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Resonances and the continuum level density

A. T. Kruppa
Institute of Nuclear Research of the Hungarian Academy of Sciences, P.O. Box 51, H-4001 Debrecen, Hungary

K. Arai
Department of Physics, Niigata University, Niigata 950-2181, Japan

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A method is suggested to find positions and widths of resonances with the use of an arbitrary real square integrable basis. The procedure is based on the fact that the parameters of a resonance are related to the continuum level density. The method is a generalization of the box quantized L^2-stabilization technique of Mandelshtam, Ravuri, and Taylor [Phys. Rev. Lett. **70**, 1932 (1993)]. For illustration, the method is applied to the s-wave potential scattering case. [S1050-2947(99)05205-1]

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I. INTRODUCTION

Since resonances have a great effect on the physical properties of quantum systems, much effort has been devoted to the calculation of the parameters of a resonance. There are several theoretical and numerical approaches to describe resonance states [1–3]. The methods that use only bound-state-type techniques are especially important since very sophisticated models and computer codes are developed to deal with bound-state problems in atomic, molecular, and nuclear physics. The so-called L^2-stabilization method [4–10] resembles most closely a bound-state-type calculation. In this approach a square integrable basis is selected; then Hamiltonian matrices are diagonalized several times. The repeated diagonalizations correspond to different matrix sizes or different values for the nonlinear parameter of the basis. The diagonalizations immediately give the energies of the bound states. The distribution of the remaining eigenvalues contains information about the positions and widths of the resonance states in a hidden way. The unfolding of this information is termed the L^2-stabilization procedure.

The L^2-stabilization method has been substantially improved recently by Mandelshtam, Ravuri, and Taylor [11]. Their method is based on the calculation of the level density of the system. Because it is assumed that the system is in a box the level density has the form $\rho(E)=\Sigma_i\delta(E-E_i)$, where E_i is an eigenvalue of the system. The Dirac δ functions of $\rho(E)$ are smoothed by an appropriate average over the size of the box. The resonances pop up as sharp peaks in the smoothed level density. It was realized [12–14] that the resonances show up more clearly if the level density of the free box system is subtracted from $\rho(E)$. The parameters of the resonances can also be calculated using the smoothed level counting function [12,13]. Since the method of Ref. [11] assumes that the system is in a box, this severely restricts the functions that can be taken as a basis. The popular basis functions of the quantum chemistry and the nuclear physics are excluded. In order to use an arbitrary basis, an approximation was considered [13,15]. The smoothing of the Dirac δ functions of the level density has been carried out by an average over the nonlinear parameter of the basis [15,16].

The aim of this paper is to show that it is possible to generalize the method of Mandelshtam, Ravuri, and Taylor in such a way that the box quantization can be avoided. Our method is based on the notion of the continuum level density. The continuum level density is the generalization of the level density for Hamiltonians with a continuous spectrum. This quantity is defined with the help of the Green operators of the interacting and the free systems. Our method has a sound mathematical foundation since it is shown that the continuum level density is connected to the scattering S matrix. We show that if we expand the eigenfunctions of the full and the free Hamiltonians on an arbitrary real square integrable basis, then the approximate continuum level density has the form $\Sigma_i\delta(E-e_i)-\Sigma_i\delta(E-e_i^0)$, where e_i and e_i^0 are the eigenvalues of the full Hamiltonian matrix and the free Hamiltonian matrix, respectively. We also have to smooth the Dirac δ functions, but we carry this out using the Strutinsky smoothing procedure [17]. Our approach is similar to the method of Ref. [11]. There is, however, a great difference between our method and the method of Mandelshtam, Ravuri, and Taylor. We neither put the system into a box nor use the approximation that a basis with a nonlinear parameter can be considered as a ‘‘soft’’ box.

The outline of the paper is the following. In Sec. II we define the continuum level density and show its relation to the parameters of a resonance. In Secs. III and IV we discuss the basis-set calculation of the continuum level density. A numerical example is given in Sec. V.

II. THE CONTINUUM LEVEL DENSITY

For simplicity we consider the radial Schrödinger equation. The kinetic energy operator in the partial wave l is denoted by $\hat{T}_l$ and the potential $\hat{V}_l$ depends only on the coordinate r. The level density of a Hamiltonian with pure point spectrum is related to the Green-operator $\hat{G}(E)$ of the system by the trace formula [18]

$$\rho(E)=-\frac{1}{\pi}\,\mathrm{Im}\{\mathrm{Tr}[\hat{G}(E+i0)]\}. \tag{1}$$

If the Hamiltonian in addition to the bound states has a continuous spectrum, the continuum level density $\Delta_l(E)$ is defined [19] with the help of the Green operators of the interacting and the free system,

$$\Delta_l(E) = -\frac{1}{\pi}\,\mathrm{Im}\{\mathrm{Tr}[\hat{G}_l(E+i0) - \hat{G}_l^0(E+i0)]\}. \qquad (2)$$

In Eq. (2) the full and free Green operators are given by the expressions $\hat{G}_l(z) = (z-\hat{H}_l)^{-1}$ and $\hat{G}_l^0(z) = (z-\hat{T}_l)^{-1}$, respectively. The notation $\hat{G}(E+i0)$ stands for the limit $\lim_{\epsilon\to+0}\hat{G}(E+i\epsilon)$, and $\mathrm{Tr}[\hat{G}(E+i0)]$ means the trace of the operator $\hat{G}(E+i0)$. Note that it is not possible to take the trace in Eq. (2) term by term because $\hat{H}_l$ and $\hat{T}_l$ have a continuous spectrum.

For spherically symmetric systems it can be shown [20,21] that $\Delta_l(E)$ is proportional to the derivative of the scattering phase shift $\delta_l(E)$,

$$\Delta_l(E) = \frac{1}{\pi}\frac{d\delta_l(E)}{dE}. \qquad (3)$$

This form of the continuum level density was introduced by Beth and Uhlenbeck [22]. Since the behavior of the phase shift around a resonance is known [23], $\Delta_l(E)$ in the vicinity of a resonance, characterized by the position E_r and width Γ_r, can be turned into the form

$$\Delta_l(E,E_r,\Gamma_r) = \Delta_l^r(E,E_r,\Gamma_r) + \Delta_l^{\mathrm{bg}}(E). \qquad (4)$$

The background term $\Delta_l^{\mathrm{bg}}(E)$ is a slowly changing function of the energy. The resonance part has a Breit-Wigner shape,

$$\Delta_l^r(E,E_r,\Gamma_r) = \frac{1}{\pi}\frac{\Gamma_r/2}{(E-E_r)^2+\Gamma_r^2/4}, \qquad (5)$$

and produces a sharp peak in the continuum level density. We can use this fact to determine the parameters of the resonance.

The continuum level density can be defined for three-dimensional problems as well. In that case there is coupling between the different partial waves and in Eq. (2) we have to use the full Green operators. The corresponding continuum level density $\Delta(E)$, according to the result of Ref. [24], can be related to the on-shell scattering S matrix $S(E,\hat{k},\hat{k}')$,

$$\Delta(E) = \frac{1}{2i\pi}\mathrm{Tr}\left[S(E,\hat{k},\hat{k}')^*\frac{d}{dE}S(E,\hat{k},\hat{k}')\right]. \qquad (6)$$

As resonances are the poles of the S matrix, the continuum level density can also be related to the resonances in the three-dimensional case. In the case of spherical symmetry this relation is simple. Here the S matrix is of the following form [25]:

$$S(E,\hat{k},\hat{k}') = \sum_{l,m} Y_{lm}(\hat{k})\exp(2i\delta_l(E))Y_{lm}(\hat{k}')^* \qquad (7)$$

and substituting Eq. (7) into Eq. (6) immediately gives back Eq. (3).

III. BASIS-SET CALCULATION OF THE CONTINUUM LEVEL DENSITY

The continuum level density can be determined using the expression (3). However, the application of Eq. (3) requires that the Schrödinger equation with the scattering boundary condition be solved. In this section we show that a suitable modified, smoothed continuum level density can be calculated using a basis-set method based on purely L^2 functions.

In order to solve the eigenvalue problem of $\hat{H}_l$, we expand the eigenfunctions on a given orthonormal basis ϕ_i. If N basis functions are used, then the eigenvalues are determined by diagonalizing the $N\times N$ Hamiltonian matrix $H_{n,m} = \langle\phi_n,\hat{H}_l\phi_m\rangle$. This procedure shows that the eigenvalue problem of the approximate Hamiltonian

$$\hat{H}_l^N = \hat{P}_N\hat{H}_l\hat{P}_N \qquad (8)$$

is solved, where

$$\hat{P}_N = \sum_{i=1}^{N}|\phi_i\rangle\langle\phi_i|. \qquad (9)$$

If $N\to\infty$, then $\hat{P}_N$ tends to the unit operator and $\hat{H}_l^N$ approaches $\hat{H}_l$. Similar to the approximate Hamiltonian, an approximate kinetic energy operator can be introduced by the definition

$$\hat{T}_l^N = \hat{P}_N\hat{T}_l\hat{P}_N. \qquad (10)$$

With the help of the operators $\hat{H}_l^N$ and $\hat{T}_l^N$, an approximate continuum level density can be defined in analogy with Eq. (2),

$$\Delta_l^N(E) = -\frac{1}{\pi}\,\mathrm{Im}\{\mathrm{Tr}[(E+i0-H_l^N)^{-1} - (E+i0-T_l^N)^{-1}]\}. \qquad (11)$$

Since both $\hat{H}_l^N$ and $\hat{T}_l^N$ have a pure point spectrum, $\Delta_l^N(E)$ can be turned into the following form:

$$\Delta_l^N(E) = \sum_{i=1}^{N}\delta(E-e_i) - \sum_{i=1}^{N}\delta(E-e_i^0), \qquad (12)$$

where e_i denotes the result of the diagonalization of the Hamiltonian matrix and e_i^0 corresponds to the eigenvalues of the $N\times N$ kinetic energy matrix $T_{n,m} = \langle\phi_n,\hat{T}_l\phi_m\rangle$.

To compare the exact density with the approximate one, we have to smooth the Dirac δ functions in Eq. (12). The smoothed density is defined by the Strutinsky procedure [17]. If we have an oscillating function $g(E)$ (or an expression containing Dirac δ functions), then a smoothed function $\overline{g(E)}$ can be introduced by the convolution integral

$$\overline{g(E)} = \frac{1}{\Gamma}\int_0^\infty w\left(\frac{E'-E}{\Gamma}\right)P_{2M}\left(\frac{E'-E}{\Gamma}\right)g(E')dE', \qquad (13)$$

where Γ is the range parameter of the smoothing. The folding function is the product of a weight function $w(E)$ and a curvature correction polynomial $P_{2M}(E)$ of order $2M$. The popular choice for the weight function is the Gaussian, $w(E)=\exp(-E^2)/\sqrt{\pi}$, although other forms are also available [27], for example the Lorentzian shape $w(E)=1/[2\pi(E^2+1/4)]$. Due to the curvature correction polynomial, the smoothing leaves an arbitrary polynomial of order M unchanged [26,27].

Using the Strutinsky smoothing to $\Delta_l^N(E)$, we get the smoothed approximate continuum level density as a difference of two densities,

$$\overline{\Delta}_l^N(E)=\sum_i^N \frac{1}{\Gamma} w\left(\frac{E-e_i}{\Gamma}\right) P_{2M}\left(\frac{E-e_i}{\Gamma}\right) - \sum_i^N \frac{1}{\Gamma} w\left(\frac{E-e_i^0}{\Gamma}\right) P_{2M}\left(\frac{E-e_i^0}{\Gamma}\right). \tag{14}$$

We mention that Eq. (14) is valid for three-dimensional problems as well. In that case the angular momentum subscript on the left-hand side should be omitted and the eigenvalues e_i and e_i^0 should be interpreted as the eigenvalues of the full Hamiltonian matrix and the full kinetic energy matrix, respectively.

IV. CALCULATION OF THE PARAMETERS OF RESONANCES

Because only the smoothed continuum level density can be calculated with the help of Eq. (14), it is therefore important to know the result of the smoothing of the exact density. The parameters of the resonance state can be extracted from the comparison of the numerically calculated smoothed density with the smoothed exact density.

For the weight function in Eq. (13) we take the Lorentzian form. The advantage of the Lorentzian form is that the smoothing of the Breit-Wigner shape can be calculated analytically in terms of elementary transcendental functions. The smoothed exact density in the vicinity of a resonance reads

$$\overline{\Delta}_l(E,E_r,\Gamma_r)=\overline{\Delta}_l^r(E,E_r,\Gamma_r)+\overline{\Delta}_l^{\mathrm{bg}}(E), \tag{15}$$

where the smoothed Breit-Wigner shape is

$$\begin{aligned}\overline{\Delta}_l^r(E,E_r,\Gamma_r)=&\frac{\Gamma_r\beta}{2\pi^2}\left\{(E-E_r)^2-\frac{(\Gamma^2-\Gamma_r^2)}{4}\right\}\\&\times\left\{\frac{\pi}{2}+\tan^{-1}\left(\frac{2E}{\Gamma}\right)\right\}+\frac{\Gamma\beta}{2\pi^2}\\&\times\left\{(E-E_r)^2+\frac{(\Gamma^2-\Gamma_r^2)}{4}\right\}\\&\times\left\{\frac{\pi}{2}+\tan^{-1}\left(\frac{2E_r}{\Gamma_r}\right)\right\}\\&+\frac{\Gamma\Gamma_r}{4\pi^2}(E-E_r)\beta\ln\left[\frac{4E^2+\Gamma^2}{4E_r^2+\Gamma_r^2}\right]\end{aligned} \tag{16}$$

and

$$\beta=[(E-E_r)^2+(\Gamma-\Gamma_r)^2/4]^{-1}[(E-E_r)^2+(\Gamma+\Gamma_r)^2/4]^{-1}. \tag{17}$$

Here and in the rest of the paper the curvature correction is neglected because it does not alter the main considerations.

The smoothed continuum level density exhibits a sharp peak around a resonance. We can use this fact to calculate the parameters of the resonance. Let us denote the location of the peak by E_{peak}. We select a region around E_{peak} and in this region n points $\{\epsilon_i|i=1,\dots,n\}$ are equidistantly distributed and then the shape of the peak is fitted using Eqs. (15)–(17). We minimize the expression

$$\sum_i^n [\overline{\Delta}_l^N(\epsilon_i)-\overline{\Delta}_l(\epsilon_i,E_r,\Gamma_r)]^2 \tag{18}$$

with respect to E_r, Γ_r, and the parameters of the background. The smoothed background term $\overline{\Delta}_l^b(E)$ is described by a first-order polynomial in E. In the numerical calculation we have chosen a narrow interval $E_{\mathrm{peak}}-\Gamma/2<E<E_{\mathrm{peak}}+\Gamma/2$ for the fit in order to avoid the influence of other resonances. In this way, if Γ is small enough, the one-level smoothed Breit-Wigner expression (16) is enough to describe the smoothed density around E_r. We will refer to this procedure as the least-square fit of the peak.

In the next section we will compare our method with another basis-set method that is based on the theory of the complex scaling (for review see, for example, [28,29]). Here the resonances are determined to be the complex eigenvalues of a non-self-adjoint operator $\hat{H}_l(\Theta)=\exp(-2i\Theta)\hat{T}_l+\hat{V}[r\exp(i\Theta r)]$, where $\hat{V}_l(r)$ is the potential in coordinate space. The scaling parameter Θ can be chosen arbitrary but in such a way as to uncover the resonance, i.e., $\arg[\Gamma_r/(2E_r)]<\Theta<\pi/4$. Basis-set calculation can be carried out in the framework of the complex scaling theory. In this approach the eigenvalue problem of the $N\times N$ complex symmetric matrix $H(\Theta)_{i,j}=\exp(-2i\Theta)T_{i,j}+\langle\phi_i,\hat{V}_l[r\exp(i\Theta)]\phi_j\rangle$ has to be solved.

V. NUMERICAL EXAMPLE

To show our method in practice and to compare it with the complex scaling method, we consider the potential $\hat{V}_0(r)=7.5r^2\exp(-r)$ in the partial wave $l=0$ and we use atomic units. This problem was studied in Ref. [11]. For the basis functions we take the Slater-type orthonormal functions $N_n\exp(-\alpha r/2)L_n^2(\alpha r)$. In Fig. 1 we show the smoothed approximate continuum level density. There are two guiding principles for the selection of the range parameter. It is obvious that Γ has to be larger than the average spacing of the eigenvalues e_i located in the energy region of interest. If we choose Γ small, then the individual eigenvalues appear as peaks in the smoothed density (see the solid line for large E in Fig. 1). It is also clear that we must not choose Γ large because then we oversmooth and all structures of the level density are washed out. For our purpose it is best to choose Γ as small as possible, but we have to avoid the appearance of the peaks corresponding to the individual energy eigenvalues. Our experience is that two or three times the average spacing of e_i is good for the range parameter. If we choose Γ

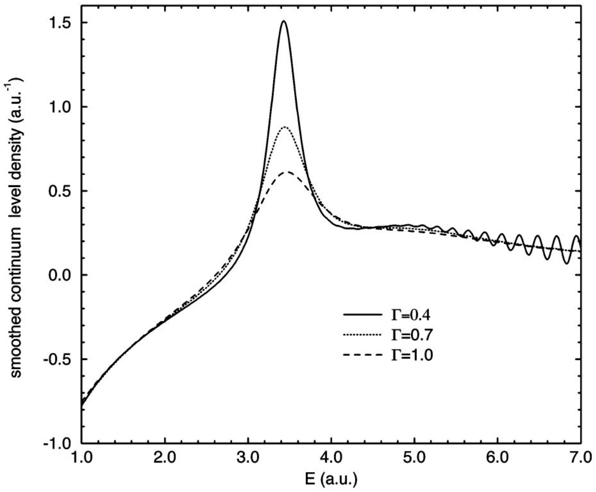

FIG. 1. The smoothed continuum level density. Three different range parameters for the smoothing are used. The basis is characterized by $\alpha=6$ and $N=180$.

properly, a sharp peak appears at the energy that roughly corresponds to E_r.

In Fig. 2 we show the position of the peak of the approximate continuum level density E_{peak} as a function of the range parameter of the smoothing. The value of E_{peak} is stable only in two digits if Γ changes. If a resonance had been completely isolated and the back-ground term had had no E dependence around E_r on the energy scale Γ, then E_{peak} should have been independent of Γ. If we look carefully at Fig. 1 we will realize that there is another resonance around $E=5.0$ with a large width. There is a small bump right to the sharp peak in Fig. 1. We checked this assumption solving the radial Schrödinger equation with the Siegert boundary condition using the code of Ref. [30]. In the numerical integration the potential was cut off at $r=16$. According to this calculation, the narrow resonance is located at $E_r=3.426\,39$ and the width is $\Gamma_r=0.025\,54$. Furthermore, there are two more resonances in this region. The second resonance is at 4.86 and its width is 1.77, the third resonance is located at 5.32 with width 1.98. The presence of the second and the third resonances explains the behavior of E_{peak}. Since the resonances are close to each other, if we smooth with large Γ, then the second and third resonance will have an enhanced effect on the density in the energy region of the first resonance and it will modify the position of the peak.

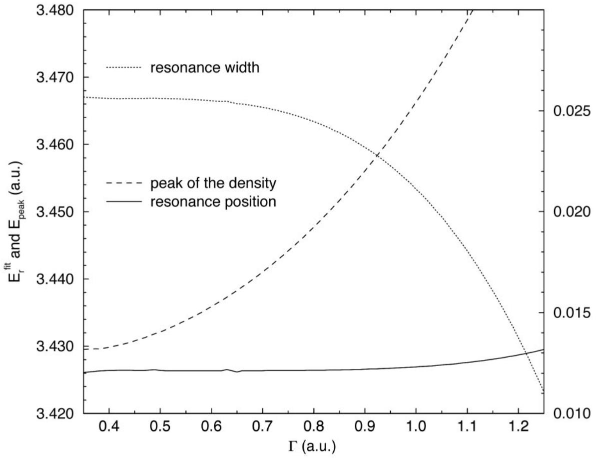

FIG. 2. The position of the peak of the continuum level density E_{peak} (use the left side scale) is shown as a function of the range of the smoothing. The least-squares fits of the resonance position E_r^{fit} (use the left side scale) and the resonance width Γ_r^{fit} (use the right side scale) are also displayed. The parameters of the basis are given in Fig. 1.

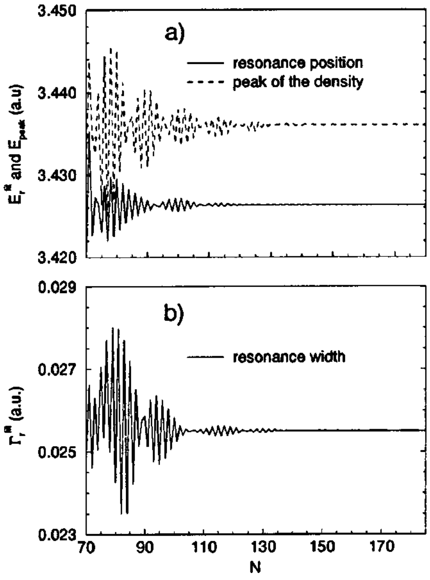

FIG. 3. The peak of the smoothed density E_{peak} and the least-squares fits of the resonance position E_r^{fit} (a) and the resonance width Γ_r^{fit} (b) are displayed as a function of the size of the basis. The nonlinear parameter of the basis was $\alpha=6$ and the range of the smoothing was $\Gamma=0.6$.

We may overcome this difficulty using the least-square fit of the peak procedure described in the preceding section. In Fig. 2, the least-square fit of the resonance position E_r^{fit} and the resonance width Γ_r^{fit} are displayed as a function of Γ. It is remarkable that on a large region of Γ the estimated values of the parameters of the resonance hardly change. In this way we demonstrated that the position and the width of the resonance can be determined independently from the range parameter of the smoothing. From Fig. 2 we can conclude that there is a resonance at $E_r^{\text{fit}}=3.426$ with width $\Gamma_r^{\text{fit}}=0.025$. These numbers agree perfectly with the exact values.

In Fig. 3 we investigate the convergence behavior of our procedure. The quantities E_{peak}, E_r^{fit}, and Γ_r^{fit} are displayed in Fig. 3(a) and Fig. 3(b) as a function of the basis size. For the nonlinear parameter of the basis we used $\alpha=6$ and for the range of the smoothing we took $\Gamma=0.6$. The position and the width of the resonance are determined using the least-square fit procedure described above. As is expected, the peak of the smoothed density and the resonance position converge to different numbers due to the presence of the other resonances. The resonance position 3.42 given in Ref. [11] is reproduced even at the smallest basis size $N=70$. Note the scale of the figure: the oscillations present in the curves E_r^{fit} and Γ_r^{fit} in Fig. 3 are in the fifth and third digits. Convergence can be achieved even in these digits if we use a not too large basis. The value of the parameter α of the basis plays a role only at small basis sizes where the oscillatory pattern is present. Using Fig. 3, we can determine a very accurate value for the parameters of the studied resonance.

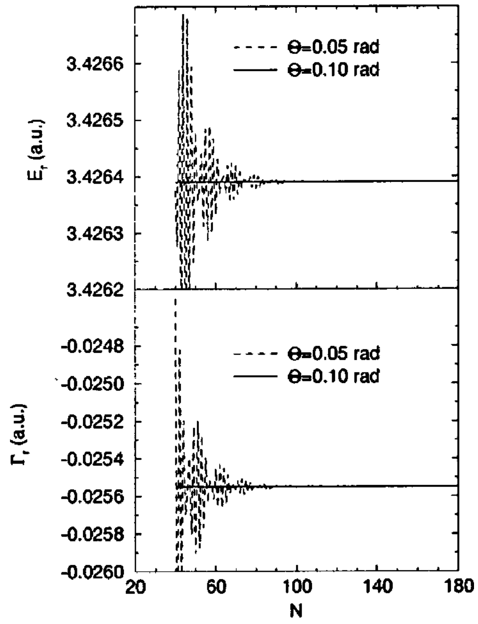

FIG. 4. The real part (upper figure) and the width (lower figure) of the resonance energy as a function of the basis size for two different values of the complex scaling parameter. The nonlinear parameter of the basis was $\alpha = 6$.

For the position we get 3.4263, and for the width we get 0.0255, in full agreement with the exact results.

In Fig. 4 we investigate the convergence behavior of the complex scaling method. We used the same nonlinear parameter for the Laguerre basis as before. The scaling parameter was $\Theta = 0.05$ rad and $\Theta = 0.1$ rad. For the smaller Θ value the convergence behavior of the complex scaling method is similar to our method. For larger Θ values the complex scaling method converges very quickly. It might be possible to speed up the convergence of our method if the parametrization of the continuum level density around a resonance can be improved. We note, however, that the complex scaling method uses a nonstandard, non-self-adjoint representation of the Hamiltonian. In contrast, our method uses only the outputs of the most standard real basis-set calculation. Comparing our method with the L^2-stabilization technique and with the improved approach of Mandelshtam, Ravuri, and Taylor, we may conclude the following.

We do not have to calculate the tedious stabilization plot and our smoothing procedure does not require the repeated digonalization of the Hamiltonian matrix.

VI. CONCLUSION

To sum up, we have shown that the L^2 stabilization method based on box quantization can be generalized to an arbitrary real square integrable basis. Our method is based on the fact that the continuum level density is connected to the scattering S matrix. The Strutinsky averaging procedure is applied to calculate smoothed quantities. We showed that the smoothed continuum level density can be related to the eigenvalues of the Hamiltonian matrix and to the eigenvalues of the kinetic energy matrix in a very simple way. Since the exact continuum level density has a Breit-Wigner shape around a resonance, the smoothed exact density can be calculated analytically. With the help of our method, the position and width of a resonance can be determined using an arbitrary real square integrable basis, which means that all the models and computer codes that are developed for bound states and based on the basis-set method are at our disposal to calculate resonances.

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