Addendum by A. Temkin and A.K. Bhatia to Chapter 25: Autoionization

Since the original chapter, we briefly review two calculational methods used for basic applications in autoionization of few body systems: (a) complex rotation and (b) a pseudopotential method.

Complex rotation, briefly mentioned above, has been extensively applied with great accuracy. Two additional basic systems to be mentioned here are H^- and Ps^- (Ps=positronium). In complex rotation the particle distances are multiplied by a common phase factor

$$r_i \rightarrow r_i e^{i\theta} \tag{25.32}$$

Under this replacement the Hamiltonian is transformed

$$H \rightarrow T e^{-2i\theta} + V e^{-i\theta} \tag{25.33}$$

(only Coulomb interactions are assumed). A real variational wave function Φ is used (for the applications here, they are of Hylleraas form, multiplied by rotational harmonics of symmetric Euler angles of the desired angular momentum, parity, and spin [39]). The functional

$$[E] = \frac{<\Phi|H|\Phi>}{<\Phi|\Phi>} = \frac{<\Phi|T|\Phi> e^{-2i\theta} + <\Phi|V|\Phi> e^{-i\theta}}{<\Phi|\Phi>} \tag{25.34}$$

is evaluated. Minimization with respect to the linear parameters, for a given value of θ, is carried in the usual way, but by virtue of the complex dependence on rotation angle the matrix elements H_{ij} in matrix eigenvalue equation

$$det|H_{ij}(\theta) - E\Delta_{ij}| = 0 \tag{25.35}$$

are complex. Thus the solution of (25.35) gives rise to complex eigenvalues $E_\lambda = E_\lambda(\theta)$. For a given λ, the optimum θ is the one for which $E_\lambda(\theta)$ is affectively stationary as a function of θ [40]. Results for $^1D^e$ states of H^- are given in the Table 25.5. Note no projection operators are used: the real part of the E_λ corresponds to the Breit-Wigner (i.e. experimental) position of the resonance, and Im(E_λ)=$\Gamma_{BW}/2$ where Γ_{BW} corresponds to the Breit-Wigner (experimental) width of the resonance. These parameters thus include the full Feshbach values plus corrections, cf. Eq. (25.31).

Using Hylleraas wave functions with up to 1230 terms in the complex rotation method, resonance parameters have been obtained for resonance states of H^- below the n=2 and 3 thresholds of H, which compare very well with those obtained using the projection-operators, R-matrix and close-coupling methods. Similar calculations for Ps^- have been carried out [44]. Complex rotation method has been applied to autoionization states of many different systems including muonic [45] systems, as well as to study the combined effect of electric field and spin-orbit interaction on resonance parameters [46].

Table 25.5. Comparison of resonance parameters (in eV) obtained from different methods for calculating $^1D^e$ states in H^-.

Threshold n	Complex-cordinate rotation[40]		R-matrix[41]		Feshbach projection[42] Cf. Eq.(25.31)	
	E	Γ	E	Γ	E_F	Γ_F
2	10.12436	0.00862	10.1252	0.00881	10.1243	0.010
3	11.81102	0.04512	11.81097*	0.04449*		

*Close Coupling (18-state), Ref. [43].

The second method that is included in this addendum is done so for the reason that it represents a rather different idea for the calculation of autoionization rather than being a more elaborate application of methodoligies that are already known, with results too numerous to be referenced here. The method, described as a pseudopotential approach, was introduced by Martin et al. [47]. An effective Hamiltonial, H_{eff}, is defined

$$H_{eff} = H + MP. \tag{25.36}$$

M is a scalar parameter (i.e. a number), which will be taken very large, multiplying the P operator, Eq. (25.16). [Applications have thus far been restricted to one-electron targets and resonances below n=3 excited state.] In practice one minimizes the expectation value of H_{eff}:

$$\delta\left[\frac{<\Psi_v|H_{eff}|\Psi_v>}{<\Psi_v\Psi_v}\right] = 0 \tag{25.37}$$

using an arbitrary, quadratically integrable, variational function Ψ_v. In order to understand the nature of the spectrum that arises from this variation, we imagine Ψ_v divided into its P and Q space components

$$\Psi_v = Q\Psi_v + P\Psi_v = \Psi_v^Q + \Psi_v^P \tag{25.38}$$

The expectation value $<\Psi_v|H_{eff}|\Psi_v>$ is written in matrix form

$$<\Psi_v|H_{eff}|\Psi_v> = \left\langle (\Psi_v^Q\ \Psi_v^P) \begin{pmatrix} H_{QQ} & H_{PQ} \\ H_{QP} & H_{PP}+M \end{pmatrix} \begin{pmatrix} \Psi_v^Q \\ \Psi_v^P \end{pmatrix} \right\rangle \tag{25.39a}$$

The eigenvalue problem resulting from Eq.(25.37) reduces to finding the eigenvalues of the determinant

$$det \begin{pmatrix} <H_{QQ}> -\lambda & <H_{PQ}> \\ <H_{QP}> & <H_{PP}> +M-\lambda \end{pmatrix} = 0 \tag{25.39b}$$

Note, only the bottom right component contains the term M. As a result the eigenvalues, which can readily be solved for from Eqs.(25.39), are in the limit of large M:

$$\lim_{M\to large} \lambda = \begin{cases} M+<H_{PP}> \\ <H_{QQ}> \end{cases} \tag{25.40}$$

The lower eigenvalue is the desired Feshbach resonant energy $\mathcal{E}_{\mathcal{F}} = <\mathcal{H}_{QQ}>$. The width is calculated from [with our normalization, cf. Eq.(25.21)]

$$\Gamma = 2k|<\Psi_\lambda|H_{eff}|\chi_E>|^2 \tag{25.41}$$

where χ_E is the solution of the exchange approximation

$$(H_{PP} - E)\chi_E = 0 \tag{25.42}$$

It is emphasized that this method only calculates the Feshbach energy, thus the shifts are not included. On the other hand the method uses no projection operators in calculating matrix elements of H, and only the matrix elements of P by itself. This is much easier than a standard QHQ calculation.

In practice the matrix in Eq.(25.39) will expand to an NxN matrix where N is the number of linear parameters in Ψ_v, and (if one uses a Hylleraas form of Ψ_v, for example) the matrix in Eq.(25.39) will not overtly divide itself into the simple form of this heuristic exposition pictured in Eq.(25.39). Nevertheless the conclusion holds; in detail the eigenvalue spectrum will span a range of values with those below the (n=2, in this example) corresponding to real resonances, and the largest eigenvalue will approach the value of M used in the specific calculation.

A sample of results for the $He(^1P)$ resonances below the n=2 threshold of He^+ taken from Ref.[47], with limited comparisons is given in Table 25.6. Note, the value of $\mathcal{E}_\mathcal{F}$ of the second resonance in the Martin et al. [47] calculation is lower than the rigorous QHQ calculation [42]. It is believed that this is due to the residual M dependence of H_{eff}.

Table 25.6. Resonance energies $\mathcal{E}_\mathcal{F}$(Ry) and widths(eV) for ^1P states of He below n=2 threshold (-1 Ry) of He^+.

State	Martin et al.[47]		Lipsky and Conneely [48]		Bhatia and Temkin [42,49]	
	Position	Width	Position	Width	Position	Width
1	-1.38400	0.0382	-1.37672	0.0341	-1.38579	0.0363
2	-1.19460	0.000146	-1.19312	0.000131	-1.19418	0.000106
3	-1.12752	0.000860	-1.12584	0.00727	-1.12772	0.0090

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