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An improved algorithm to determine the density of resonance states using the stabilization method

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Abstract. By using properties of the Sturm sequences related to tridiagonal matrices we describe a very efficient algorithm to determine the density of resonance states based on the stabilization method.

In a recent paper Mandelshtam *et al* [1] calculated the density of resonance states by enclosing the system in a box of length, L, and studying the behaviour of the energy eigenvalues $E(L)$ as functions of the box length L. More precisely, assume that the radial part of the s-wave Schrödinger equation is

$$\left[-\frac{\partial^2}{\partial r^2}+V(r)\right]\Psi(r)=E\Psi(r) \tag{1}$$

with the boundary condition at the origin (regular solution) $\Psi(0)=0$. Mandelshtam *et al* [1] solved equation (1) with the boundary conditions $\Phi_L(0)=\Phi_L(L)=0$. The eigenvalues $E(L)$ decrease with L according to

$$\frac{\partial E(L)}{\partial L}=-\frac{\Phi_L'^2(L)}{\int_0^L \Phi(r)^2\,\mathrm{d}r}. \tag{2}$$

Although always negative, the gradient of equation (2) changes dramatically when $E(L)$ is close to one of the resonance energies, E_R, of equation (1). In fact, since the resonance states are localized in some region of space (typically a potential well with a penetrable barrier) the absolute value of the gradient is considerably small when $E(L)\simeq E_R$. This fact is referred to as *stabilization* of the resonance energy.

To determine the density of resonance states Mandelshtam *et al* [1] averaged the density of states

$$\rho_L(E)=\sum_j \delta[E_j(L)-E] \tag{3}$$

where $E_j(L)$ are the eigenvalues of the caged model, in a wide region of L values, so as to obtain a continuous function of E:

$$\langle\rho_L(E)\rangle=\frac{1}{\Delta L}\int_{L-\Delta L/2}^{L+\Delta L/2}\rho_{L'}(E)\,\mathrm{d}L'. \tag{4}$$

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This averaging was inspired by the work of Kim and Ezra [2]. Finally, by using properties of Dirac's delta function they rewrote equation (4) as

$$\langle \rho_L(E) \rangle = \frac{1}{\Delta L} \sum_j \left[\frac{\partial E_j(L')}{\partial L'} \right]^{-1}_{E_j(L')=E} \tag{5}$$

where the sum in equation (5) includes only the eigenvalues $E_j(L')$ satisfying $E_j(L') = E$ in the interval $L - \Delta L/2 < L' < L + \Delta L/2$ chosen for averaging.

The rationale behind the last transformation is that, according to [1], equation (5) is less costly to evaluate than equation (4).

Later [3], the method was modified to deal directly with the eigenphase sum, and applied to the study of the van der Waals complex NeICl [4]. Very recently, Salzgeber and coworkers [5] realized the importance of properly removing the background phase to simplify the identification of resonances.

The method to find the position and width of the resonances consists of collecting information from a large set of values of L in the range $[L - \Delta L/2, L + \Delta L/2]$ and constructing a histogram representing the averaged density of states [1]. One obtains the parameters of the resonance from a least-square fit of the histogram to a Lorentzian function

$$\rho_R(E) = \frac{C}{(E - E_R)^2 + \Gamma^2/4}$$

plus a background. The procedure requires a large number of matrix diagonalizations to build up the distribution of resonances. The Hamiltonian matrix is usually constructed by using a set of basis functions (typically sinusoidal) which vanish at both ends of the box.

The purpose of this note is to show that the process of accumulating information to build up the histogram may be carried out *very efficiently* by using equation (4) instead of equation (5), if the Schrödinger equation is discretized by the simple replacement $\partial^2/\partial r^2 \to \delta^2/h^2$ (δ being the centred difference operator), because of the special properties of the resulting Sturm sequences.

After this transformation there results a tridiagonal matrix with diagonal elements

$$a_k = \frac{2}{h^2} + V_k$$

and all upper-diagonal elements are equal to $b_k = -1/h^2$. Here h is the constant step of integration and $V_k = V(kh)$ is the potential function at the discretization point.

From a symmetric tridiagonal matrix one can construct a *Sturm sequence* [6, 7] for the polynomials $p_r(E) = \det(T_r - EI)$, where T_r is the matrix with the first r rows and columns, and I is the identity matrix of the same dimension. One easily verifies that

$$p_r(E) = (a_r - E)p_{r-1}(E) - b_{r-1}^2 p_{r-2}(E).$$

This sequence is *unreduced*, because the off-diagonal elements are non-zero. The important property of this sequence is that the number of zeros to the left of E equals the number of changes of sign of the sequence

$$\{p_0(E), p_1(E), \ldots, p_r(E)\}.$$

Calling $\nu_r(E)$ the number of such sign changes, the number of eigenvalues between two given values E_1 and E_2 is $|\nu_r(E_1) - \nu_r(E_2)|$. This method is especially well suited to find the distribution or density of eigenvalues as a function of E.

For an efficient evaluation of the *cumulative* distribution related to equation (4) one proceeds by storing the number $\nu_r(E)$ at each r, which corresponds to a box length

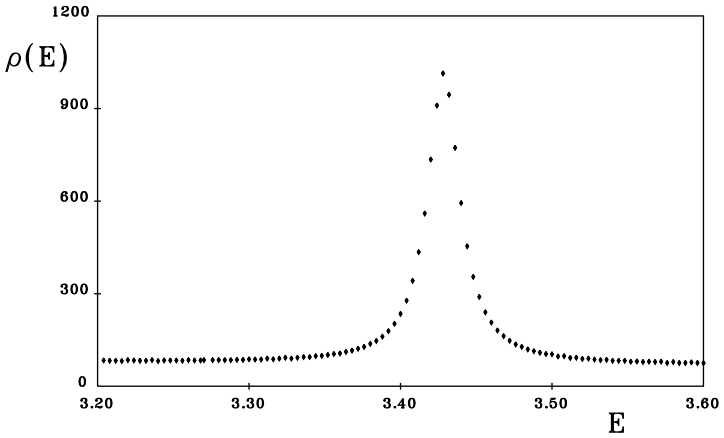

Figure 1. Histogram representing the averaged density of resonance states for the Hamiltonian model. The calculation corresponds to $L = 13$ and $\Delta L = 6$.

$L_r = rh$, along a single evaluation of the Sturm sequence up to a value of $N_{\max}$ given by $L + \Delta L = N_{\max}h$. The cumulative number of eigenvalues is

$$\langle \rho(E) \rangle \approx \frac{1}{\Delta E \Delta L} \sum_{r=N_{\min}}^{N_{\max}} |\nu_r(E) - \nu_r(E + \Delta E)|. \tag{6}$$

The evaluation of the Sturm sequence involves $O(N_{\max})$ flops, so the determination of a histogram with N_{bin} bins involves $O(N_{\max}N_{\text{bin}})$ flops only.

We have used this algorithm to determine an s-wave resonance of the Hamiltonian

$$H = -\nabla^2/2 + 7.5r^2 \exp(-r) \text{ au}. \tag{7}$$

This simple model is a reference problem for the determination of resonances (see [1], and also [8, 9]). Figure 1 shows the distribution of eigenvalues corresponding to $L = 16$ au and $\Delta L = 6$ au, with $N_{\max} = 30\,000$, corresponding to the average of around 8000 distributions. To give an idea of the efficiency of the method we mention that the determination of the histogram took only 7 s in a Pentium at 60 MHz. The least-squares fit of the Lorentzian gave $E_R = 3.4284$ and $\Gamma = 0.0255$. These results are in agreement with previous ones [1, 8, 9]. One may improve the results by a Richardson extrapolation that requires repeated calculation with different mesh steps h.

It was suggested by one of the referees to test this method on potentials with singularities or with discontinuities. So we considered the potential

$$V(r) = 30\frac{r - b}{\sqrt{|r - b|}} \exp(-r) \tag{8}$$

which has a discontinuous derivative at $r = b$. This potential has recently been studied by Čížek and Horáček [10] for solving the Lippmann–Schwinger differential equation and also the equivalent integral equation. Note that in this case the kinetic energy part is $-\nabla^2$ (i.e. without the factor of $\frac{1}{2}$ from equation (7)). The resonance distributions obtained by us for two values of $b = 0.40$ and $b = 0.65$ are shown in figure 2.

The first case presents a broad resonance with $E_R = 8.03$ and $\Gamma = 0.93$. The energy of the resonance is slightly smaller than the maximum of the potential. The second case shows a narrow resonance with $E_R = 0.9362$ and $\Gamma = 0.000\,11$. Both results agree with the values obtained in [10], which for comparison should be multiplied by 2 [11]. The

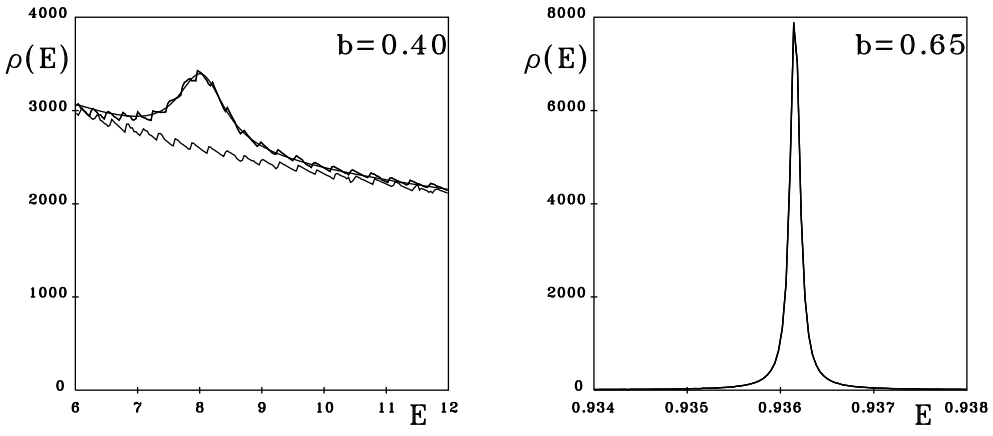

Figure 2. Histogram representing the averaged density of resonance states for the discontinuous potential (equation (8)). The calculation was carried out from $L_1 = 15$ up to $L_2 = 65$, with a total of 50 000 samples. The left-hand figure shows the obtained density (jigsaw line showing a peak), the Lorentzian fit (smooth line) and also the free density.

conclusion is that the discontinuity does not affect the accuracy of the results. The same conclusion was drawn from the singular potential

$$V(r) = -100\frac{\exp(-4r)}{r} + \lambda\frac{\exp(-r)}{r} \tag{9}$$

also considered in [10] (due to a printing error, this equation was missed in [10]).

However, the presence of very broad resonances has drawn our attention to the importance of the background. The left plot in figure 2 ($b = 0.40$) shows a characteristic jigsaw pattern. The actual resonance appears as a bump on top of a jigsaw background, which on average behaves as $1/\sqrt{E}$ [1]. The staircase pattern is not a consequence of the numerical approximation, but of the finite size of the box enclosing the system.

Going back to equation (5), in which for a free particle

$$E_j(L) = \frac{j^2\pi^2}{L^2} \tag{10}$$

one may easily obtain the background density distribution

$$\rho_0(E) = \frac{\pi}{4\Delta L E^{3/2}}[k_M(k_M+1) - k_m(k_m+1)] \tag{11}$$

where k_M (k_m) is the largest (smallest) integer less (greater) than $(L + \Delta L/2)\sqrt{E}/\pi$ ($(L - \Delta L/2)\sqrt{(E)}/\pi$). Consequently, each time these quantities cross an integer value it results in a step in the distribution. In the left-hand plot of figure 2, such discontinuities appear at $E = 6.075, 6.316, 6.562, \ldots$, as follows from $L + \Delta L/2 = 65$ which arises from the largest box considered. On the other hand, narrow resonances may lay within a step, without any special behaviour, as in the right-hand plot of figure 2 ($b = 0.65$) or in figure 1.

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