Determination of Resonance Energy and Width
by Calculation of the Density of Resonance States Using
the Stabilisation Method

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The energies and widths for the 2s^2^1S^0 and 2s2p^3P_0 doubly-excited states of H^- are determined by calculation of the density of resonance states using the stabilisation method. Highly correlated Hylleraas-type wave functions are used. Our results are compatible with the other most accurate calculations in the literature.

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PACS. 32.80.De - Autoionization.

I. Introduction

Recently, Mandelshtam et al. [1] have proposed a procedure to calculate resonance energy E_r and width Γ by calculating the density of resonance states using the stabilisation method. The use of the stabilization method to investigate atomic resonances has a long history [2, 3]. The method has been used to estimate resonance positions (but not the widths) for different atomic systems [4-6]. Efforts have been made to calculate autoionization widths by combining the stabilisation method and the L^2-technique[7]. The latest development [1] of the stabilisation method to calculate resonance positions and widths requires only L^2 functions. This method, which does not require the use of complex analytic continuation [8], nor does it require the solutions of scattering functions [9], is an interesting alternative in the field of theoretical investigations of atomic resonances. Muller et al. [10] have applied the method to calculate doubly excited S-wave resonances in He. In order to test the method for a highly correlated atomic system, we apply it to investigate the 2s^2^1S^0 and 2s2p^3P_0 resonant states in e^- - H scattering below the N = 2 hydrogen threshold. Hylleraas-type wave functions with N = 525 and N = 680 terms are used for the S and P states, respectively. Our objective of the present work is to apply the method to calculate some well-documented atomic resonances and to examine how accurate the results are as compared with the most accurate values in the literature.

II. Theory and method

The spectral density of states p(E) has two parts: p^P(E) and p^Q(E) where P and Q are referred to the open (P) and closed (Q) space, respectively, used in the Feshbach
projection formalism. The $\rho^P(E)$ is a smooth function of energy $E$, and $\rho^Q(E)$ is a result of complex poles of the Green's function. The spectral density of resonance pole is given by

$$\rho^Q(E) = -\frac{1}{\pi} \text{Im} \left[ \sum_k \frac{1}{(E - E_k) + i\Gamma_k} \right], \quad (1)$$

where $E_k - i\Gamma_k$ is the $k$th complex pole of the Green's function. Recently Mandelshtam et al [1] have shown that $\rho^Q(E)$ can be obtained by

$$\rho^Q(E) = \frac{1}{L_2 - L_1} \int_{L_1}^{L_2} \rho_L(E) dL, \quad (2)$$

where

$$\rho_L(E) = \sum_j \delta(E_j(L) - E), \quad (3)$$

and $L$ is the size of the box in which the Hamiltonian is diagonalized. For atomic system, we can replace the "hard wall" by a "soft wall" [10], and Eq. (2) can be replaced by the following

$$\rho^Q(E) = \frac{1}{\alpha_{\text{max}} - \alpha_{\text{min}}} \int_{\alpha_{\text{min}}}^{\alpha_{\text{max}}} \rho_o(E) d\alpha, \quad (4)$$

where $\alpha$ is a non-linear parameter in the wave function. Eq. (3) becomes

$$\rho_o(E) = \sum_j \delta(E_j(\alpha) - E). \quad (5)$$

Using the equation

$$\int \delta(f - f(x))g(x) dx = g(x) \left| \frac{df}{dx} \right|_{f(x)=f}^{-1}, \quad (6)$$

Eq. (4) can be evaluated as

$$\rho^Q(E) = \frac{1}{\alpha_{\text{max}} - \alpha_{\text{min}}} \sum_j \left| \frac{dE_j(\alpha)}{d\alpha} \right|_{E_j(\alpha)=E}^{-1} \quad (7)$$

For an isolated resonance $\rho^Q(E)$ can be shown as [11]

$$\rho^Q(E) \equiv \pi^{-1} \frac{\Gamma/2}{(E - E_r)^2 + \Gamma^2/4}. \quad (8)$$
The $\rho^2(E)$ can be calculated from the stabilisation graph using Eq. (7), and the resonance parameters ($E_r$ and $\Gamma$) can be obtained by fitting $\rho^2(E)$ to Eq. (8).

### III. Wave functions and calculations

For the singlet S-wave states in $e^-\cdot H$ scattering, we use the Hylleraas-type wave functions

$$\Psi = \sum C_{\alpha \beta \gamma \delta} \exp[-\alpha(r_1 + r_2)] r_1^{1/2} r_2^{1/2}$$

with $\omega \geq k + m + n$, and $k$, $m$, $n$, and $w$ being positive integers or zero, and $k \geq m$. The coordinates $r_1$ and $r_2$ are for electron 1 and 2, respectively, relative to the proton, and $r_{12}$ is the distance between the two electrons. We use $N=525$ terms ($w = 15$) in our present investigation for the S-wave calculation. For the triplet P-wave states with odd parity, the wave function is also of Hylleraas-type,

$$\Psi = \sum C_{k m n} \exp[-\alpha(r_1 + r_2)] r_1^{k-1} r_2^{m-1} Y_{10}(1) Y_{00}(2)$$

We use expansion length of $N=680$ ($w = 14$) to construct the stabilisation plot. Figure 1 shows the plot for S-wave energy eigenvalues $\psi_{10}$, the non-linear parameters of the wave function. We use 300 points to cover the range of $\alpha$ from $\alpha = 0.2$ to $\alpha = 0.8$. The 10th to 27th eigenvalues in the energy range of -0.20 Ryd to -0.34 Ryd are shown here. It is seen that an eigenvalue near $E = -0.3$ Ryd exhibits stabilisation character. Of course, such a stabilised eigenvalue represents the well known lowest doubly-excited $2s^21^1S^0$ state of $H^-$. From the stabilisation plot we take the 13th eigenvalue in the interval of $\alpha = 0.4$ to 0.5, and apply the following function to obtain the inverse of the slope.

![Fig. 1. Energy eigenvalues vs. $\alpha$ parameters for $1^1S^0$ states of $H^-$.](image1.png)

![Fig. 2. Calculated density (in circles) and the fitted Lorentzian (in solid line) for the $2s^21^1S^0$ resonance state.](image2.png)
\[ \rho_n = \frac{a_{n+1} - a_{n-1}}{\alpha_{n+1} - \alpha_{n-1}} = \frac{dE^{-1}}{d\alpha |_{\alpha=E}} . \]  

(11)

It is seen that \( \rho_n \) in Eq. (11) differs from \( \rho^Q(E) \) in Eq. (7) only by an overall multiplication constant of \( (a_{\text{max}} - a_{\text{min}})^{-1} \). Such a difference would not affect the determination of \( E_r \) and \( \Gamma \) when we use \( \rho_n \) to fit to the following equation

\[ \rho_n(E) = \frac{a(\Gamma/2)}{(E - E_r)^2 + \Gamma^2/4} + b . \]  

(12)

Later in the text, we will discuss the effects on \( E_r \) and \( \Gamma \) when different ranges of \( (a_{\text{max}} - a_{\text{min}}) \) are used. In Fig. 2, the circles are the actual calculations of \( \rho_n \) using Eq. (11). The solid line is the fitted curve using the Lorentzian form of Eq. (12). The fit gives \( E_r = -0.29755 \) Ryd and \( \Gamma = 0.00346 \) Ryd.

In Fig. 3, we plot the P-wave eigenvalues \( \psi_s(\alpha) \), the non-linear parameters in the wave function. Again, we use 300 points to cover the range of \( \alpha \) from \( \alpha = 0.2 \) to \( \alpha = 0.8 \). The 9th to 27th eigenvalues are shown here in the energy range of -0.20 Ryd to -0.32 Ryd. The stabilised eigenvalue near \( E = -0.284 \) Ryd represents the doubly excited \( 2s2p^3P^o \) state of \( H^- \). Next, we take the 12th eigenvalue in the \( \alpha \) interval from \( \alpha = 0.36 \) to \( \alpha = 0.46 \), and apply Eq. (11) to calculate \( \rho_n \). The circles in Fig. 4 are the actual calculations of \( \rho_n \), and they are then fitted to Eq. (12). The solid line in Fig. 4 is the best fit, and from which we obtain \( E_r = -0.28427 \) Ryd and \( \Gamma = 0.000426 \) Ryd.

In order to assign the uncertainties for the resonance parameters in our investigation, we repeat the above fitting procedure for different intervals of \( \alpha \). In general, slightly different \( E_r \) and \( \Gamma \) are obtained when different regions of \( \alpha \) are used. By keeping \( \Delta \alpha = \alpha_{\text{max}} - \alpha_{\text{min}} = 0.1 \), we systematically scan through the stabilisation curves shown in Figs. 1 and 3. For example, we use \( \Delta \alpha = (0.30 - 0.20), (0.35 - 0.25), \) and \( (0.40 - 0.30) \), etc.. By performing such a procedure, we are looking for a region of \( \alpha \) that exhibits the 1st second-order stabilisation.”
Fig. 5 shows the result for the $2s^2p^3P^0$ state. From that we assign the resonance energy and width with uncertainties of $E_r = -0.284270$ Ryd $\pm 0.000008$ Ryd and $\Gamma = 0.000426$ Ryd $\pm 0.000016$ Ryd. It should also be mentioned that we have repeated the above procedure by using $\Delta \alpha = 0.2$ and $\Delta \alpha = 0.3$. The results are not much different from those shown in Fig. 5 when $\Delta \alpha = 0.1$ is used. As for the $2s^21S^e$ state, we employ the similar procedure as described above, and the resonance parameters with uncertainties are determined as $E_r = -0.29756$ Ryd $\pm 0.00006$ Ryd and $\Gamma = 0.00346$ Ryd $\pm 0.00012$ Ryd. Table I shows our results, and the comparison with other accurate calculations in the literature [8,12-13]. It is seen that the results obtained by using the stabilisation method compare well with other accurate results, although our present estimated uncertainties are slightly larger than those of the other elaborate calculations. One of the reasons for the present procedure would lead to slightly larger uncertainties is that, in constructing the stabilisation curves, a finite mesh size in $\alpha$ is used. As a result, inevitable errors are introduced when we use Eq. (11) to calculate $dE/da$ and its inverse. It should be mentioned that a stabilisation method was used to investigate the highly correlated doubly-excited $^1S^e$ resonance using CI functions [15]. Their width was determined from the avoided crossings of the stabilisation curves. In comparison, our present results are closer to the most accurate values in the literature than those of Ref. [15].

In summary, this work presents a calculation of resonance energies and widths for the highly correlated doubly excited $2s^21S^e$ and $2s^2p^3P^0$ states of H$^-$ by calculating the...
TABLE I. The 2s\(^{2}\)1\(^{S}\) and 2s2p\(^{3}\)P\(^{0}\) resonances in e--H scattering below the N=2 threshold.

<table>
<thead>
<tr>
<th></th>
<th>(E_r) (Ryd)</th>
<th>(\Gamma) (Ryd)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)(^{S})</td>
<td>-0.29756 ± 0.00006</td>
<td>0.00346 ± 0.00012</td>
</tr>
<tr>
<td>Complex-rotation(^a)</td>
<td>-0.297555 ± 0.000004</td>
<td>0.003467 ± 0.000002</td>
</tr>
<tr>
<td>Other theory(^b)</td>
<td>-0.297553 ± 0.000004</td>
<td>0.003462 ± 0.000008</td>
</tr>
<tr>
<td>Other theory(^c)</td>
<td>-0.29718</td>
<td>0.0035</td>
</tr>
<tr>
<td>(3)(^{P})</td>
<td>-0.284270 ± 0.000008</td>
<td>0.000426 ± 0.000016</td>
</tr>
<tr>
<td>Present</td>
<td>-0.284273</td>
<td>0.000426</td>
</tr>
<tr>
<td>Complex-rotation(^d)</td>
<td>-0.284265</td>
<td>0.00043</td>
</tr>
</tbody>
</table>

\(^a\): Complex-rotation, Hylleraas functions [8, 12].
\(^b\): Feshbach projection formalism, Hylleraas functions [13].
\(^c\): Stabilisation method with CI functions [15].
\(^d\): Kohn variational method, Hylleraas functions [14].

density of resonance states using the stabilisation method. It is shown that quite accurate results can be obtained. The method is an interesting alternative to calculate atomic resonance parameters including both energy positions and widths, as only \(L^2\) functions are needed for the entire calculation. Furthermore, this method can be combined with the use of model potentials to investigate resonances in a many-electron atomic system. For example, the four-electron (beryllium-like) systems can be treated as a two-electron system by including a model Hamiltonian to represent the interaction between the core electrons and the outer electrons. The doubly-excited states of beryllium-like ions can then be calculated [16] using the stabilisation method as described in this work.

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