=[0,\infty)$. The spectral representation

$$\Phi_0 f(E) := \frac{E^{1/4}}{\sqrt{\pi}}\int_0^\infty \frac{\sin(\sqrt{E}r)}{\sqrt{E}}f(r)dr, \quad E>0,$$

is isometric from $L^2(\mathbb{R}_+,dr)$ onto $L^2(\mathbb{R}_+,dE)$. The inverse transformation is given by

$$\Phi_0^{-1}g(r) = \frac{1}{\sqrt{\pi}}\int_0^\infty \frac{\sin(\sqrt{E}r)}{E^{1/4}}g(E)dE.$$

C. Wave matrices and scattering matrix

The scattering system $\{H,H_0\}$ is asymptotically complete, the wave operators

$$W_\pm := s-\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}$$

exist and they are isometric from $L^2(\mathbb{R}_+,dr)$, the absolutely continuous subspace of H_0 onto the absolutely continuous subspace $P^{\mathrm{ac}}L^2(\mathbb{R}_+,dr)$ of H. The operators $\Phi W_\pm \Phi_0^{-1}$ are unitary on $L^2(\mathbb{R}_+,dE)$, they commute with the spectral measure of M, therefore they act as multiplication operators by so-called wave matrices $E\to W_\pm(E)$:

$$(\Phi W_{\pm}\Phi_0^{-1}f)(E) = W_{\pm}(E)f(E), \quad f \in L^2(\mathbb{R}_+, dE),$$

where $|W_{\pm}(E)|=1$, $E>0$. Rewriting the wave operators as spectral integrals, the calculation of the wave matrices yields

$$W_{\pm}(E) = \frac{F(\pm\sqrt{(E+i0)_+})}{|F(\sqrt{E})|} = \frac{F(\pm k)}{|F(k)|}, \quad E>0, \quad k>0.$$

The scattering matrix, corresponding to the scattering operator $S:=W_+^*W_-$ is then given by

$$S(E) = \frac{W_-(E)}{W_+(E)} = \frac{F(-k)}{F(k)} =: \tilde{S}(k), \quad E>0, \quad k>0. \tag{15}$$

(15) shows that the function $k \to \tilde{S}(k)$ is meromorphic on $\mathbb{C}$. The function $E \to S(E)$ is well defined on the Riemannian surface of $\sqrt{E}$, and one has

$$S(E_-) = S(E_+)^{-1}. \tag{16}$$

Note that $|\tilde{S}(k)|=1$ for $k \in \mathbb{R}$ and $\tilde{S}(0)=1$, also in the case $F(0)=0$. That is, poles of $\tilde{S}(\cdot)$ are at most in the upper half plane or in the lower half plane. Since $F(k)=0$ implies $F(-k)\neq 0$ this means that k_0 is a pole of $\tilde{S}(\cdot)$ if and only if $F(k_0)=0$. The poles of $\tilde{S}(\cdot)$ in the lower half plane are called *resonances*. They correspond to points on the second sheet of $S(\cdot)$. In the following we omit the symbol tilde and we write $S(\cdot)$ also for the scattering matrix as a function of k.

D. Eigenvalues

The function $r \to \psi_+(r,k_0)$, $k_0 \in \mathbb{C}_+$, is crucial for the eigenvalue problem of H. Note that $\psi_+(\cdot,k_0) \in L^2(\mathbb{R}_+,dr)$. By partial integration of $(Hf,\psi_+(\cdot,k_0))_{L^2(\mathbb{R}_+,dr)}$, one obtains the *basic identity*

$$(Hf,\psi_+(\cdot,k_0)) = \overline{f'(0)}F(k_0) + E_0(f,\psi_+(\cdot,k_0)), \quad E_0 = k_0^2, \quad f \in \text{dom } H. \tag{17}$$

The functions $f \in \text{dom } H$ are sometimes called the *test functions* in relation (17). It shows that a necessary condition for $\psi_+(\cdot,k_0)$ to be an eigenvector of H for the eigenvalue E_0 is $F(k_0)=0$, and this is also sufficient because then $\psi_+(\cdot,k_0) \in \text{dom } H$. This means that the scattering matrix $S(\cdot)$ has a pole at $(E_0)_+$, i.e., in the first sheet. Note that the self-adjointness of H implies that only points $k_0=i\alpha_0$, $\alpha_0>0$ are possible. Since H is bounded below and 0 cannot be an accumulation point of zeros $i\alpha$, there are at most finitely many eigenvalues.

III. SPECTRAL THEORY OF THE RESONANCES

In the following it is pointed out that the resonances can be characterized as distinguished generalized eigenvalues of H whose (generalized) eigenvectors are antilinear forms of an appropriate Gelfand triplet for the absolutely continuous subspace and which satisfy a *boundary condition*. First, with respect to this triplet, the *characteristic* antilinear form

$$f \to (f,\psi_+(\cdot,k)), \tag{18}$$

given by the Hilbert space vector $\psi_+(\cdot,k)$, holomorphic in the upper half plane, which occurs in the basic identity, is analytically continuable into the lower half plane $k \in \mathbb{C}_-$. Second, the boundary condition requires that generalized eigenvectors, associated with a generalized eigenvalue $k \in \mathbb{C}_-$, coincide with the analytic continuation of the *renormalized* characteristic antilinear form

$$f \to S(k)^{1/2}(f,\psi_+(\cdot,k)), \tag{19}$$

i.e., they coincide with the analytic continuation of (18) at this point up to the *renormalization factor* $S(k)^{1/2}$. In other words, they are required to satisfy the analytic continuation of the renormalized basic identity (17). This implies immediately that the analytic continuation of the renormalized characteristic antilinear form is an eigenantilinear form if and only if the associated point k is a resonance. Moreover, in this case this antilinear form coincides with the Dirac form at this point (in the spectral representation). For all other points it is not of the Dirac type. Thus the boundary condition represents the link between the true eigenvectors and the generalized eigenvectors associated to resonances.

A. The antilinear form $f \to (f, \psi_+(\cdot, k))$ restricted to the absolutely continuous subspace

For simplicity in the following we assume $F(0) \neq 0$. We restrict the test functions f to $f \in \mathrm{dom}\, H \cap P^{\mathrm{ac}} L^2(\mathbb{R}_+, dr)$. Then the characteristic antilinear form is given by

$$(f, \psi_+(\cdot, k)) = (\Phi f, \Phi \psi_+(\cdot, k)) = \frac{F(k)}{\sqrt{\pi}} \int_0^\infty \overline{g(E)} \frac{E^{1/4}}{|F(\sqrt{E})|} \frac{1}{E - k^2} dE, \quad k \in \mathbb{C}_+ \tag{20}$$

because of (12), where $g := \Phi f \in L^2(\mathbb{R}_+, dE)$. Obviously, the integral in (20) is for each g a holomorphic function for all $k^2 \in \mathbb{C} \backslash [0, \infty)$ or $k \notin \mathbb{R}$. This means that expression (20) defines also a holomorphic function in the lower half plane $k \in \mathbb{C}_-$. For clarity we distinguish these two functions notationally. We put

$$l_\pm(f, k) := \frac{F(k)}{\sqrt{\pi}} \int_0^\infty \overline{g(E)} \frac{E^{1/4}}{|F(\sqrt{E})|} \frac{1}{E - k^2} dE, \quad k \in \mathbb{C}_\pm. \tag{21}$$

The boundary condition, mentioned in the introduction of Sec. III, requires analytic continuability of $l_+(f, k)$ into the lower half plane $k \in \mathbb{C}_-$. From (21) it can be seen that this condition is satisfied if $g(\cdot)$ is analytically continuable. The renormalized antilinear form (19) is given by

$$S(k)^{1/2} l_+(f, k) = \frac{1}{\sqrt{\pi}} |F(k)| \int_0^\infty \frac{1}{E - k^2} \overline{g(E)} \frac{E^{1/4}}{|F(\sqrt{E})|} dE. \tag{22}$$

Note that $F(k)F(-k) = |F(k)|^2$ for $k \in \mathbb{R}$, i.e., $k \to |F(k)|^2 =: G(k^2)$ is an entire function of $E = k^2$, i.e., the function $k \to |F(k)| = \sqrt{G(E)}$ is an analytic function whose Riemannian surface has two sheets like that of $\sqrt{E}$ but where the zeros of $G(\cdot)$ are branching points. Note that $G(E) = 0$, i.e., $|F(k)| = 0$ if and only if $F(k) = 0$.

B. The Gelfand triplet

We define an appropriate Gelfand space $\mathcal{G} \subset P^{\mathrm{ac}} L^2(\mathbb{R}_+, dr)$ by conditions on its spectral transformation $\Phi \mathcal{G} \subset L^2(\mathbb{R}_+, dE)$. It is defined to be the submanifold of all test functions $f \in P^{\mathrm{ac}} L^2(\mathbb{R}_+, dr)$ such that their spectral transformations $g := \Phi f$ satisfy the following conditions:

(i) $g \in \mathrm{dom}\, M^n$ for $n = 1, 2, 3, \ldots$,
(ii) the function $g \in \Phi \mathcal{G}$ is an entire function on $\mathbb{C}$.

The topology of $\mathcal{G}$ is defined by the collection of norms

$$|g|_{K,n} := \sup_{0 \le j \le n} \|M^j g\|_{L^2(\mathbb{R}_+, dE)} + \sup_{E \in K} |g(E)|,$$

where K runs through all compact subsets $K \subset \mathbb{C}$.

Obviously $\mathcal{G}$ is closed with respect to its topology and dense in $P^{\mathrm{ac}} L^2(\mathbb{R}_+, dr)$ with respect to the Hilbert norm.

The corresponding Gelfand triplet satisfies

$$\mathcal{G} \subset P^{\mathrm{ac}} L^2(\mathbb{R}_+, dr) \subset \mathcal{G}^\times, \tag{23}$$

where $\mathcal{G}^\times$ denotes the corresponding manifold of all continuous antilinear forms on the Gelfand space $\mathcal{G}$.

The extension $H^\times$ of $H\upharpoonright P^{ac}L^2(\mathbb{R}_+,dr)$ with respect to the Gelfand triplet (23) is defined by

$$\langle Hf|\phi_0^\times\rangle = \langle g|H^\times\phi_0^\times\rangle, \quad \phi_0^\times \in \mathcal{G}^\times, \quad f\in\mathcal{G},$$

where $H^\times$ maps $\mathcal{G}^\times$ into $\mathcal{G}^\times$. The (generalized) eigenvalue equation reads

$$\langle f|H^\times\phi_0^\times\rangle = \langle f|E_0\phi_0^\times\rangle \quad \text{or} \quad \langle Hf-\overline{E_0}f|\phi_0^\times\rangle = 0, \ f\in\mathcal{G}.$$

An eigenantilinear form $\phi_0^\times$ for the generalized eigenvalue $E_0=k_0^2$, $k_0\in\mathbb{C}_-$, satisfies the boundary condition if $\phi_0^\times$ coincides with the analytic continuation of the renormalized antilinear form (22), originally defined on $\mathbb{C}_+$, at the point $k_0\in\mathbb{C}_-$, $k_0^2=E_0$.

Note that the spectral transformation Φ induces a bijection $\Phi^\times$ between the antilinear forms on $\mathcal{G}$ and $\Phi\mathcal{G}$, $\mathcal{G}^\times \ni \phi^\times \to \Phi^\times\phi^\times \in (\Phi\mathcal{G})^\times$, defined by

$$\langle \Phi f|\Phi^\times\phi^\times\rangle := \langle f|\phi^\times\rangle.$$

In the following, for convenience, we denote the renormalized characteristic antilinear form for the upper half plane of k by $\phi^\times(k)$, i.e.,

$$\langle f,\phi^\times(k)\rangle := S(k)^{1/2}l_+(f,k), \quad f\in\mathcal{G}.$$

C. Result

Theorem 1: *The point $k_0\in\mathbb{C}_-$ is an eigenvalue of the extension $H^\times$ with respect to the Gelfand triplet* (23) *with an eigenantilinear form $\phi_0^\times$ satisfying the boundary condition if and only if k_0 is a resonance. In this case the antilinear form $\Phi^\times\phi_0^\times$ is realized up to a constant factor by the Dirac antilinear form on $\Phi\mathcal{G}$.*

Proof: If $f\in\mathcal{G}$ and $g:=\Phi f$ then, according to (21) and (22) the analytic continuation of the renormalized characteristic antilinear form $\phi^\times(k)$ into the lower half plane is given by

$$\langle f|\phi^\times(k)\rangle = S(k)^{1/2}l_+(f,k) = S(k)^{1/2}l_-(f,k) + \frac{1}{\sqrt{\pi}}|F(k)|\cdot 2\pi i\overline{g(\bar{k}^2)}\frac{k^{1/2}}{|F(k)|}, \quad k\in\mathbb{C}_-$$

or

$$\langle f|\phi^\times(k)\rangle = \frac{1}{\sqrt{\pi}}|F(k)|\int_0^\infty \frac{1}{E-k^2}\overline{g(E)}\frac{E^{1/4}}{|F(\sqrt{E})|}dE + 2i\sqrt{\pi}k^{1/2}\overline{g(\bar{k}^2)}, \quad k\in\mathbb{C}_-. \tag{24}$$

The basic identity for the renormalized characteristic antilinear forms reads as

$$\langle Hf|\phi^\times(k)\rangle = \overline{f'(0)}|F(k)| + E\langle f|\phi^\times(k)\rangle, \quad k\in\mathbb{C}_+, \quad E=k^2.$$

The analytic continuation of the renormalized characteristic antilinear form satisfies the basic identity, too. Therefore it is an eigenantilinear form for $k:=k_0$ if and only if $F(k_0)=0$, i.e., if and only if k_0 is a resonance. Then $\phi_0^\times := \phi^\times(k_0)$. In this case one has, according to (24)

$$\langle g|\Phi^\times\phi^\times(k_0)\rangle = 2i\sqrt{\pi}E_0^{1/4}\overline{g(\overline{E_0})}, \quad E_0=k_0^2, \quad g\in\Phi\mathcal{G},$$

i.e., the eigenantilinear form (in the spectral representation) coincides with the Dirac antilinear form up to a constant. □

Note that in the case $F(k)\neq 0$, Eq. (24) shows that the renormalized characteristic antilinear form is *not* of the Dirac type.

If the boundary condition is removed then all points of the complex plane are generalized eigenvalues of the extension of the absolutely continuous part of H with respect to the Gelfand triplet (23), i.e., then the *distinguished* character of the resonances as generalized eigenvalues of the Hamiltonian is lost. That is, a spectral characterization of the resonances requires absolutely taking into account the original Hamiltonian H because the boundary condition is due to the interplay between H and its spectral representation. If one neglects this origin, then the only topic to treat is the spectral representation, i.e., the multiplication operator on $L^2(\mathbb{R}_+,dE)$, which is not sufficient for a spectral characterization.

IV. HARDY SPACES AND GAMOV VECTORS

In this section only the spectral representation of the absolutely continuous part of H is considered, i.e., the multiplication operator on the Hilbert space of the spectral representation.

Lemma: *Let M be the multiplication operator on $L^2(\mathbb{R}_+,dE)$ and*

$$\Phi\mathcal{G} \subset L^2(\mathbb{R}_+,dE) \subset (\Phi\mathcal{G})^{\times}$$

the spectral transform of the Gelfand triplet (23). Then the Dirac antilinear form δ_{E_0} for each point $E_0 \in \mathbb{C}$, defined by

$$\langle g|\delta_{E_0}\rangle := \overline{g(\overline{E_0})}, \quad g \in \Phi\mathcal{G},$$

is an element of $(\Phi\mathcal{G})^{\times}$ and it is an eigenantilinear form for $M^{\times}$, i.e.,

$$\langle Mg - \overline{E_0}g|\delta_{E_0}\rangle = 0, \quad g \in \Phi\mathcal{G}.$$

Proof: Obvious. □

In the following we use a modified Gelfand triplet where the functions from the Gelfand space act on the complex plane cutted by the positive half line. The aim is to obtain representations of the Dirac antilinear form for nonreal points by Hilbert space vectors from $L^2(\mathbb{R},dE)$. For this purpose we collect some facts on Hardy spaces. The projections defined on the Hilbert space $L^2(\mathbb{R},dE)$ given by multiplication with the characteristic functions $\chi_{\mathbb{R}_\pm}(\cdot)$ are denoted by $P_\pm$. The Hardy spaces for $\mathbb{C}_\pm$ [subspaces of $L^2(\mathbb{R},dE)$] are denoted by $\mathcal{H}^2_\pm$.

We put

$$\mathcal{H}^2_\pm \ni f \to f_- := P_- f \in \mathcal{D}_\pm := P_-\mathcal{H}^2_\pm \subset L^2(\mathbb{R}_-,dE).$$

Note that on $\mathcal{H}^2_\pm$ the projection P_- is a bijection and the inclusion is dense. Note further that

$$\mathcal{D} := \mathcal{D}_+ \cap \mathcal{D}_- \tag{25}$$

is an infinite-dimensional manifold of functions which are holomorphic on $\mathbb{C}_{>0}$. We define a new norm on $\mathcal{D}_\pm$ by

$$\mathcal{D}_\pm \ni f_- \to [f]_\pm := \|P_-^{-1}f\|.$$

Then with respect to the new norm, $\mathcal{D}_\pm$ is a Hilbert space, canonically isomorphic to $\mathcal{H}^2_\pm$ and $\text{clo}_{[\cdot]_\pm}\mathcal{D}_\pm = \mathcal{H}^2_\pm$. One obtains the following result.

Theorem 2: *For $\zeta_0 \in \mathbb{C}_\mp$ the Dirac antilinear form $\delta_{\zeta_0}(\cdot)\restriction\mathcal{D}$ is also continuous with respect to the norm $\|\cdot\|_\pm$, hence a fortiori continuous on its closure $\mathcal{H}^2_\pm$, and*

$$\delta_{\zeta_0}(g) = \overline{g(\overline{\zeta_0})} = \pm\frac{1}{2\pi i}\int_{-\infty}^{\infty} g(E \pm i0)\frac{1}{\zeta_0 - E}dE, \quad g \in \mathcal{D}.$$

Proof: Obvious by the Paley–Wiener theorem. □

The vector

$$\mathbb{R} \ni E \to \frac{1}{\zeta_0 - E}$$

is called *Gamov vector* for ζ_0. This denotation is due to Bohm–Gadella.[4] Note that this realization of $\delta_{\zeta_0}(\cdot)$ on $\mathcal{D}$ with respect to the injected stronger norms $\|\cdot\|_\pm$ by the (Hilbert space) Gamov vector uses the full real line. It is valid for all $\zeta_0 \in \mathbb{C}_{\pm}$, i.e., there is no distinction between the resonances and other nonreal points.

V. RESONANCES AND TRANSITION PROBABILITIES

In the foregoing sections a spectral characterization of the resonances in terms of H is pointed out. In this section we present relations between resonances and special transition probabilities. These relations are obtained by using only the spectral type of H (in other words the free reference Hamiltonian H_0) and the scattering matrix $S(\cdot)$. Relations of this type are known (see, e.g., Gadella[7,8]). Formula (29) for a finite number of resonances was given for the first time by Bohm.[9] We present conditions such that certain infinite sums of residual terms for all pairs of complex-conjugated resonances of the scattering matrix for the resonance poles are convergent and can be expressed by special transition probabilities for vectors from Hardy spaces.

We focus on the second sheet of $\sqrt{E}$, where the resonances are located. Then the scattering matrix $S(\cdot)$ on the second sheet satisfies

$$S(E-i0) =: S(E), \quad S(E+i0) = S(E)^{-1}, \quad E>0,$$

where $E\to S(E)$ is the *physical* scattering matrix, corresponding to the scattering operator S. The set $\mathcal{M}=\mathcal{M}_0\cup\mathcal{M}_+\cup\mathcal{M}_-$ of resonances consists of an at most finite set $\mathcal{M}_0$ of real resonances $\xi<0$ and the set of pairs of complex-conjugated resonances $\{\zeta,\bar{\zeta}\}\in\mathcal{M}_-\times\mathcal{M}_+$, where $\operatorname{Im}\zeta<0$, i.e., its corresponding k is from the fourth quadrant, $\operatorname{Im} k<0$, $\operatorname{Re} k>0$.

As in Sec. IV we use holomorphic functions f on $\mathbb{C}_{>0}$, $f\in\mathcal{D}$.

Theorem 3: *Let V be a step function and f, $g\in\mathcal{D}$. Assume the following condition.*

(i) *There is a sequence $\{\beta_n\}_{n=1}^{\infty}$, $\beta_n>0$, $\beta_n\to\infty$ for $n\to\infty$, such that for the parameter representation $P_n^+:=\{E_n^+(t),t>0\}$ of the branch of a parabola $y^2=A_n(\beta_n-x)$, $A_n>0$ in the upper half plane $x+iy$ of the second sheet with vertex $E_n^+(+0)=\beta_n$ and $\lim_{t\to\infty}\operatorname{Re} E_n^+(t)=-\infty$ one has*

$$\inf_{n,t>0}\left|F\left(\sqrt{E_n^+(t)}\right)\right|>0. \tag{26}$$

Then

$$(f_+,Sg_-)-\overline{(g_+,Sf_-)}=-2\pi i\sum_{\zeta\in\mathcal{M}}(f(\bar{\zeta}),S_{-1,\zeta}g(\zeta)), \tag{27}$$

i.e., the infinite sum on the right hand side is convergent and (27) is satisfied. The term $S_{-1,\zeta}$ denotes the coefficient of $(z-\zeta)^{-1}$ in the Laurent expansion of the scattering matrix at ζ, i.e.,

$$(f(\bar{\zeta}),S_{-1,\zeta}g(\zeta))=\operatorname{res}_{z=\zeta}(f(\bar{z}),S(z)g(z)).$$

Note that then the complex-conjugated parabolic branch P_n^- in the lower half plane of the second sheet

$$E_n^-(t):=\overline{E_n^+(t)}, \quad E_n^-(+0)=\beta_n$$

satisfies

$$F\left(\sqrt{E_n^-(t)}\right)=\overline{F\left(\sqrt{E_n^+(t)}\right)}$$

such that (26) is also true for P_n^-. Note further that in the present case (multiplicity 1) we have $(f(\bar{\zeta}),S_{-1,\zeta}g(\zeta)):=\overline{f(\bar{\zeta})}S_{-1,\zeta}g(\zeta)$.

Proof: Let $R>0$ and $L_{n,R}^{\pm}:=-R\pm i[0,y_{n,R}]$ be the segment such that $-R\pm iy_{n,R}\in P_n^{\pm}$. Let $\mathcal{C}_{n,R}$ be the positively oriented closed path shown in Fig. 1, consisting of the upper and lower border $E\pm i0$ for $0\le E\le\beta_n$, the piece $P_{n,R}^+$ of the parabolic path P_n^+ from β_n up to the intersection with the segment $L_{n,R}^+$, its complex conjugate $P_{n,R}^-$ and the segments $L_{n,R}^{\pm}$. Then, according to (10) and (8), and condition (i) for sufficiently large n and R, one has

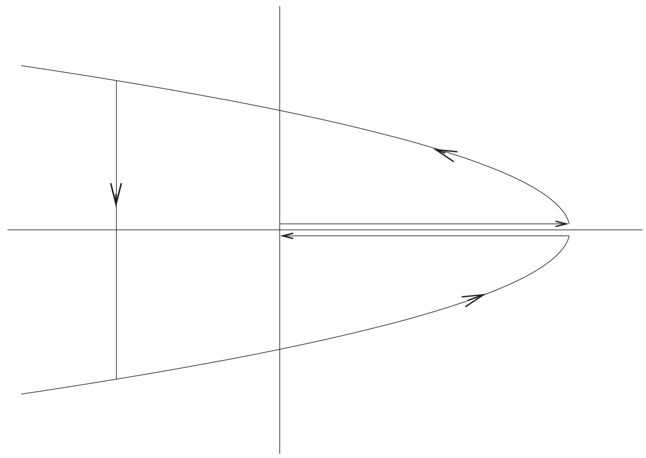

FIG. 1. The contour $\mathcal{C}_{n,R}$ in the second sheet of $\sqrt{E}$.

$$\sup_{z\in\mathcal{C}_{n,R}} |S(z)| =: K < \infty .$$

Then we investigate the integral

$$\int_{\mathcal{C}_{n,R}} (f(\bar{z}),S(z)g(z))dz,$$

where along the lower border $\mathbb{R}_+ - i0$ the function f means f_+, g means g_-, and $S(z)$ means $S(E - i0)$, along the upper border $\mathbb{R}_+ + i0$ the function f is f_-, g is g_+ and $S(z)$ is $S(E+i0)$. Obviously one has

$$\int_{\mathcal{C}_{n,R}} (f(\bar{z}),S(z)g(z))dz = 2\pi i \sum_{\zeta\in\mathcal{M}_{n,R}} (f(\bar{\zeta}),S_{-1,\zeta}g(\zeta)), \qquad (28)$$

where $\mathcal{M}_{n,R}$ consists of all resonances inside the path $\mathcal{C}_{n,R}$. We know *a priori* that the integrals

$$\int_0^\infty (f_+(E),S(E-i0)g_-(E)dE \ , \quad \int_0^\infty (f_-(E),S(E+i0)g_+(E))dE$$

exist. The remaining integrals we consider in the upper and lower half plane, separately. First, for $\mathcal{C}^+_{n,R} := P^+_{n,R} \cup L^+_{n,R}$ we have

$$\left| \int_{\mathcal{C}^+_{n,R}} (f(\bar{z}),S(z)g(z))dz \right| \leq K \int_{\mathcal{C}^+_{n,R}} |f(\bar{z})| \cdot |g(z)| \cdot |dz| \leq K \left(\int_{\mathcal{C}^+_{n,R}} |f(\bar{z})|^2 |dz| \right)^{1/2} \left(\int_{\mathcal{C}^+_{n,R}} |g(z)|^2 |dz| \right)^{1/2} .$$

Now

$$\int_{\mathcal{C}^+_{n,R}} = \int_{P^+_{n,R}} + \int_{L^+_{n,R}} \leq \int_{P^+_n} + \int_{L^+_R} ,$$

where $L^+_R := -R + i[0,\infty]$ and

$$\int_{P_n^+} |f(\bar{z})|^2 |dz| = \int_{w(P_n^+)} |\tilde{f}(w)|^2 \frac{|dw|}{|1+w|^2}, \quad \tilde{f}(w) := \overline{f(\bar{z})},$$

where $w=(1+iz)/(1-iz)$ is a conformal mapping of the upper half plane onto the unit disk. This integral is finite because

$$\int_{|w|=1} |\tilde{f}(w)|^2 \frac{|dw|}{|1+w|^2} = \int_{-\infty}^{\infty} |f_+(x+i0)|^2 dx < \infty.$$

Similarly

$$\int_{L_R^+} |f(z)|^2 |dz| = \int_{w(L_R^+)} |\tilde{f}(w)|^2 \frac{|dw|}{|1+w|^2} < \infty.$$

The Euclidean length $|w(P_n^+)|$ of $w(P_n^+)$ tends to zero for $n \to \infty$ and $|w(L_R^+)|$ tends to zero for $R \to \infty$. The same procedure for the function g yields the result that the left hand side of (28) tends to zero if n and R tend to infinity. Similarly we obtain a corresponding result for the path $\mathcal{C}_{n,R}^-$ in the lower half plane. Then we carry out the limits $n \to \infty$ and $R \to \infty$ in Eq. (28) which implies assertion (27). □

Condition (i) can be replaced by other ones such that the paths $E^{\pm}(t)$, $t>0$ in the second sheet are more general. Form (i) we have used allows a simple verification in the case of the square well potential.

Remark: There is a modified relation between (f_+, Sg_-) and the modified sum of the residual terms where only the resonances from $\mathcal{M}_-$ appear. To obtain this relation, one has to choose a negatively oriented path

$$\mathcal{B}_{n,R} := [0, \beta_n] \cup P_{n,R}^- \cup L_{n,R}^- \cup B_{R,\epsilon}^-,$$

where R is sufficiently large and $B_{R,\epsilon}^-$ is the segment $[-R, 0]$ but where the real resonances $\xi<0$ are surrounded in the lower half plane by semicircles with radius $\epsilon>0$. Further put $B_\epsilon^- := (-\infty, -R] \cup B_{R,\epsilon}^-$. Then by the same arguments as before one obtains

$$\int_{B_\epsilon^-} (f(\bar{z}), S(z)g(z))dz + (f_+, Sg_-) = -2\pi i \sum_{\zeta \in \mathcal{M}_-} (f(\bar{\zeta}), S_{-1,\zeta} g(\zeta)). \tag{29}$$

Correspondingly, for the upper half plane and the positively oriented path B_ϵ^+, complex conjugated with respect to B_ϵ^-, one obtains

$$\int_{B_\epsilon^+} (f(\bar{z}), S(z)g(z))dz + (f_-, S^{-1} g_+) = 2\pi i \sum_{\zeta \in \mathcal{M}_+} (f(\bar{\zeta}), S_{-1,\zeta} g(\zeta)). \tag{30}$$

Subtracting (30) from (29) one gets

$$\int_{B_\epsilon^-} - \int_{B_\epsilon^+} = \sum_{\xi \in \mathcal{M}_0} \int_{\mathcal{C}_{\xi,\epsilon}^+} = 2\pi i \sum_{\xi \in \mathcal{M}_0} (f(\bar{\xi}), S_{-1,\xi} g(\xi)),$$

where $\mathcal{C}_{\xi,\epsilon}^+$ denotes the positively oriented circle around ξ with radius ϵ. Thus one arrives again at (27). The integral $\int_{B_\epsilon^-} (f(\bar{z}), S(z)g(z))dz$ is sometimes called the *background integral* (see e.g., Bohm and Harshman[12]).

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APPENDIX: THE SQUARE WELL POTENTIAL

The square well potential is defined by

$$V(r) = \begin{cases} -V^2, & 0 \le r \le R \\ 0, & r > R. \end{cases}$$

For convenience we put $R=1$ and assume $V>1$. Introducing the variables $z := k/V$ and

$$w := \sqrt{1+z^2} \tag{A1}$$

the Jost function is given by

$$F(k) = e^{ik}\left(\cos Vw - iz\frac{\sin Vw}{w}\right). \tag{A2}$$

Note that $F(0)=\cos V$. That is, $F(0)=0$ for $V:=\pi/2+n\pi$, $n=0,1,2,\ldots$. In the following we assume $F(0)\neq 0$.

The zeros of F in the first sheet $z\in\mathbb{C}_+$ are well known [see, e.g., Flügge (Ref. 13, p. 161)]. If $z\in\mathbb{C}_-$ then $z^2\in\mathbb{C}\backslash[0,\infty)$ and $w^2\in\mathbb{C}\backslash[1,\infty)$, i.e., for w the points $w\in(-\infty,-1]\cup[1,\infty)$ are excluded. For $z=-i\alpha$, $\alpha\geq 1$ there are no zeros, but for $0<\alpha<1$, one has $F(-iV\alpha)=0$ if and only if $\tan V\beta=\beta(1-\beta^2)^{-1/2}$, $0<\beta:=\sqrt{1-\alpha^2}$, i.e., if V is large enough then there are (at most finitely many) zeros. One has $\mathbb{C}_-\backslash i\mathbb{R}_-=\mathbb{C}_{-,-}\cup\mathbb{C}_{+,-}$ where $\mathbb{C}_{-,-},\mathbb{C}_{+,-}$ denote the third and fourth quadrant, respectively. The conformal mapping (A1) maps $\mathbb{C}_{+,-}$ bijectively onto $\mathbb{C}_{+,-}$ and $\mathbb{C}_{-,-}$ onto $\mathbb{C}_{+,+}$ (first quadrant). Therefore z is a zero of $z\to F(Vz)$ if and only if

$$\sin Vw = \pm w, \quad w\in\mathbb{C}_{+,+}\cup\mathbb{C}_{+,-}. \tag{A3}$$

If w is a solution of (A3) then also $\bar{w}$ is a solution. Hence, without loss of generality, one can choose $w=u+iv$ from the first quadrant. (A1) implies

$$u = \cosh(Vv)\sqrt{1-\left(\frac{v}{\sinh(Vv)}\right)^2}, \quad \cos(Vu) = \pm\frac{v}{\sinh(Vv)}.$$

Choose a Cartesian (u,η)-plane and v as the parameter of the two paths

$$u(v) := \cosh(Vv)\sqrt{1-\eta(v)^2}, \quad \eta_\pm(v) := \pm\frac{v}{\sinh(Vv)}, \quad v\geq 0.$$

Then z is a zero of $z\to F(Vz)$ with corresponding $w=u+iv$ if and only if

$$\cos Vu(v) = \eta_\pm(v). \tag{A4}$$

The set of solutions of (A3) can be described, except for possibly one point, as a set of two-point clusters $w_{\pm,n}=u_{\pm,n}+iv_{\pm,n}$, $n\geq N\geq 0$, where $u_{\pm,n}=u(v_{\pm,n})$. The n-cluster is associated with $u_n := (\pi/2V)+n(\pi/V)$ such that $u_{+,n}>u_n>u_{-,n}$ and $|u_{\pm,n}-u_n|\to 0$ for $n\to\infty$. For $n=N$ there is possibly only one resonance.

The corresponding E-values in the second sheet are given by

$$E = V^2 z^2 = V^2(w^2 - 1) = V^2(u^2 - v^2 - 1 + 2ivu), \quad w = u + iv, \ v > 0 \tag{A5}$$

and the corresponding complex-conjugated values $\bar{E}$. By straightforward calculation one obtains for the asymptotics of the resonances with respect to the z-plane

$$y = V^{-1}(2x^{1/2})\log(2x^{1/2}), \quad x \to \infty, \quad z = x + iy.$$

To verify condition (i) in Theorem 3, we choose

$$w_n^+(t) \coloneqq V^{-1}(-n\pi - it), \quad t \geq 0.$$

Then

$$E_n^+(t) = V^2(w_n^+(t)^2 - 1) = n^2\pi^2 - t^2 - V^{-2} + i \cdot 2n\pi t,$$

i.e., in this case one has $\beta_n \coloneqq n^2\pi^2 - V^{-2}$ and $A_n \coloneqq 4n^2\pi^2$, and

$$k_n^+(t) = \sqrt{E_n^+(t)} = Vw_n^+(t)(1 - w_n^+(t)^{-2})^{1/2} \in \mathbb{C}_-. \tag{A6}$$

Note that

$$\sup_{t>0} |w_n^+(t)|^{-1} \leq \frac{V}{n\pi}.$$

For $F(k_n^+(t))$ one obtains by straightforward calculation using the expansion of the square root in (A6) the expression

$$\exp\left(-\frac{iV}{2w_n^+(t)} + \frac{1}{w_n^+(t)^3}O(1)\right)\left(1 + \frac{1}{4w_n^+(t)^2}(e^{2t} - 1) + \frac{1}{2w_n^+(t)^4}(e^{2t} - 1)O(1)\right).$$

where $O(1)$ is a uniform bound with respect to t related to $n \to \infty$. The modulus of the first factor is larger than 1. A lengthy but straightforward lower estimation of the second factor yields condition (i).

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