

## Spectral sum rules for the three-body problem

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This paper derives a number of sum rules for nonrelativistic three-body scattering. These rules are valid for any finite region  $\Sigma$  in the six-dimensional coordinate space. They relate energy moments of the trace of the on-shell time-delay operator to the energy-weighted probability for finding the three-body bound-state wave functions in the region  $\Sigma$ . If  $\Sigma$  is all of the six-dimensional space, the global form of the sum rules is obtained. In this form the rules constitute higher-order Levinson's theorems for the three-body problem. Finally, the sum rules are extended to allow the energy moments to have complex powers.

## I. INTRODUCTION

This paper derives a set of sum rules for the nonrelativistic three-body scattering problem. The type of rule we obtain is a statement of spectral stability. The addition of pairwise potentials to the three-particle free Hamiltonian changes the spectrum in two ways. First, the continuous spectrum, associated with scattering phenomena, is shifted by a finite amount along the energy axis. The free-particle continuum begins at zero energy whereas the perturbed continuum has its threshold at the energy of the most tightly bound two-body eigenstate. Secondly, the perturbation may cause a point spectrum to appear. The sum rules we derive in this paper relate the change in the shifted continuum-state density to the point spectrum.

In the simpler two-body collision problem these spectral sum rules have been extensively studied, e.g., Refs. 1–15. The earliest version of these rules is that found by Levinson.<sup>1</sup> This rule states that for a given partial wave  $l$ , the value of the phase shift at the threshold energy is proportional to the number of distinct bound states having total angular momentum  $l$ . Extensions of these results include the study of arbitrary energy moments of the continuum state density shift induced by the perturbing potential. The partial-wave case for central potentials was analyzed by Percival<sup>6</sup> and Percival and Roberts<sup>7</sup> and the noncentral global problem solved by Buslaev<sup>5,8</sup> and Bollé.<sup>14</sup> Recently, much of the work on these sum rules has emphasized the role played by time-delay theory.<sup>11,14,15</sup> This was a natural development since the trace of the time-delay

operator for scattering at energy  $E$  is equal to the shift of the two-body continuum-state density at  $E$ . For a recent review of time-delay theory and its applications we refer to Ref. 16. The understanding of the higher-order Levinson's theorems as a moment relation involving time delay has led to the discovery of their analogs in classical scattering.<sup>17–19</sup>

In spite of the extensive literature on the single-channel two-body spectral sum rules there is no corresponding effort for the few-body multichannel scattering problem. The one exception we know of is the paper by Wright<sup>20</sup> on the generalization of Levinson's theorem to the three-body problem having fixed total angular momentum  $J$ . In the present study we shall describe a variety of three-body spectral sum rules. These rules are stated for both local regions in coordinate space and in their global form for all of space. In this global form, they constitute higher-order Levinson's theorems. The sum rules are given for both integer and complex powers of the total energy variable. Throughout this discussion the two-body interactions are assumed to be local potentials that are smooth and decay at large distances, but are not necessarily central.

Our general approach is to employ the recently developed high-energy asymptotic expansion of the coordinate space  $N$ -body Green's function,<sup>21</sup> together with known analyticity properties of these Green's functions in the complex energy variable. Time-delay theory is then used in the description of the local version of the sum rules.

Section II summarizes the aspects of three-body scattering theory needed in our subsequent analyses.

Section III obtains the sum rules for integer powers of the energy. Finally, Sec. IV extends the rules to complex power moments of the connected Green's-function discontinuity across the real energy axis. The Appendix contains the definition of time-delay suitable for the three-body problem in finite space regions.

## II. THREE-BODY THEORY

In this section we summarize the known results from three-body scattering theory that are required in our derivation. In the center-of-mass coordinate frame the positions of the three spinless particles are given by the Jacobi variables  $\vec{x}_\alpha, \vec{y}_\alpha$ . The variable  $\vec{x}_\alpha$  is the vector separation of the particle  $\alpha$  from the center of mass of the cluster ( $\beta, \gamma$ ). The remaining independent coordinate variable  $\vec{y}_\alpha$  gives the vector separation of the constituents  $\beta$  and  $\gamma$  of the  $\alpha$  cluster. The canonically conjugate momenta related to  $\vec{x}_\alpha$  and  $\vec{y}_\alpha$  are denoted by  $\vec{p}_\alpha$  and  $\vec{k}_\alpha$ .

Let  $m_\alpha$  ( $\alpha = 1, 2, 3$ ) be the masses of the three particles, then

$$n_\alpha = m_\alpha(m_\beta + m_\gamma)/(m_\alpha + m_\beta + m_\gamma)$$

represents the reduced mass of particle  $\alpha$  and cluster  $\alpha$ . The kinetic energy of this relative motion is  $\vec{p}_\alpha^2/2n_\alpha$ . The cluster  $\alpha$  has reduced mass  $\mu_\alpha = m_\beta m_\gamma/(m_\beta + m_\gamma)$  and an internal kinetic energy given by  $\vec{k}_\alpha^2/2\mu_\alpha$ , where  $\vec{k}_\alpha$  is the internal momentum of the fragments of cluster  $\alpha$ . With this notation the free three-particle kinetic-energy Hamiltonian  $H_0$  is

$$H_0 = \frac{\vec{p}_\alpha^2}{2n_\alpha} + \frac{\vec{k}_\alpha^2}{2\mu_\alpha} = \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + \frac{\vec{p}_3^2}{2m_3}. \quad (2.1)$$

The position of the three particles can be stated in terms of any one of the three Jacobi systems ( $\alpha = 1, 2, 3$ ). Clearly  $H_0$  is invariant with respect to the choice of  $\alpha$ . Associated with the invariant  $H_0$  is the coordinate space metric invariant

$$\rho^2 = \frac{n_\alpha}{m_0} x_\alpha^2 + \frac{\mu_\alpha}{m_0} y_\alpha^2 = \frac{1}{m_0} (m_1 r_1^2 + m_2 r_2^2 + m_3 r_3^2), \quad (2.2)$$

where  $\vec{r}_1, \vec{r}_2, \vec{r}_3$  are the individual position vectors of particles 1, 2, 3 in the center-of-mass system, and

$$m_0^2 = m_1 m_2 m_3 / (m_1 + m_2 + m_3).$$

The six-dimensional vector  $(\vec{x}_\alpha, \vec{y}_\alpha)$  is denoted by  $\vec{\rho}$ .

The dynamical behavior of the three-body problem is governed by the various Hamiltonians the system admits. Let  $V_\alpha$  represent the local potential acting between particles  $\beta$  and  $\gamma$ . So in coordinate space we have

$$V_\alpha(\vec{x}_\alpha, \vec{y}_\alpha) = v_\alpha(\vec{y}_\alpha), \quad (2.3)$$

where it is assumed that  $v_\alpha(\vec{y}_\alpha)$  vanishes as  $|\vec{y}_\alpha| \rightarrow \infty$ . More specifically, we suppose that  $v_\alpha$  belongs to the class of short-ranged interactions that Faddeev used in his proof of asymptotic completeness.<sup>22</sup> In terms of  $V_\alpha$  we may define the following Hamiltonians:

$$H_\alpha = H_0 + V_\alpha, \quad \alpha = 1, 2, 3 \quad (2.4)$$

$$H = H_0 + U, \quad U = \sum_\alpha V_\alpha. \quad (2.5)$$

These Hamiltonians are linear operators on the Hilbert space  $\mathcal{H}$  of square-integrable functions over the six coordinate degrees of freedom  $\vec{x}_\alpha, \vec{y}_\alpha$ . Since the potentials  $v_\beta$  and  $v_\gamma$  are decaying,  $H_\alpha$  will approximately govern the time evolution of the three-particle system if particle  $\alpha$  and cluster  $\alpha$  are far apart.

Consider the multichannel Møller operators that define two-Hilbert-space scattering theory.<sup>22-24</sup> We begin with the two-particle subsystems contained within the three-particle problem. Let  $h_\alpha$  be the two-particle Hamiltonian for particles  $\beta$  and  $\gamma$ , and let  $\phi_{\alpha,i}$  be a unit normalized eigenfunction of  $h_\alpha$  having binding energy  $-\chi_{\alpha,i}^2$ , i.e.,

$$\begin{aligned} h_\alpha \phi_{\alpha,i} &= \left[ \frac{1}{2\mu_\alpha} k_\alpha^2 + v_\alpha \right] \phi_{\alpha,i} \\ &= -\chi_{\alpha,i}^2 \phi_{\alpha,i}, \quad \alpha = 1, 2, 3. \end{aligned} \quad (2.6)$$

The index  $i$  labels the distinct eigenfunctions of  $h_\alpha$ . The scattering solutions defined by  $h_\alpha$  are given in terms of the Møller wave operator

$$\omega_\alpha^{(+)} = s\text{-lim}_{t \rightarrow -\infty} e^{ih_\alpha t} e^{-ih_0 t}, \quad (2.7)$$

where  $h_\alpha^0 = k_\alpha^2/2\mu_\alpha$ . In formula (2.7)  $e^{ih_\alpha t}$  and  $e^{-ih_0 t}$  are the unitary time evolution operators for the Hamiltonians  $h_\alpha$  and  $h_\alpha^0$ , respectively. The symbol  $s\text{-lim}$  denotes the strong limit in the two-particle Hilbert space. The operator  $\omega_\alpha^{(+)}$  is an isometry on the space  $L^2(\vec{y}_\alpha)$  having a range that is the orthogonal complement of the linear subspace spanned by the bound-state wave functions  $\{\phi_{\alpha,i}\}$ .

The three-body Møller operators are defined in a way similar to the  $\omega_\alpha^{(+)}$ , except that the channel

structure is introduced via a channel identification operator  $J_{\alpha,i}$ . For each stable two-particle cluster  $\phi_{\alpha,i}$  we define a channel Hilbert space by  $\mathcal{H}_{\alpha,i} = L^2(\vec{x}_\alpha)$ . The identification operator  $J_{\alpha,i}$  then maps each  $f_{\alpha,i} \in \mathcal{H}_{\alpha,i}$  into an element of  $\mathcal{H}$  by

$$(J_{\alpha,i}f_{\alpha,i})(\vec{x}_\alpha, \vec{y}_\alpha) = \phi_{\alpha,i}(\vec{y}_\alpha)f_{\alpha,i}(\vec{x}_\alpha). \quad (2.8)$$

In terms of the  $J_{\alpha,i}$  the wave operators are

$$\Omega_{\alpha,i}^{(+)} = s\text{-}\lim_{t \rightarrow -\infty} e^{iHt} e^{-iH_\alpha t} J_{\alpha,i}. \quad (2.9)$$

In both (2.7) and (2.9) it is understood that the argument of the exponential function is divided by the rationalized value of Planck's constant  $\hbar$ . The multichannel wave operators  $\Omega_{\alpha,i}^{(+)}$  map functions from an incident channel space  $\mathcal{H}_{\alpha,i}$  into the full space  $\mathcal{H}$ .

Next, we recall the form asymptotic completeness takes in terms of the wave operators. Denote the normalized eigenfunctions of  $H$  by

$$H\Psi_i = E_i\Psi_i, \quad i = 1, \dots, N_3 \quad (2.10)$$

where  $N_3$  is the total number of three-body bound states. We suppose that the strength of the potentials  $v_\alpha$  do not assume the exceptional values that lead to the Efimov effect,<sup>25</sup> whereby  $N_3 = \infty$  and the point spectrum has zero energy as an accumulation point. Take  $B$  to be the projector onto the subspace spanned by  $\{\Psi_i\}$ . Then the statement of asymptotic completeness is

$$\sum_{\alpha,i} \Omega_{\alpha,i}^{(+)} \Omega_{\alpha,i}^{(+)\dagger} + B = 1, \quad (2.11)$$

where  $\dagger$  denotes the adjoint between the spaces  $\mathcal{H}_{\alpha,i}$  and  $\mathcal{H}$ . The completeness statement (2.11) is that defined by the Hamiltonian pair  $(H, H_0)$ . Related completeness statements are defined by the pairs  $(H_\alpha, H_0)$ .

Finally, we summarize the spectral property of multichannel time-delay theory.<sup>16,26-32</sup> Take  $\Sigma$  to be an arbitrary region of the six-dimensional coordinate space having finite Lebesgue measure

$$\nu(\Sigma) = \int_\Sigma d\vec{x}_\alpha d\vec{y}_\alpha < \infty. \quad (2.12)$$

For an incoming scattering state in channel  $\alpha i$ , with energy  $E$  and incident plane-wave direction  $\hat{p}_\alpha$  there exists an on-shell time-delay operator  $q_{\alpha,i}(E; \Sigma)$ . The operator  $q_{\alpha,i}(E; \Sigma)$  maps  $L^2(\hat{p}_\alpha)$  into  $L^2(\hat{p}_\alpha)$  and is defined in detail by its momentum-space kernel representation  $q_{\alpha,i}(E; \Sigma; \hat{p}_\alpha, \hat{p}'_\alpha)$ . The definition of multichannel time delay together with the explicit formulas for these momentum-space kernels are stated in the Ap-

pendix. At this point we furthermore introduce the connected resolvent difference. For complex energy  $Z$  we define the resolvents  $R(Z)$  and  $R_\alpha(Z)$  by  $(H - Z)^{-1}$  and  $(H_\alpha - Z)^{-1}$ . We then decompose  $R(Z)$  into a point spectrum part and an absolutely continuous spectrum part, viz.,

$$R(Z) = R_p(Z) + R_{ac}(Z), \quad (2.13)$$

where

$$R_{ac}(Z) \equiv \sum_{\alpha,i} \Omega_{\alpha,i}^{(+)} \Omega_{\alpha,i}^{(+)\dagger} R(Z) \quad (2.14)$$

and

$$R_p(Z) \equiv BR(Z). \quad (2.15)$$

The orthogonality and completeness properties of  $B$  and  $\Omega_{\alpha,i}^{(+)} \Omega_{\alpha,i}^{(+)\dagger}$  justify the decomposition (2.13). The absolutely continuous connected resolvent difference  $\tilde{R}(Z)$  is then

$$\tilde{R}(Z) \equiv R_{ac}(Z) - R_0(Z) - \sum_{\alpha>0} [R_\alpha(Z) - R_0(Z)]. \quad (2.16)$$

Let  $\text{Tr}$  be the trace on the space  $\mathcal{H}$ , and let  $\text{tr}$  be the trace on the space  $L^2(\hat{p}_\alpha)$  ( $\alpha=0,1,2,3$ ). The spectral property of time delay relates then the trace of  $\text{Im}\tilde{R}(Z)$  to the traces of  $q_{\alpha,i}(E; \Sigma)$  in the following way: For each energy  $E$  and each finite region  $\Sigma$  one has

$$\begin{aligned} 2 \text{Tr} P(\Sigma) \text{Im}\tilde{R}(E + i0) P(\Sigma) \\ = \hbar^{-1} \sum_{\alpha,i} \text{tr} q_{\alpha,i}(E; \Sigma), \end{aligned} \quad (2.17)$$

where  $P(\Sigma)$  is the projection operator for the space region  $\Sigma$ . If  $E$  is less than the threshold in channel  $\alpha, i$  then the term  $\text{tr} q_{\alpha,i}(E; \Sigma)$  is zero. The right-hand side (rhs) of Eq. (2.17) is, of course, the total time delay in all channels  $\alpha, i$  for scattering states with energy  $E$ . The left-hand side (lhs) is  $2\pi$  times the change in the total density of continuum states having energy  $E$ , with support on  $\Sigma$ . Identity (2.17) can be derived<sup>30</sup> using the momentum-space behavior of the kernels of  $q_{\alpha,i}(E; \Sigma)$ , or alternatively by using trace-class methods and direct-integral representations of Hilbert spaces.<sup>31,32</sup> In the limit  $\Sigma \rightarrow \infty$ , both members of equality (2.17) can be related to the three-body  $S$  matrices.<sup>16,26,28-31,33</sup>

### III. INTEGER MOMENT SUM RULES

We begin with an investigation of the behavior of the resolvent kernels  $R(Z)$ ,  $R_\alpha(Z)$ , and  $R_0(Z)$  in coordinate space. In particular, we want to obtain the large- $Z$  expansion for these kernels. Let us re-

call that the problem of obtaining the high-temperature expansion of the heat-equation kernel is completely solved.<sup>21</sup> Given  $H$  as defined by Eq. (2.5), the kernel of the operator  $e^{-\beta H}$  has the following asymptotic expansion in the inverse temperature variable  $\beta$ :

$$e^{-\beta H}(\vec{\rho}, \vec{\rho}') \sim e^{-\beta H_0}(\vec{\rho}, \vec{\rho}') \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \beta^n P_n(\vec{\rho}, \vec{\rho}'), \quad (3.1)$$

where the free heat kernel is the standard expression

$$e^{-\beta H_0}(\vec{\rho}, \vec{\rho}') = \frac{1}{(4\pi q\beta)^3} \exp\left[-\frac{1}{4\beta q}(\vec{\rho} - \vec{\rho}')^2\right]. \quad (3.2)$$

Here, the metric length squared  $(\vec{\rho} - \vec{\rho}')^2$  is given by formula (2.2). The basic quantum scale factor for the system is

$$q = \frac{\hbar^2}{2m_0}. \quad (3.3)$$

The coefficient functions  $P_n(\vec{\rho}, \vec{\rho}')$  are completely determined in terms of the three-body potential  $U$ . These functions satisfy a simple recursion relation.<sup>34</sup> In Ref. 21 the recursion relation has been solved to provide a parametric integral formula for all  $P_n(\vec{\rho}, \vec{\rho}')$ . The  $P_n(\vec{\rho}, \vec{\rho}')$  are polynomials of order  $n$  in the potential and certain coordinate-space derivatives of the potential. Furthermore, they are polynomials of order  $2(n-1)$  in Planck's constant  $\hbar$ . Our final results require only the diagonal value  $\vec{\rho} = \vec{\rho}'$  of these coefficient functions. We denote this value by  $P_n(\vec{\rho})$ .

The resolvent  $R(Z)$  is obtained from the operator  $e^{-\beta H}$  by Laplace transforming. Take  $\sigma(H)$  to be the spectrum of  $H$  then  $R(Z)$  is given by

$$R(Z) = \int_0^{\infty} d\beta e^{Z\beta} e^{-\beta H}, \quad \text{Re}Z < \inf \sigma(H). \quad (3.4)$$

This operator identity has the following kernel form:

$$R(Z; \vec{\rho}, \vec{\rho}') = \int_0^{\infty} d\beta e^{Z\beta} e^{-\beta H}(\vec{\rho}, \vec{\rho}'). \quad (3.5)$$

Inserting the asymptotic expansion (3.1) into the transform (3.5) gives us an asymptotic expansion for the resolvent kernel

$$R(Z; \vec{\rho}, \vec{\rho}') \sim \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} P_n(\vec{\rho}, \vec{\rho}') \times \int_0^{\infty} d\beta e^{Z\beta} \beta^n e^{-\beta H_0}(\vec{\rho}, \vec{\rho}'). \quad (3.6)$$

Both Eqs. (3.1) and (3.6) are uniform asymptotic expansions with respect to  $\vec{\rho}, \vec{\rho}'$  having values in some finite region of coordinate space.<sup>35</sup>

The integrals in expression (3.6) can be explicitly evaluated. Representing  $Z$  by the polar variables  $Z = |Z| e^{i\theta}$ , where  $\theta \in [0, 2\pi)$ , and setting  $\Delta^2 = |\vec{\rho} - \vec{\rho}'|^2$ , these integrals can be written as<sup>36</sup> [recall Eq. (3.2)]

$$I_n \equiv \int_0^{\infty} d\beta e^{Z\beta} \beta^{n-3} \exp(-\Delta^2/4q\beta) = \frac{2i^{n-2}}{Z^{n-2}} \left[ \frac{Z^{1/2} q^{-1/2} \Delta}{2} \right] K_{n-2}(-i(Z^{1/2} q^{-1/2} \Delta)), \quad (3.7)$$

where  $K_{n-2}$  is the modified Bessel function of the third kind. Formula (3.7) is valid for  $\theta \in (\pi/2, 3\pi/2)$ , or equivalently for  $\text{Re}Z < 0$ . Let  $\Pi \equiv \{Z: Z \notin \mathcal{R}^+\}$  be the  $Z$  plane with a cut along the positive real axis. The result (3.7) can then be extended to the domain  $\Pi$  by analytic continuation in the following way. Introducing the Hankel function  $H_\nu^{(1)}$ , connected to  $K_\nu$  by<sup>37</sup>

$$K_\nu(Z') = \frac{\pi i}{2} e^{v\pi i/2} H_\nu^{(1)}(e^{i\pi/2} Z'), \quad -\pi < \arg Z' \leq \frac{\pi}{2} \quad (3.8)$$

the analytically continued form of integral  $I_n$  is

$$I_n = \frac{\pi i (-1)^n}{Z^{n-2}} \left[ \frac{Z^{1/2} q^{-1/2} \Delta}{2} \right]^{n-2} \times H_{n-2}^{(1)}(Z^{1/2} q^{-1/2} \Delta), \quad (3.9)$$

for all  $Z \in \Pi$ . In this way the expansion (3.6) now reads

$$R(Z; \vec{\rho}, \vec{\rho}') \sim a\pi i \sum_{n=0}^{\infty} \frac{1}{n!} P_n(\vec{\rho}, \vec{\rho}') \frac{1}{Z^{n-2}} \left[ \frac{Z^{1/2} q^{-1/2} \Delta}{2} \right]^{n-2} \times H_{n-2}^{(1)}(Z^{1/2} q^{-1/2} \Delta), \quad (3.10)$$

where the constant  $a$  is given by  $(4\pi q)^{-3}$ .

To proceed further it is useful to understand the behavior of the first few terms in the series (3.10). Consider the exact and free resolvent kernels  $R(Z; \vec{\rho}, \vec{\rho}')$  and  $R_0(Z; \vec{\rho}, \vec{\rho}')$  [the latter is exactly given by the  $n=0$  term in the expansion (3.10)] as functions of  $\vec{\rho}$  and  $\vec{\rho}'$  for fixed  $Z$ . By using well-known properties of the Hankel functions<sup>37</sup> we see that the  $n=0$  term in expression (3.10) is propor-

tional to  $|\vec{\rho}-\vec{\rho}'|^{-4}$  for  $\vec{\rho}'\rightarrow\vec{\rho}$ . The second term  $n=1$  is also singular in that limit and behaves like  $|\vec{\rho}-\vec{\rho}'|^{-2}$ . Finally, the  $n=2$  term goes then as  $\ln|\vec{\rho}-\vec{\rho}'|$ . In fact, all this singular behavior is confined to the real part of the functions  $R(Z;\vec{\rho},\vec{\rho}')$  and  $R_0(Z;\vec{\rho},\vec{\rho}')$ . Their imaginary part is always nonsingular as  $\vec{\rho}\rightarrow\vec{\rho}'$ . For  $n\geq 3$  the terms in the series (3.10) are no longer singular. Thus by subtracting the  $n=0,1,2$  terms from  $R(Z;\vec{\rho},\vec{\rho}')$  in (3.10), it is possible to define a regularized Green's function that has a smooth, well-defined diagonal value.

Since the spectral sum rules involve the change in the total continuum-state density, we need to ex-

pand the connected resolvent difference given by

$$R_c(Z)\equiv R(Z)-R_0(Z)-\sum_{\alpha>0}[R_\alpha(Z)-R_0(Z)]. \tag{3.11}$$

For the resolvent  $R(Z)$  we employ the expansion (3.10). In the case of the resolvent  $R_\alpha(Z)$  ( $\alpha>0$ ), defined for the Hamiltonian  $H_\alpha$ , this expansion is just Eq. (3.10) with  $P_n(\vec{\rho},\vec{\rho}')$  replaced by  $P_n^\alpha(\vec{\rho},\vec{\rho}')$ . The notation  $P_n^\alpha(\vec{\rho},\vec{\rho}')$  means that the potential entering the expressions for  $P_n^\alpha(\vec{\rho},\vec{\rho}')$  is  $V_\alpha(\vec{x}_\alpha,\vec{y}_\alpha)$ . So the connected resolvent difference (3.11) allows the expansion

$$R_c(Z;\vec{\rho},\vec{\rho}')\sim a\pi i\sum_{n=2}^\infty\frac{1}{n!}P_n^c(\vec{\rho},\vec{\rho}')\frac{1}{Z^{n-2}}\left[\frac{Z^{1/2}q^{-1/2}\Delta}{2}\right]^{n-2}H_{n-2}^{(1)}(Z^{1/2}q^{1/2}\Delta), \tag{3.12}$$

where  $P_n^c$  denotes the connected coefficient function

$$P_n^c(\vec{\rho},\vec{\rho}')=P_n(\vec{\rho},\vec{\rho}')-\sum_{\alpha>0}P_n^\alpha(\vec{\rho},\rho'). \tag{3.13}$$

Here we have used the fact that the  $n=0$  term for  $R_c(Z)$  clearly vanishes. Furthermore, the  $n=1$  term is also zero because of the linearity of  $P_1(\vec{\rho},\vec{\rho}')$  in the potential, viz. [see Ref. 21, Eq. (2.23)],

$$P_1^c(\vec{\rho},\vec{\rho}')=\int_0^1d\xi U[\xi\vec{\rho}+(1-\xi)\vec{\rho}']-\sum_\alpha\int_0^1d\xi V_\alpha[\xi\vec{\rho}_\alpha+(1-\xi)\vec{\rho}'_\alpha]=0. \tag{3.14}$$

This last result is a consequence of the assumption that the total three-body potential  $U$  is a sum of pairwise forces. If  $U$  has a true three-body force then  $P_1^c\neq 0$ .

The last stage of the derivation is to use Cauchy's theorem to extract the sum rules from the analyticity of  $R_c(Z;\vec{\rho},\vec{\rho}')$ . Let  $N$  be a non-negative integer. (It will be the order of the sum rule.) For a fixed value of  $\vec{\rho}$  and a given  $N$  we consider the analytic function

$$F_N(Z;\vec{\rho})\equiv Z^N\left[r(Z;\vec{\rho})-a\sum_{n=3}^{N+3}\frac{P_n^c(\vec{\rho})}{n(n-1)(n-2)}\frac{1}{Z^{n-2}}\right], \tag{3.15}$$

where the term  $r(Z;\vec{\rho})$  is the diagonal value of the regularized connected resolvent difference, viz.,

$$r(Z;\vec{\rho})\equiv\lim_{\Delta\rightarrow 0}\left[R_c(Z;\vec{\rho},\vec{\rho}')-\frac{\pi ia}{2}P_2^c(\vec{\rho},\vec{\rho}')H_0^{(1)}(Z^{1/2}q^{-1/2}\Delta)\right]. \tag{3.16}$$

The terms  $n=3\sim N+3$  are the diagonal values of the corresponding terms in Eq. (3.12), namely,

$$\lim_{\Delta\rightarrow 0}a\pi i\sum_{n=3}^{N+3}\frac{1}{n!}P_n^c(\vec{\rho},\vec{\rho}')\frac{1}{Z^{n-2}}\left[\frac{Z^{1/2}q^{-1/2}\Delta}{2}\right]^{n-2}H_{n-2}^{(1)}(Z^{1/2}q^{-1/2}\Delta)=\sum_{n=3}^{N+3}a\frac{(n-3)!}{n!}P_n^c(\vec{\rho})\frac{1}{Z^{n-2}}, \tag{3.17}$$

where we have used the standard small argument series expansion for the Hankel functions.<sup>37</sup>

The function  $F_N(Z;\vec{\rho})$  is analytic in the domain  $\Pi_\sigma\equiv\{Z:Z\notin\sigma(H)\}$ . Since  $F_N(Z;\vec{\rho})$  contains the first  $N+3$  terms in the asymptotic expansion of  $R_c(Z;\vec{\rho},\vec{\rho}')$ , the order of the next term will be  $Z^{-N-2}$ . This means that the large- $Z$  behavior of

$F_N(Z,\vec{\rho})$  will be

$$F_N(Z;\vec{\rho})=O(|Z|^{-2}). \tag{3.18}$$

Cauchy's theorem then states that for each closed contour whose interior is within  $\Pi_\sigma$ ,

$$\oint dZ F_N(Z;\vec{\rho})=0. \tag{3.19}$$

Decompose the closed contour into two segments  $C_\Gamma$  and  $C_\eta$ , as indicated in Fig. 1. First we infer from Eq. (3.18) that the total contribution around  $C_\Gamma$  vanishes in the limit  $\Gamma \rightarrow \infty$ . Secondly, we calculate the contribution from the point spectrum part of  $r(Z; \vec{\rho})$  by using Eqs. (2.13)–(2.15) to write

$$R_p(Z; \vec{\rho}, \vec{\rho}') = \sum_{i=1}^{N_3} \frac{\Psi_i(\vec{\rho}) \Psi_i^*(\vec{\rho}')}{E_i - Z}. \quad (3.20)$$

In that way we obtain

$$\begin{aligned} \int_{C_\eta} dZ Z^N R_p(Z) (\vec{\rho}, \vec{\rho}') \\ = 2\pi i \sum_{i=1}^{N_3} (E_i)^N |\Psi_i(\vec{\rho})|^2. \end{aligned} \quad (3.21)$$

Note that there is no restriction about the location of the point spectrum. It may coincide with the continuous spectrum. Next we discuss the subtraction terms in Eq. (3.15). Their contribution to  $C_\eta$  is finite and is straightforward to evaluate as a line integral from  $\Gamma - i0$  to  $\Gamma + i0$ . Only the  $n = N + 3$  term is nonzero, so

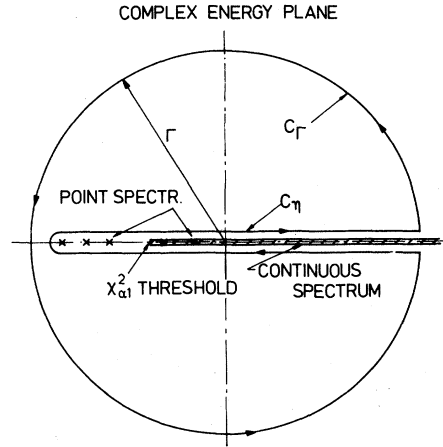


FIG. 1. Contour in the complex energy plane around the spectrum of  $H$ .

$$\begin{aligned} \int_{C_\eta} dZ Z^N \left[ -a \sum_{n=3}^{N+3} \frac{P_n^c(\vec{\rho})}{n(n-1)(n-2)} \frac{1}{Z^{n-2}} \right] \\ = 2\pi i \frac{a}{b} P_{N+3}^c(\vec{\rho}), \end{aligned} \quad (3.22)$$

where  $b = (N+3)(N+2)(N+1)$ . Finally, we determine the contribution from the rest of  $r(Z; \vec{\rho})$ . Utilizing Eq. (2.16) we set

$$r(Z; \vec{\rho}) - R_p(Z; \vec{\rho}, \vec{\rho}') = \lim_{\Delta \rightarrow 0} [\tilde{R}(Z; \vec{\rho}, \vec{\rho}') - \frac{1}{2} \pi i a P_2^c(\vec{\rho}, \vec{\rho}') H_0^{(1)}(Z^{1/2} q^{-1/2} \Delta)]. \quad (3.23)$$

Take  $-\chi_{\alpha,1}^2$  to be the threshold energy for three-body scattering. Then, with the use of the reflection property

$$\tilde{R}(Z^*; \vec{\rho}, \vec{\rho}') = \tilde{R}^*(Z; \vec{\rho}, \vec{\rho}'), \quad (3.24)$$

we arrive at

$$\int_{C_\eta} dZ Z^N [r(Z; \vec{\rho}) - R_p(Z; \vec{\rho}, \vec{\rho}')] = \int_{-\chi_{\alpha,1}^2}^{\infty} dE E^N 2i [\text{Im} \tilde{R}(E + i0; \vec{\rho}, \vec{\rho}') - \frac{1}{2} \pi a P_2^c(\vec{\rho})]. \quad (3.25)$$

Adding all these results we get

$$\int_{-\chi_{\alpha,1}^2}^{\infty} dE E^N 2i [\text{Im} \tilde{R}(E + i0; \vec{\rho}, \vec{\rho}') - \frac{1}{2} \pi a P_2^c(\vec{\rho})] = -2\pi \sum_{i=1}^{N_3} (E_i)^N |\Psi_i(\vec{\rho})|^2 - \frac{2\pi a}{b} P_{N+3}^c(\vec{\rho}). \quad (3.26)$$

This identity holds for each value of  $\vec{\rho}$ . Consider the precise form of the function  $P_2^c(\vec{\rho})$ . From Ref. 21, the formula for  $P_2(\vec{\rho})$  is

$$P_2(\vec{\rho}) = U(\vec{\rho})^2 - \frac{1}{3} q \Delta_p U(\vec{\rho}), \quad (3.27)$$

where  $\Delta_p$  is the six-dimensional Laplacian. Because the Laplacian term is linear in the potential we have

$$P_2^c(\vec{\rho}) = 2 \sum_{\alpha} \sum_{\beta > \alpha} v_{\alpha}(\vec{x}_{\alpha}) v_{\beta}(\vec{x}_{\beta}). \quad (3.28)$$

The  $P_{N+3}^c(\vec{\rho})$  on the rhs of Eq. (3.26) can be obtained in a similar way, e.g., formally

$$P_3^c = 6v_{\alpha} v_{\beta} v_{\gamma} + 3 \sum_{\alpha} \sum_{\beta \neq \alpha} v_{\alpha} v_{\beta}^2 - q \sum_{\alpha} \sum_{\beta \neq \alpha} v_{\alpha} \Delta_p v_{\beta} - q \sum_{\alpha} \sum_{\beta > \alpha} \vec{\nabla}_{\rho} v_{\alpha} \cdot \vec{\nabla}_{\rho} v_{\beta}. \quad (3.29)$$

In order to introduce time delay into the sum rules we integrate Eq. (3.26) with respect to  $\vec{\rho}$  in an arbitrary,

but finite, region  $\Sigma$ . If  $P(\Sigma)$  is the projection operator for this region [see Eq. (A2)] then

$$\int_{\Sigma} d\vec{\rho} \operatorname{Im} \tilde{R}(E + i0; \vec{\rho}, \vec{\rho}) = \operatorname{Tr} P(\Sigma) \operatorname{Im} \tilde{R}(E + i0) P(\Sigma). \tag{3.30}$$

The rhs of equality (3.30) may be replaced with the trace of the three-body time-delay operators by the spectral property (2.17). Thus Eq. (3.26) implies the spectral sum rule

$$\begin{aligned} \int_{-\chi_{\alpha,1}^2}^{\infty} dE E^N \left[ \hbar^{-1} \sum_{\alpha,i} \operatorname{tr} q_{\alpha,i}(E; \Sigma) - \frac{\pi}{(4\pi q)^3} \int_{\Sigma} P_2^c(\vec{\rho}) d\vec{\rho} \right] \\ = -2\pi \sum_{i=1}^{N_3} (E_i)^N \int_{\Sigma} d\vec{\rho} |\Psi_i(\vec{\rho})|^2 - \frac{2\pi}{(4\pi q)^3 (N+3)(N+2)(N+1)} \int_{\Sigma} d\vec{\rho} P_{N+3}^c(\vec{\rho}). \end{aligned} \tag{3.31}$$

Statement (3.31) is the principal result of this paper. For every space region  $\Sigma$  having finite Lebesgue measure and all integers  $N \geq 0$ , the sum rule (3.31) gives the precise inter-relationship between the  $N$ th energy moment of the time-delays of all open channels and the energy-weighted probability for finding the bound-state wave functions in the region  $\Sigma$ . As presented in formula (3.31) the form of the sum rule has several features found earlier in the study of sum rules for classical scattering. The validity of expression (3.31) in arbitrary regions of space was first observed in the classical rules.<sup>18</sup> The presence of the surface term  $P_{N+3}^c(\vec{\rho})$  is also a characteristic of the classical rules in even-dimensional spaces.<sup>18,19</sup>

The derivation just outlined for identity (3.31) is clearly heuristic. The step that is most difficult to make rigorous is the demonstration of the fact that the estimate (3.18) is uniform in  $\arg Z$ . Assume that the potential interaction can be written as the Fourier transform of a signed measure  $\mu(\vec{\alpha})$ , having finite bounded variation, i.e.,

$$U(\vec{\rho}) = \int d\mu(\vec{\alpha}) e^{i\vec{\alpha} \cdot \vec{\rho}}, \tag{3.32}$$

$$\begin{aligned} \int_{-\chi_{\alpha,1}^2}^{\infty} dE E^N \left[ 2 \operatorname{Tr} \operatorname{Im} \tilde{R}(E + i0) - \frac{\pi}{(4\pi q)^3} \int d\vec{\rho} P_2^c(\vec{\rho}) \right] \\ = -2\pi \sum_{i=1}^{N_3} (E_i)^N - \frac{2\pi}{(4\pi q)^3 (N+1)(N+2)(N+3)} \int d\vec{\rho} P_{N+3}^c(\vec{\rho}). \end{aligned} \tag{3.34}$$

Note that  $\operatorname{Tr} \operatorname{Im} \tilde{R}(E + i0)$  on the lhs of (3.34) can also be written in terms of the three-body  $S$  matrices.<sup>33</sup> In this form (3.34) the sum rules constitute higher-order three-body Levinson's theorems.

#### IV. FRACTIONAL MOMENT SUM RULES

Let us derive the forms for the complex power moment sum rules. Starting from the formulas (3.15) and (3.16), we obtain by setting  $N = 0$

where

$$\|\mu\| = \int d|\mu|(\vec{\alpha}) < \infty. \tag{3.33}$$

For potentials of this class it is not difficult to prove the following.<sup>35</sup> Let  $Z_0$  be a point on the negative real axis to the left of the spectrum of  $H$ . From the Laplace transform (3.5) one can establish that the statement (3.18) is valid if  $\arg(Z - Z_0) \in (\pi/2, 3\pi/2)$ . Furthermore, this result may be extended by analytic continuation [using integral (3.5)], if the real parameter  $\beta$  is rotated in the complex plane. Thus, for every  $\delta > 0$  one can obtain that (3.18) is valid in the domain  $\arg(Z - Z_0) \in (\delta, 2\pi - \delta)$ . Our derivation, however, assumes the stronger result that (3.18) is also valid for  $\delta = 0$ .

The global sum rules follow from (3.31) if the limit  $P(\Sigma) \rightarrow 1$  is taken. Since this limit, for trace quantities, has not yet been rigorously characterized in three-body time-delay theory for all possible channels (see the Appendix), we state the result in terms of  $\operatorname{Tr} \operatorname{Im} \tilde{R}(E + i0)$ . Thus the rule (3.31) has the global form

$$F_0(Z; \vec{\rho}) = r(Z; \vec{\rho}) - \frac{a}{3!} P_3^c(\vec{\rho}) \frac{1}{Z}. \tag{4.1}$$

Next, we recall that the function  $F_0(Z; \vec{\rho})$  is analytic for all  $Z \in \Pi_{\sigma}$ , i.e., for all  $Z$  away from the spec-

trum of  $H$ . So for the contour shown in Fig. 1, we have that

$$\oint dZ Z^{\lambda+i\mu} F_0(Z; \vec{\rho}) = 0, \tag{4.2}$$

where  $0 \leq \lambda < 1$  and  $\mu \in \mathcal{R}$ . Using these constraints and the fact that  $F_0(Z; \vec{\rho})$  behaves as  $Z^{-2}$  for large  $Z$ , one obtains that the  $C_\Gamma$  line-integral contribution to (4.2) is zero in the limit  $\Gamma \rightarrow \infty$ . In this way we see that all the nontrivial contributions to the in-

tegral (4.2) are associated with the  $C_\eta$  line integral.

Consider first the point spectrum contribution to  $C_\eta$ . Clearly, this is

$$\int_{C_\eta} dZ Z^{\lambda+i\mu} R_p(Z)(\vec{\rho}, \vec{\rho}) = 2\pi i \sum_{j=1}^{N_3} (E_j)^{\lambda+i\mu} |\Psi_j(\vec{\rho})|^2. \tag{4.3}$$

Secondly, the continuous spectrum contribution to  $C_\eta$  is defined as the sum

$$I = \int_{-\chi_{\alpha,1}^2}^\Gamma dE (E+i\eta)^{\lambda+i\mu} \tilde{F}_0(E+i\eta; \vec{\rho}) - \int_{-\chi_{\alpha,1}^2}^\Gamma dE (E-i\eta)^{\lambda+i\mu} \tilde{F}_0(E-i\eta; \vec{\rho}), \tag{4.4}$$

where  $\tilde{F}_0$  denotes  $F_0$  minus the point spectrum component of the Green's function. In terms of the notation of Sec. II it reads

$$F_0(Z; \vec{\rho}) \equiv \lim_{\Delta \rightarrow 0} [\tilde{R}(Z; \vec{\rho}, \vec{\rho}') - \frac{1}{2} a \pi i P_2(\vec{\rho}, \vec{\rho}') H_0^{(1)}(Z^{1/2} q^{-1/2} \Delta)] - \frac{a}{3!} P_3^c(\vec{\rho}) \frac{1}{Z}. \tag{4.5}$$

Representing  $Z^{\lambda+i\mu}$  in polar variables with the origin at  $Z=0$ ,

$$(E+i\eta)^{\lambda+i\mu} = (E^2 + \eta^2)^{(\lambda+i\mu)/2} \exp[i(\lambda+i\mu) \arctan(\eta/E)], \tag{4.6}$$

and defining

$$T(E+i\eta; \vec{\rho}) \equiv \exp[i(\lambda+i\mu) \arctan(\eta/E)] \tilde{F}_0(E+i\eta; \vec{\rho}), \tag{4.7}$$

we can write the integral  $I$  in the form

$$I = \int_{-\chi_{\alpha,1}^2}^\Gamma dE (E^2 + \eta^2)^{(\lambda+i\mu)/2} \{ T(E+i\eta; \vec{\rho}) - \exp[2\pi i(\lambda+i\mu)] T(E+i\eta; \vec{\rho})^* \}. \tag{4.8}$$

To obtain Eq. (4.8) we have also employed the reflection property (3.24). In terms of the real and imaginary parts of  $T(E+i\eta; \vec{\rho})$  the curly bracket part of Eq. (4.8) can be written as

$$\{ \} = -2i(-1)^{\lambda+i\mu} \sin(\lambda+i\mu)\pi \operatorname{Re} T + 2i(-1)^{\lambda+i\mu} \cos(\lambda+i\mu)\pi \operatorname{Im} T. \tag{4.9}$$

The last step in this calculation is to take the limit  $\eta \rightarrow 0$  and  $\Gamma \rightarrow \infty$  in the definition of  $I$ . The boundary values of  $\operatorname{Re} T(E+i\eta; \vec{\rho})$  and  $\operatorname{Im} T(E+i\eta; \vec{\rho})$  are found to be

$$\operatorname{Re} T(E+i0; \vec{\rho}) = G(E; \vec{\rho}) - \frac{a}{3!} P_3^c(\vec{\rho}) \frac{1}{E}, \tag{4.10}$$

where

$$G(E; \vec{\rho}) \equiv \lim_{\Delta \rightarrow 0} [\operatorname{Re} \tilde{R}(E+i0; \vec{\rho}, \vec{\rho}') + \frac{1}{2} a \pi P_2^c(\vec{\rho}, \vec{\rho}') Y_0(E^{1/2} q^{-1/2} \Delta)] \tag{4.11}$$

with  $Y_0$  the Bessel function of the second kind, and

$$\operatorname{Im} T(E+i0; \vec{\rho}) = \operatorname{Im} \tilde{R}(E+i0; \vec{\rho}, \vec{\rho}') - \frac{1}{2} a \pi P_2^c(\vec{\rho}). \tag{4.12}$$

Substituting Eqs. (4.9), (4.10), and (4.12) into Eq. (4.8) gives us the value of  $I$  for  $\eta = +0$  and  $\Gamma = \infty$ . Altogether, expression (4.2) becomes the identity

$$\begin{aligned} -2(-1)^{\lambda+i\mu} \sin(\lambda+i\mu)\pi \int_{-\chi_{\alpha,1}^2}^\infty dE E^{\lambda+i\mu} \left[ G(E; \vec{\rho}) - \frac{a}{3!} P_3^c(\vec{\rho}) \frac{1}{E} \right] \\ + 2(-1)^{\lambda+i\mu} \cos(\lambda+i\mu)\pi \int_{-\chi_{\alpha,1}^2}^\infty dE E^{\lambda+i\mu} [\operatorname{Im} \tilde{R}(E+i0; \vec{\rho}, \vec{\rho}') - \frac{1}{2} a \pi P_2^c(\vec{\rho})] \\ = -2\pi \sum_{j=1}^{N_3} (E_j)^{\lambda+i\mu} |\Psi_j(\vec{\rho})|^2. \end{aligned} \tag{4.13}$$



The relations (4.13) for all  $\lambda \in (0,1)$  and all  $\mu \in \mathcal{R}$  constitute the general complex power sum rules. It is seen that these rules couple the discontinuity of the imaginary part of the connected resolvent difference with that of the real part of the regularized resolvent difference. Identity (4.13) holds for each  $\vec{\rho}$ . The rules for finite-space regions or the global-trace form can be obtained by integrating (4.13) with respect to  $\vec{\rho}$ . In addition the higher-order complex rules can be derived similarly if  $F_0(Z; \vec{\rho})$  is replaced by  $F_N(Z; \vec{\rho})$ .

In particular, we note that the complex rule (4.13) has no surface term on the right-hand side as does the integer rule [e.g., Eq. (3.26) with  $N=0$ ]. The mechanism of this discontinuity arises from the imaginary part of the  $Z^{-1}$  term present in  $\tilde{F}_0(Z; \vec{\rho})$ . This term is explicitly the integral

$$\int_{-\chi_{\alpha,1}^2}^{\Gamma} dE (E^2 + \eta^2)^{(\lambda+i\mu)/2} \frac{\eta}{E^2 + \eta^2} \tag{4.14}$$

times the constant  $-a(3!)^{-1}P_3^c(\vec{\rho})$ . This integral may be evaluated and gives<sup>38</sup>

$$\eta^{\lambda+i\mu} \left\{ \left[ \frac{\Gamma}{\eta} \right] {}_2F_1 \left[ \frac{-\lambda-i\mu+2}{2}, \frac{1}{2}, \frac{3}{2}, - \left[ \frac{\Gamma}{\eta} \right]^2 \right] + \left[ \frac{\chi_{\alpha,1}^2}{\eta} \right] {}_2F_1 \left[ \frac{-\lambda-i\mu+2}{2}, \frac{1}{2}, \frac{3}{2}, - \left[ \frac{\chi_{\alpha,1}^2}{\eta} \right]^2 \right] \right\}. \tag{4.15}$$

The hypergeometric function  ${}_2F_1$ , behaves as  $[1 + (\Gamma/\eta)^2]^{-1/2}$  for a large argument, thus the  $\eta \rightarrow 0$  limit is well defined. The result may then be written

$$\eta^{\lambda+i\mu} \frac{\Gamma(\frac{1}{2})\Gamma \left[ -\frac{\lambda}{2} + \frac{1}{2} - i\frac{\mu}{2} \right]}{\Gamma \left[ -\frac{\lambda}{2} + 1 - i\frac{\mu}{2} \right]}. \tag{4.16}$$

This factor gives zero in the  $\eta \rightarrow 0$  limit if  $\lambda > 0$  and  $\mu \in \mathcal{R}$ . But if  $\mu=0$  and  $\lambda=0$  then this term is exactly the surface term appearing on the right-hand side of Eq. (3.26).

Returning to the general behavior of the complex rules, one case of special interest of (4.13) is the rule for  $\lambda = \frac{1}{2}$  and  $\mu=0$ , viz.,

$$\int_{-\chi_{\alpha,1}^2}^{\infty} dE E^{1/2} \left[ G(E; \vec{\rho}) - \frac{a}{3!} P_3^c(\vec{\rho}) \frac{1}{E} \right] = \pi \sum_{j=1}^{N_3} |E_j|^{1/2} |\Psi_j(\vec{\rho})|^2. \tag{4.17}$$

Since in this case the  $\cos(\lambda+i\mu)\pi$  factor vanishes we see that only the real part of the connected resolvent difference appears in statement (4.17).

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APPENDIX

In this appendix, the definition of multichannel time delay appropriate for the three-body problem is given. A detailed account of time delay, its spectral property and the relation to the logarithmic derivative of the  $S$  matrix can be found in Refs. 16 and 26–32. Here we recount only enough of the general theory in order to specify the time-delay operators  $q_{\alpha,i}(E; \Sigma)$ .

Consider a fixed finite region  $\Sigma$ , and an exact time-dependent wave-packet solution of the Schrödinger equation

$$\Psi_{\alpha,i}(t) = e^{-iHt} \Omega_{\alpha,i}^{(+)} f_{\alpha,i} \tag{A1}$$

for an incident state  $f_{\alpha,i} \in \mathcal{H}_{\alpha,i}$ . Take  $P(\Sigma)$  to be the projection operator in  $\mathcal{H}$  on the region  $\Sigma$ , viz.,

$$[P(\Sigma)f](\vec{x}_\alpha, \vec{y}_\alpha) = \begin{cases} f(\vec{x}_\alpha, \vec{y}_\alpha) & \text{if } (\vec{x}_\alpha, \vec{y}_\alpha) \in \Sigma \\ 0 & \text{otherwise.} \end{cases} \tag{A2}$$

Then the transit time of  $\Psi_{\alpha,i}(t)$  through the region  $\Sigma$  is given by the integral

$$\int_{-\infty}^{\infty} dt ||P(\Sigma)\Psi_{\alpha,i}(t)||^2. \tag{A3}$$

The corresponding “free” transit time for the incident state  $f_{\alpha,i}$  is generated by the time evolution under  $H_\alpha$  rather than  $H$  and is represented by the integral

$$\int_{-\infty}^{\infty} dt ||P(\Sigma)e^{-iH_\alpha t}J_{\alpha,i}f_{\alpha,i}||^2. \quad (\text{A4})$$

Doing the time integration in both the expressions (A3) and (A4) gives an energy-conserving delta function and provides us with a time-independent operator whose matrix elements give us the difference of the transit times (A3) and (A4). Specifically, for all  $\alpha > 0$ ,

$$(f_{\alpha,i}, Q_{\alpha,i}(\Sigma)f_{\alpha,i}) = \int_{-\infty}^{\infty} dt [||P(\Sigma)\Psi_{\alpha,i}(t)||^2 - ||P(\Sigma)e^{-iH_\alpha t}J_{\alpha,i}f_{\alpha,i}||^2], \quad (\text{A5})$$

where the momentum-space representation of  $Q_{\alpha,i}(\Sigma)$  is given by

$$(f_{\alpha,i}, Q_{\alpha,i}(\Sigma)f_{\alpha,i}) = \int \int d\vec{p}_\alpha d\vec{p}'_\alpha f_{\alpha,i}^*(\vec{p}'_\alpha) \frac{\delta(E' - E)}{n_\alpha p_\alpha} q_{\alpha,i}(E, \Sigma; \hat{p}'_\alpha, \hat{p}_\alpha) f_{\alpha,i}(\vec{p}_\alpha). \quad (\text{A6})$$

In formula (A6),  $E$  and  $E'$  are given by  $\vec{p}_\alpha^2/2n_\alpha - \chi_{\alpha,i}^2$  and  $\vec{p}'_\alpha^2/2n_\alpha - \chi_{\alpha,i}^2$ ;  $\hat{p}_\alpha, \hat{p}'_\alpha$  are the unit direction vectors defined by  $\vec{p}_\alpha, \vec{p}'_\alpha$ , and  $q_{\alpha,i}(E, \Sigma; \hat{p}'_\alpha, \hat{p}_\alpha)$  is the kernel

$$q_{\alpha,i}(E, \Sigma; \hat{p}'_\alpha, \hat{p}_\alpha) = hn_\alpha p_\alpha [\Omega_{\alpha,i}^{(+)\dagger} P(\Sigma) \Omega_{\alpha,i}^{(+)} - J_{\alpha,i}^\dagger P(\Sigma) J_{\alpha,i}] (\vec{p}'_\alpha, \vec{p}_\alpha). \quad (\text{A7})$$

The right-hand side of Eq. (A7) is the momentum-space kernel defined by the operator  $\Omega_{\alpha,i}^{(+)\dagger} P(\Sigma) \Omega_{\alpha,i}^{(+)} - J_{\alpha,i}^\dagger P(\Sigma) J_{\alpha,i}$ . The momenta appearing there are those restricted to the on-shell momenta in channel  $\alpha i$  specified by the energy  $E$ .

The  $\alpha=0$  case is the three-particle collision initiated from an incoming state of three asymptotically free particles. An arbitrary incoming wave packet may have a component that leads to the collision of two particles while the third is a remote noninteracting spectator. This is not a true three-particle scattering and so the definition of time delay should remove the contribution of these disconnected three-particle collisions. So from the difference

$$T(f_0) \equiv \int_{-\infty}^{\infty} dt [||P(\Sigma)e^{-iHt}\Omega_0^{(+)}f_0||^2 - ||P(\Sigma)e^{-iH_0 t}f_0||^2] \quad (\text{A8})$$

we subtract

$$T_\alpha(f_0) \equiv \sum_{\alpha>0} \int_{-\infty}^{\infty} dt [||P(\Sigma)e^{-iH_\alpha t}W_\alpha^{(+)}f_0||^2 - ||P(\Sigma)e^{-iH_0 t}f_0||^2], \quad (\text{A9})$$

where  $W_\alpha^{(+)}$  is the two-body wave operator for the system  $(\beta, \gamma)$  in the three-particle space  $\mathcal{H}$ , viz.,

$$W_\alpha^{(+)} = 1_\alpha \otimes \omega_\alpha^{(+)}, \quad (\text{A10})$$

with  $\omega_\alpha^{(+)}$  defined by Eq. (2.7) and  $1_\alpha$  the identity operator on the space  $\mathcal{H}_{\alpha,i}$ . This defines the connected time delay for a region  $\Sigma$  and an incoming channel  $\alpha=0$ . The time-independent operator  $Q_0(\Sigma)$  for this process is then

$$(f_0, Q_0(\Sigma)f_0) = T(f_0) - T_\alpha(f_0). \quad (\text{A11})$$

Let  $\vec{p}_0$  denote the six-dimensional momentum pair  $(\vec{p}_\alpha, \vec{q}_\alpha)$  and

$$\frac{\vec{p}_0^2}{2m_0} = \frac{\vec{p}_\alpha^2}{2n_\alpha} + \frac{\vec{k}_\alpha^2}{2\mu_\alpha}. \quad (\text{A12})$$

With this notation the kernel for  $Q_0(\Sigma)$  is

$$(f_0, Q_0(\Sigma)f_0) = \int \int d\vec{p}_0 d\vec{p}'_0 f_0^*(\vec{p}'_0) \frac{\delta(E - E')}{m_0 p_0^4} q_0(E, \Sigma; \hat{p}'_0, \hat{p}_0) f_0(\vec{p}_0), \quad (\text{A13})$$

where the on-energy shell operator is  $(E = p_0^2/2m_0 = p_0'^2/2m_0)$

$$q_0(E, \Sigma; \hat{p}'_0, \hat{p}_0) = hm_0 p_0^4 \left[ \Omega_0^{(+)\dagger} P(\Sigma) \Omega_0^{(+)} - P(\Sigma) - \sum_{\alpha>0} [W_\alpha^{(+)\dagger} P(\Sigma) W_\alpha^{(+)} - P(\Sigma)] \right] (\vec{p}'_0, \vec{p}_0). \quad (\text{A14})$$

Here  $(p_0, \hat{p}_0)$  is the spherical coordinate description of the point  $\vec{p}_0$ . Formulas (A7) and (A14) provide explicit momentum-space kernel representations of  $q_{\alpha,i}(E; \Sigma)$  and  $q_0(E; \Sigma)$ . They are valid for all  $E$  and any finite measurable set  $\Sigma$ . However, modifi-

cations of these formulas need to be introduced if one wants to analyze the limit where  $\Sigma$  becomes all of the six-dimensional space. For more details we refer to Refs. 16 and 28–30.

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