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Calculation of resonances in a $dt\mu$ molecule by the R-matrix method

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Using the spectral representation of Green's function, we calculate the density of states and extract parameters of resonances in the scattering system. The method is implemented for the resonances in the $dt\mu$ molecule below the $t\mu$ $(n=2)$ threshold.

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The R-matrix method [1] is widely used in time-independent scattering calculations. It was first shown by Wigner and Eisenbud [2] that the R matrix permits a convergent spectral expansion. A similar representation was used by Schneider and Walker to derive the R-matrix propagation equations within the scope of the diabatic-by-sector scheme [3]. Essentially, the same method was also given later by Baluja Burke, and Morgan [4] and the modifications for adiabatic-by-sector approach were proposed in Refs. [5], [6].

We have shown recently that the spectral representation can be obtained also for the scattering wave function itself [7]. This provides a very stable numerical technique for solving both homogeneous and inhomogeneous Schrödinger equations with arbitrary boundary conditions. The method has been used for studying dissociative electron attachment to di-atomic molecules and proved to be very efficient [8]. In these previous papers, the emphasis was mostly given to the numerical efficiency, but the significance of the method can go far beyond just the numerical method. In the case of inhomogeneous Schrödinger equation, the spectral expansion of the solution leads to the same representation for Green's function. The latter yields, in principle, full information about the system, which can be easily extracted due to well established properties of the basis functions in the spectral expansion. In the present work, we calculate the density of states in the scattering system and illustrate the method by calculating the resonances in the three-body Coulombic system of $dt\mu$ molecule.

We start with a brief derivation of Green's function, appropriate for the three-body problem. We use the mass-scaled hyperspherical coordinates $\mathbf{R}=(R,\boldsymbol{\varphi})$, where $\boldsymbol{\varphi}$ denotes a set of angle variables on the hypersphere Ω. We confine the system in the box $R\in[0,R_f]$ and consider the inhomogeneous problem

$$[K+H_{\mathrm{ad}}(\boldsymbol{\varphi};R)-E]\Psi(R,\boldsymbol{\varphi})=\chi(R,\boldsymbol{\varphi}), \tag{1}$$

$$\text{with}\quad K=-\,(1/2R^2)\,(\partial/\partial R)\,R^2\,(\partial/\partial R)+(15/8R^2) \tag{2}$$

$$\text{and}\quad \Psi(0,\boldsymbol{\varphi})=0. \tag{3}$$

Here, $\Psi(R,\boldsymbol{\varphi})$ is the wave function of the three-body system multiplied by $R^{3/2}$ and the adiabatic Hamiltonian H_{ad} depends on R parametrically. Inhomogeneous part $\chi(R,\boldsymbol{\varphi})$ is an arbitrary L^2 function. In order to introduce Green's function, we impose the additional homogeneous condition at $R=R_f$. Let $\Phi_\nu(\boldsymbol{\varphi})$ be the real-valued hyperspherical adiabatic channel functions (i.e., the eigenfunctions of H_{ad}) calculated at $R=R_f\Phi_\nu$ form a complete basis set on the hypersphere and we assume the boundary condition at $R=R_f$ in a general form

$$\left\langle \Phi_\nu \middle| \frac{d\Psi}{dR} \right\rangle = \sum_{\mu=1}^{N_{\mathrm{ch}}} A_{\nu\mu}\langle \Phi_\mu|\Psi\rangle, \tag{4}$$

where $\langle\Phi_\nu|\Psi\rangle$ stands for the integral on the hypersphere $R=R_f$,

$$\langle\Phi_\nu|\Psi\rangle \equiv \int_\Omega \Phi_\nu(\boldsymbol{\varphi};R_f)\Psi(R_f,\boldsymbol{\varphi})\,d\mu(\boldsymbol{\varphi}), \tag{5}$$

with $d\mu(\boldsymbol{\varphi})$ being an appropriate measure. Hereafter, we will use the notation $(\cdots|\cdots)$ for integration over the full-dimensional configuration space $\Omega\times[0,R_f]$ with the measure $R^2 dR\, d\mu(\boldsymbol{\varphi})$. The matrix $A_{\nu\mu}$ is a complex-valued boundary matrix determined from the type of Green's function and the corresponding boundary condition. Below we will discuss the case of outgoing Green's function.

The Hamiltonian $K+H_{\mathrm{ad}}$ is not Hermitian due to the surface term at $R=R_f$ in the kinetic-energy operator. The latter can be recast in the form $K=\tilde{K}-L$, where $\tilde{K}$ is the symmetrized operator and the *Bloch operator* L represents the asymmetric part. In the space of square integrable functions satisfying zero boundary condition at the origin [Eq. (3)], $\tilde{K}$ and L are completely determined by the corresponding matrix elements,

$$(\Psi_1|\tilde{K}\Psi_2)\equiv \frac{1}{2}\int_\Omega d\mu(\boldsymbol{\varphi})\int_0^{R_f} dR\,R^2\frac{\partial\Psi_1}{\partial R}\,\frac{\partial\Psi_2}{\partial R} + \frac{15}{8}\int_\Omega d\mu(\boldsymbol{\varphi})\int_0^{R_f} dR\,\Psi_1\Psi_2 \tag{6}$$

and

$$(\Psi_1|L|\Psi_2)\equiv (R_f^2/2)\,\langle\Psi_1|(\partial/\partial R)\Psi_2\rangle. \tag{7}$$

The R-matrix basis is now defined in the usual way by the equation

$$(\Psi_n|\tilde{K}+H_{\mathrm{ad}}|\Psi_m)=E_n\delta_{nm}. \tag{8}$$

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This eigenvalue problem supplies real-valued Ψ_n and E_n which are futher used to expand the solution of interest Ψ as

$$\Psi = \sum_n C_n \Psi_n . \tag{9}$$

It is worth noting that the coefficients in this expansion are generally complex valued and so are the wave function Ψ, which is determined by the boundary condition [Eq. (4)], and the inhomogeneous term χ. Substituting Eq. (9) into Eq. (1) and using Eq. (7), one obtains

$$C_n = \frac{1}{E_n - E}\left[(\Psi_n|\chi) + \frac{R_f^2}{2}\left\langle \Psi_n \middle| \frac{\partial}{\partial R}\Psi \right\rangle \right]. \tag{10}$$

Now the unknown solution $\boldsymbol{\Psi}$ enters only into the surface term and the boundary condition at $R=R_f$ can be used to determine C_n. Using the orthogonality of the adiabatic channel functions on the hypersphere, the last term in Eq. (10) is rewritten as

$$\left\langle \Psi_n \middle| \frac{\partial}{\partial R}\Psi \right\rangle = \sum_\mu \langle \Psi_n | \Phi_u \rangle \lambda_\mu , \tag{11}$$

where by definition $\lambda_\mu \equiv \langle \Phi_\mu | (\partial/\partial R)\Psi \rangle$. From Eqs. (9)–(11) and the boundary condition [Eq. (4)], λ_ν are easily found as

$$\lambda_\nu = \sum_\mu [(1 - A\mathcal{R})^{-1}A]_{\nu\mu} \sum_n \frac{\langle \Phi_\mu | \Psi_n \rangle (\Psi_n | \chi)}{E_n - E}, \tag{12}$$

where

$$\mathcal{R}_{\nu\mu} = \frac{R_f^2}{2} \sum_n \frac{\langle \Phi_\nu | \Psi_n \rangle \langle \Psi_n | \Phi_n \rangle}{E_n - E} \tag{13}$$

is the R matrix at $R=R_f$. Once λ_ν are found, Ψ is given by Eqs. (9)–(11). The solution can be written in the integral form

$$\Psi(R,\boldsymbol{\varphi}) = \int_0^{R_f} R'^2 dR' \int_\Omega d\mu(\boldsymbol{\varphi}') G(R,\boldsymbol{\varphi},R',\boldsymbol{\varphi}') \chi(R',\boldsymbol{\varphi}'), \tag{14}$$

where the kernel is nothing but Green's function

$$G(\mathbf{R},\mathbf{R}',E) = \sum_n \frac{\boldsymbol{\Psi}_n(\mathbf{R})\Psi_n(\mathbf{R}')}{E_n - E} + \frac{R_f^2}{2} \sum_{nm} \frac{C_{nm}\Psi_n(\mathbf{R})\Psi_m(\mathbf{R}')}{(E_n - E)(E_m - E)} \tag{15}$$

with

$$C_{nm} = \sum_{\nu\mu=1}^{N_{ch}} \langle \Psi_n | \Phi_\nu \rangle [(1 - A\mathcal{R})^{-1}A]_{\nu\mu} \langle \Phi_\mu | \Psi_m \rangle. \tag{16}$$

Note the essential difference of Eq. (15) from the ordinary spectral expansion of Green's function in the formal *R*-matrix theory [9,10]. In the latter case, Green's function appears as a kernel of the integral representation which relates the value of the wave function in the inner region $R<R_f$ with its derivatives at the boundary $R=R_f$. On the contrary, the present result is valid for arbitrary values of the arguments $\mathbf{R}$, $\mathbf{R}'$, and Green's function explicitly includes the boundary conditions for the scattering wave function. Starting from Eq. (15), one can obtain similar representation for any physical quantity of interest. Here, we derive a useful expression for the density of states $\rho(E)$ and study resonances in the scattering system.

We introduce $\rho(E)$ by the standard formula

$$\rho(E) = (1/\pi)\,\mathrm{Im}[\mathrm{Tr}\hat{G}^+(E)] = (1/\pi)\,\mathrm{Im}\int_0^{R_f} R^2 dR \sum_\Omega d\mu(\boldsymbol{\varphi}) G^+(\mathbf{R},\mathbf{R},E), \tag{17}$$

where $G^+(\mathbf{R},\mathbf{R},E)$ is the outgoing Green's function. In scattering problems, one usually defines $\hat{G}^+$ by attaching an infinitesimal positive imaginary quantity to the energy *E*. In our formulation, *E* is real while the matrix $A_{\nu\mu}$ in Eq. (4) must correspond to outgoing solutions of the inhomogeneous equation. Inserting Eq. (15) into Eq. (17) and using the orthogonality of Ψ_n, we obtain

$$\rho(E) = \frac{1}{\pi}\,\mathrm{Im}\left[\frac{R_f^2}{2} \sum_{n\nu\mu} \frac{\langle \Psi_n | \Phi_\nu \rangle [(1 - A\mathcal{R})^{-1}A]_{\nu\mu} \langle \Phi_\mu | \Psi_n \rangle}{(E_n - E)^2} \right]. \tag{18}$$

The summation over *n* just gives the *E* derivative of the *R* matrix in Eq. (13) and we come to the following practically useful formula:

$$\rho(E) = (1/\pi)\,\mathrm{Im}\{\mathrm{Tr}[(d\mathcal{R}/dE)\,(1 - A\mathcal{R})^{-1}A]\}. \tag{19}$$

It is worthwhile to note that the spectral representation is not required any more to evaluate $\rho(E)$ in Eq. (19). Any of the well developed methods of *R*-matrix propagation can be implemented to calculate $\mathcal{R}$ at $R=R_f$.

Our purpose is to determine the energy position E_0 and the width Γ of the resonance from the behavior of $\rho(E)$. It is known from the general scattering theory that the density of states [Eq. (17)] contains the resonant contribution $(1/\pi)[d\delta(E)/dE]$ [11], where $\delta(E)$ is the scattering phase shift $\exp[2i\delta(E)] = \det \mathbf{S}(E)$ [12,13]. For a short-range potential, the same result follows directly from Eq. (19). Thus, by cutting off the nonadiabatic couplings between channels at $R=R_f$, we can define the asymptotic states as $f_\nu^\pm = (1/\sqrt{k_\nu}R)e^{\pm i k_\nu R}|\Phi_\nu\rangle$. In this approximation, $A_{\nu\mu} = [ik_\nu(E) - (1/R_f)]\delta_{\nu\mu}$ and Eq. (19) gives

$$\rho(E) = (1/\pi)\,[R_f\ \mathrm{Tr}(1/\hat{k}) - \mathrm{Tr}((1 + \hat{k}\tilde{\mathcal{R}}\hat{k}\tilde{\mathcal{R}})^{-1}(1/\hat{k})\,\tilde{\mathcal{R}}) + (d\delta(E)/dE)], \tag{20}$$

where $\hat{k}$ stands for the corresponding diagonal matrix and $\tilde{\mathcal{R}} \equiv [1 + (1/R_f)\mathcal{R}]^{-1}\mathcal{R}$ is the *R* matrix for the wave function multiplied by the hyper-radius *R*. We assume that the lifetime Γ^{-1} of the resonance is much longer than the characteristic scattering time $R_f \mathrm{Tr}(1/k)$. Then, at *E* close to E_0, the term $d\delta/dE \sim \Gamma$ dominates and the resonant behavior of $\rho(E)$ has the Breit-Wigner form

$$\rho(E)\sim\frac{\Gamma}{2\pi}\frac{1}{(E-E_0)^2+(\Gamma^2/4)}. \tag{21}$$

The short-range approximation is twofold. First, it implies that R_f is much larger than the size of the resonance wave function. If this is not the case, the resonance component of $\rho(E)$ is R_f dependent. This can be easily seen, for example, by expressing Green's function in Eq. (19) via Siegert states [14]. Generally, Eq. (21) must be multiplied by a smooth function of R_f which approaches unity at infinite R_f. Second, the above analysis is based on the diagonal adiabatic boundary matrix $A_{\nu\mu}$. There are such cases, of course, that the long-range part of the interaction should be properly taken into account outside the radius R_f. In general, the boundary condition reads [see Eq. (4)]

$$\mathbf{A}=\mathbf{O}'\mathbf{O}^{-1} \tag{22}$$

with

$$O_{\nu i}=\langle\Phi_\nu|\Psi_i^+\rangle \quad\text{and}\quad O'_{\nu i}=\langle\Phi_\nu|(d/dR)\Psi_i^+\rangle, \tag{23}$$

where Ψ_i^+ are the appropriately found outgoing solutions in the outer region $R>R_f$. The diagonal form of A corresponds to the simplest approximation $\Psi^+=f^+$.

We implemented the method described above to study resonances in $dt\mu$ molecule for zero total angular momentum. Recently, there has been a lot of attention on this system due to its important role in muon catalyzed fusion [15–20]. The lowest resonances in $dt\mu$ have been detected previously and a number of results [14,21–25] are available. Although the different methods give fairly close values for the resonance energies, there are orders of magnitude discrepancy in the widths. The present results resolve this discrepancy.

To propagate the R matrix, we divide the whole interval $[0,R_f]$ into small equal sectors of the size of 5 ma.u. At the boundaries of sectors, the adiabatic eigenvalue problem for $H_{\rm ad}$ is solved using the hyperspherical elliptic coordinates. In these coordinates, one can nicely remove the singularities due to Coulombic potential from $H_{\rm ad}$ [26]. The adiabatic channel functions have been calculated using direct product of DVR (discrete variable representation) basis sets for two hyperangles with the accuracy not worse than six significant digits in the adiabatic energies. Within each sector $[R_l,R_r]$, the R matrix $\mathcal{R}(R)$ is propagated according to the conventional relation [4,5]

$$\mathcal{R}(R_r)=M^{(r,r)}-M^{(r,l)}[M^{(l,l)}+\mathcal{R}(R_l)]^{-1}M^{(l,r)}, \tag{24}$$

where the auxiliary sector matrices $M^{(\alpha,\beta)}$ explicitly depend on the total energy E and are evaluated by the method of Ref. [6]. Differentiation of Eq. (24) with respect to E gives the second equation for propagating $d\mathcal{R}/dE$. We have first calculated $\rho(E)$ taking the logarithmic derivative matrix $A_{\nu\mu}=\delta_{\nu\mu}(ik_\nu-1/R_f)$, where k_ν is the local momentum for the channel ν at R_f. We have found a series of distinct resonance peaks ranging from about six to seven orders of magnitude higher than the nonresonant part of $\rho(E)$. The observed peaks can be perfectly fitted to the Breit-Wigner form of Eq. (21) in a very wide interval of magnitude of $\rho(E)$ (see Fig. 1). The accuracy of the calculations was verified by changing R_f within the interval [500, 640] and using 30, 40, and 50 adiabatic channels. For the lowest eight resonances, the results were stable but for the next two resonances, the widths did not converge with respect to R_f. This indicates the delocalized character of the resonance wave function and strong influence of the long-range interaction. This can be taken into account properly by taking more accurate outgoing boundary conditions without cutting off the couplings at $R=R_f$.

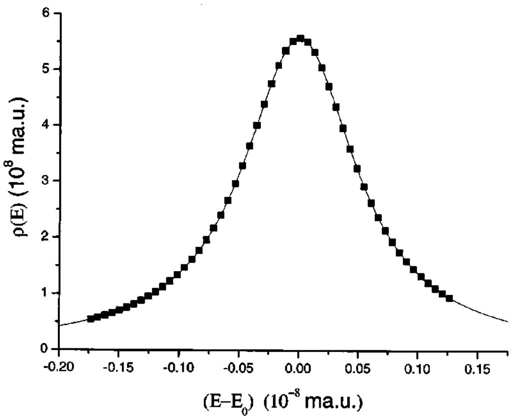

FIG. 1. Density of states in the vicinity of the resonance at $E=-0.134\,529$. The points represent numerical results obtained by Eq. (19). The solid line is the Breit-Wigner formula, Eq. (21), with the parameters from the table.

For this purpose, it is most essential to consider the dipole interaction in the $d+t\mu$ channel. In the corresponding mass-weighed Jacobi coordinates X, Y, θ, with Y for the internal coordinate, the wave function has the form $\Psi=\Sigma_{nl}\chi_{nl}(X)f_{nl}(Y,\theta)$, where f_{nl} are the Coulomb functions. To define the boundary condition correctly, one needs to find $\chi_{nl}(X)$ in the outer region. In the present work, we take into account only the most important long-range part of the interaction ($\sim X^{-2}$), which comes from the dipole matrix elements between degenerate states [27]. In this approximation, n functions χ_{nl}, $l=0,1,\ldots,n-1$ satisfy the system of equations

$$\left[\frac{1}{X^2}\frac{d}{dX}X^2\frac{1}{X^2}-\frac{1}{X^2}[\hat{l}(\hat{l}+1)+\hat{D}_n]+2\left(E+\frac{m}{2n^2}\right)\right]\hat{\chi}=0, \tag{25}$$

where m is the reduced mass of $t\mu$ atom, $\hat{l}$ is the diagonal matrix of angular momentum, and $\hat{D}_n$ is the off-diagonal matrix of the dipole interaction. After diagonalization of the constant matrix $[\hat{l}(\hat{l}+1)+\hat{D}_n]$, Eq. (25) is solved analytically. This gives the adiabatic outgoing solutions in the outer region and the logarithmic derivative matrix is determined by the matching procedure given by Eq. (22). Let us estimate the validity of the short-range potential approximation for the energies below $t\mu$ ($n=2$) threshold. In the case of $n=2$, the nondiagonal elements of $\hat{D}_2$ are $-6(M/m)$, where M is the reduced mass for the relative motion $d+t\mu$. The corresponding eigenvalues of $[\hat{l}(\hat{l}+1)+\hat{D}_2]$ are $1\pm\sqrt{1+36M^2/m^2}$, the negative component of which corresponds to the attractive potential that supports infinite num-

TABLE I. The lowest $L=0$ resonances in $dt\mu$ (in ma.u.)

Ref. [21]	Ref. [24]		Present		Ref. [14]	Ref. [22]	Ref. [23]
$-E_0$	$-E_0$	$10^9\Gamma$	$-E_0$	$10^9\Gamma$	$10^9\Gamma$	$10^9\Gamma$	$10^9\Gamma$
0.159 195	0.159 194	0.640	0.159 193 9	0.341	0.354	0.64×10^4	0.36×10^3
0.145 302	0.145 302	5.56	0.145 301 9	0.829	0.839	0.14×10^5	0.50×10^4
0.134 526	0.134 530	0.37×10^2	0.134 529	1.14	1.15	0.20×10^6	0.12×10^5
0.126 967	0.126 976	0.59×10^3	0.126 978	0.960		0.12×10^4	
0.123 569	0.123 572	0.12×10^2	0.123 573	0.270		0.15×10^5	
0.122 497	0.122 498	0.36×10^2	0.122 500	0.108		0.50×10^5	
0.121 753	0.121 756	0.76×10^2	0.121 758	0.267			
0.121 102	0.121 104	0.62×10^2	0.121 105	0.095			
0.1207	0.120 776	0.16×10^2	0.120 777	0.029			
	0.120 61	2.84	0.120 61	0.03			

ber of bound states. The analysis of this equation shows that the approximation becomes invalid (the first significant digit in the logarithmic derivative of the wave function disagrees) when $\sqrt{2(E+m/8)}X<\sim10$. If we take $X=500$, this condition indicates that the approximation does not hold at energies higher than ~-0.1207. This rough estimate correlates well with our numerical results. We redefined the part of the matrix A for $d+t\mu$ channel and repeated the calculations. We reproduced the lowest eight resonances and also could obtain the stabilized widths of the resonances at $E_0=-0.120\,777$ and $-0.120\,61$. Table I presents our final results. The positions of the resonances are in perfect agreement with the previous scattering calculations [24] and somewhat better than the results by the variational method [21]. For the highest four resonances, they are well described by the formula $E_{t\mu}\ (n=2)-E_v\sim0.4614^v$ [28]. However, the calculated widths differ by the order of magnitude from that of [22–24] which, in turn, disagree with each other. At the same time, for the lowest three resonances, we have confirmed the widths obtained by the Siegert-states method [14]. This supports our confidence in the present method.

In conclusion, we have implemented the novel representation of Green's function to evaluate density of states and resonances. The method has been applied to the three-body Coulombic $dt\mu$ system, and demonstrated to reproduce the results well for the lowest three resonances obtained by the Siegert-states method. We have also calculated the higher resonances, the energies of which are in good agreement with the previous calculations. Finally, we would like to note that in comparison with the Siegert-state representation, the present method is much easier to implement numerically and may find applications in a variety of collision processes.

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