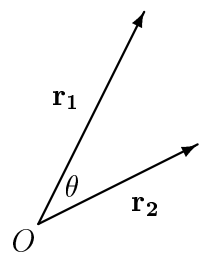
Chapter 2

The Temkin-Poet model

The Temkin-Poet model of electron scattering from atomic hydrogen has proved to be a very important model in electron-atom scattering physics, as evidenced by the considerable number of papers discussing it [1, 8, 9, 13, 14, 18, 19, 20, 23, 24, 32, 33, 34, 64, 65, 66, 67, 68, 69, 70]. In the Temkin-Poet model only the monopole component of the electron-electron interaction is included in the scattering Hamiltonian and the solution of the Schrödinger equation is restricted to the $l = 0$ partial wave. Under these circumstances the three-body potentials are separable in their respective radial coordinates. A sum of separable solutions to the Schrödinger equation satisfying physical boundary condition can then be generated, enabling a convergent and highly accurate numerical result for the S-matrix to be obtained.

2.1 Theory

Temkin proposed a solution by assuming the wavefunction describing the system to be dependent only the size and shape of the triangle comprising the three particles, and not on its orientation, as illustrated below.



This is equivalent to solving the Schrödinger equation for the zero total angular momentum component of the wavefunction Ψ. We will write this component as

$$\Psi(\mathbf{r_1}, \mathbf{r_2}, \hat{\mathbf{r}}_1.\hat{\mathbf{r}}_2) = \Psi(\mathbf{r_1}, \mathbf{r_2}, \cos\theta) \tag{2.1}$$

where θ is the angle is the angle between $\mathbf{r_1}$ and $\mathbf{r_2}$.

The boundary conditions to be satisfied for the scattering wave function are

$$\begin{aligned} \Psi^S \text{ finite as } r_1 \text{ or } r_2 &\to 0 \text{ or } \infty \\ \Psi^S \to 0 \text{ as } r_1 \text{ or } r_2 &\to \infty. \end{aligned} \tag{2.2}$$

The wave equation then takes the form

$$\begin{aligned} \Bigg(\frac{\partial^2}{\partial {r_1}^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial {r_2}^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \\ + \frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}} + E\Bigg)\Psi^S(\mathbf{r_1}, \mathbf{r_2}, \cos\theta) = 0. \end{aligned} \tag{2.3}$$

To project out the angle dependence Temkin [2] expanded the wavefunction in a series of partial waves:

$$\Psi(r_1, r_2, \cos\theta) = \frac{1}{r_1 r_2}\sum_{l=0}^{\infty}(2l+1)^{1/2}\psi_l(r_1, r_2)P_l(\cos\theta). \tag{2.4}$$

Then substituting into Eq. (2.3) the multipole expansion of the electron-electron potential

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \left(\frac{r_<^l}{r_>^{l+1}} \right) P_l(\cos\theta), \tag{2.5}$$

where $r_>$ is the greater of r_1 and r_2, folding with P_l and integrating over r_1 and r_2 he obtained [2, 71]

$$\left(\frac{\partial^2}{\partial {r_1}^2} + \frac{\partial^2}{\partial {r_2}^2} - l(l+1)\left(\frac{1}{{r_1}^2} + \frac{1}{{r_2}^2} \right) + \frac{2Z}{r_1} + \frac{2Z}{r_2} + E - M_{ll} \right) \psi_l = \sum_{m=1}^{\infty} M_{lm}\psi_m \tag{2.6}$$

where

$$M_{lm} \;=\; [(2l+1)(2m+1)]^{1/2} \sum_{m=0}^{l+m} \left(\frac{r_<^n}{r_>^{n+1}} \right) \int_0^{\pi} P_l P_m P_n \; d\theta \sin\theta. \tag{2.7}$$

If we consider the zero-order solution (right hand side of Eq. (2.6) set to zero) and retain only $l = 0$ partial waves in the expansion, Eq. (2.6) reduces to

$$\left(\frac{\partial^2}{\partial {r_1}^2} + \frac{\partial^2}{\partial {r_2}^2} + \frac{2Z}{r_1} + \frac{2Z}{r_2} - \frac{2}{r_>} + E \right) \psi(r_1, r_2) = 0 \tag{2.8}$$

with the spin symmetry

$$\psi^S(r_1, r_2) = (-1)^S \psi^S(r_2, r_1) \tag{2.9}$$

satisfied on account of Eq. (1.7).

If we now restrict the domain to the region $r_1 > r_2$, Eq. (2.8) becomes

$$\left(\frac{\partial^2}{\partial {r_1}^2} + \frac{\partial^2}{\partial {r_2}^2} + \frac{2(Z-1)}{r_1} + \frac{2Z}{r_2} + E \right) \psi(r_1, r_2) = 0 \tag{2.10}$$

which is separable so that the physical solution can be expressed as a linear combination of the separable solutions. Through the symmetry condition (2.9) the solution can then be transferred to the other region, $r_1 < r_2$.

In order to ensure continuity of ψ and its partial derivatives across $r_1 = r_2$, extra boundary conditions must be imposed on the form of the solution. For an antisymmetric wavefunction (triplet $S = 1$) it follows from Eq. (2.9) that

$$\psi^1(r_1, r_1) = 0. \tag{2.11}$$

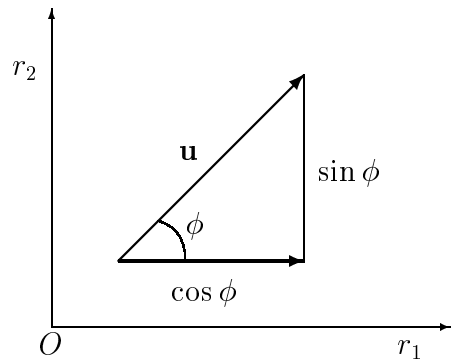
For the symmetric wavefunction (singlet $S = 0$) we require

$$\psi^0(r_1, r_2) = \psi^0(r_2, r_1) \tag{2.12}$$

implying a maximum (or minimum) and hence a vanishing directional derivative along the perpendicular to the line $r_1 = r_2$. The directional derivative of the function $w = \psi(r_1, r_2)$ is given by

$$\frac{d\psi}{dr} = \frac{\partial\psi}{\partial r_1}\cos\phi + \frac{\partial\psi}{\partial r_2}\sin\phi = \nabla\psi.\mathbf{u} \tag{2.13}$$

where ϕ is the angle measured from the r_1 axis as shown in the figure below and $r^2 = r_1^2 + r_2^2$.



Now, perpendicular to the line $r_1 = r_2$, $d\psi/dr = 0$ and $\phi = 3\pi/4$ so that

$$\frac{\partial\psi}{\partial r_1} = \frac{\partial\psi}{\partial r_2}. \tag{2.14}$$

The full boundary conditions for the problem in the triangle $r_2 \leq r_1$ are thus

$$\begin{aligned}
\psi &\to 0 && \text{as} \quad r_2 \to 0,\ \forall\ r_1 \\
\psi &\ \text{finite} && \text{as} \quad r_1 \to \infty,\ \forall\ r_2 \\
\psi &= 0 && \text{on} \quad r_1 = r_2\ \text{(triplet)} \\
\frac{\partial \psi}{\partial r_1} &= \frac{\partial \psi}{\partial r_2} && \text{on} \quad r_1 = r_2\ \text{(singlet)}.
\end{aligned} \tag{2.15}$$

It should be noted that although Eq. (2.10) is separable, the boundary conditions that must be satisfied on $r_1 = r_2$ ensure the physical wave function will not be of a separable form.

2.2 Separable Solutions

Substituting $\psi(r_1, r_2) = X(r_1)Y(r_2)$ into Eq. (2.10) and separating variables yields the equations

$$\left[\frac{\partial^2}{\partial {r_1}^2} + \frac{2(Z-1)}{r_1} + \epsilon_1\right] X(r_1) = 0 \tag{2.16}$$

and

$$\left[\frac{\partial^2}{\partial {r_2}^2} + \frac{2Z}{r_2} + \epsilon_2\right] Y(r_2) = 0 \tag{2.17}$$

which together may be written compactly as

$$\left[\frac{\partial^2}{\partial r^2} + \frac{\alpha}{r} - q^2\right] W(r) = 0 \tag{2.18}$$

where

$$\alpha = \begin{cases} 2Z \\ 2(Z-1) \end{cases} \quad \text{and} \quad -q^2 = \begin{cases} \epsilon_1 & \text{target} \\ \epsilon_2 & \text{projectile} \end{cases} \tag{2.19}$$

with $\epsilon_1 + \epsilon_2 = \epsilon_{tot}$.

Let us seek a solution of the form $W(r) = re^{-qr}w(r)$.

Substitution into Eq. (2.18) gives us

$$r\frac{d^2w}{dr^2} + (2 - 2qr)\frac{dw}{dr} + (\alpha - 2q)w = 0 \tag{2.20}$$

and then transforming to the variable $\rho = 2qr$ we arrive at the equation

$$\rho\frac{d^2w}{d\rho^2} + (2 - \rho)\frac{dw}{d\rho} + (1 - \frac{\alpha}{2q})w = 0 \tag{2.21}$$

known as Kummer's equation and has regular and irregular solutions. For the physical wave function we need the solution regular at the origin $r = 0$ and this is provided by the confluent hypergeometric function ${}_1F_1(1 - \alpha/2q; 2; \rho)$. Hence the required radial function is

$$W_\epsilon(r) = N\ r\ e^{-qr}\ {}_1F_1(1 - \frac{\alpha}{2q}; 2; 2qr) \tag{2.22}$$

where N is a normalisation constant. A regular solution exists for $\epsilon < 0$ only for discrete negative energies.

The separable solutions $\psi(r_1, r_2)$ satisfying Eq. (2.10) may be constructed from products of these one-electron wavefunctions which represent the projectile X and target Y in their respective domains:

$$u^I_\epsilon(r_1, r_2) = X^-_k(r_1)\, Y_\epsilon(r_2) \qquad \text{incident} \tag{2.23}$$

$$u^R_\epsilon(r_1, r_2) = X^+_k(r_1)\, Y_\epsilon(r_2) \qquad \text{reflected} \tag{2.24}$$

where $\frac{1}{2}k^2 = \epsilon_{tot} - \epsilon$. However it is easy to see that a particular separable solution does not on its own satisfy the scattering boundary condition, Eq. (1.11), which requires the presence of incoming and outgoing waves.

2.2.1 Target States

The energies of the target state radial functions $Y_\epsilon(r_2)$ are

$$q = \begin{cases} Z/n & \text{if } \epsilon < 0, \text{ with n = 1, 2, 3...(a bound state)} \\ \pm ik & \text{if } k^2 = \epsilon > 0 \text{ (a continuum state).} \end{cases}$$

In order to preserve the continuity of the target wavefunctions across $\epsilon = 0$, where the transition from bound states to continuum functions takes place, we choose the normalisation

$$Y_\epsilon(r_2) \to r_2 \quad as \quad r_2 \to 0 \tag{2.25}$$

so that for bound states we have

$$\begin{aligned} Y_n(r_2) &= r_2 e^{-\frac{Z}{n} r_2} \, {}_1F_1(1-n, 2; \frac{2Z}{n} r_2) \\ &= (2)^{1/2} \left(\frac{n}{2Z}\right)^{3/2} R_{n0}(r_2) \end{aligned} \tag{2.26}$$

where $R_{n0}(r_2)$ is the normalised hydrogenic s-state orbital given by [72]

$$R_{n0}(r_2) = \left(\frac{2Z}{n}\right)^{3/2} \left\{\frac{(n-1)!}{2n(n!)^2}\right\}^{1/2} e^{-\frac{Z}{n} r_2} \, L_n(\frac{2Z}{n} r_2), \tag{2.27}$$

whilst for continuum states

$$\begin{aligned} Y_\epsilon(r_2) &= r_2 e^{-ikr_2} {}_1F_1(1-i\eta, 2; 2ikr_2) \\ &= [C_o(\eta)k]^{-1} F_0(\eta, kr_2) \end{aligned} \tag{2.28}$$

where $F_0(\eta, kr_2)$ is the regular Coulomb function defined by Eq. (A.1) with $l = 0$ and $C_o^2(\eta) = 2\pi\eta(e^{2\pi\eta} - 1)^{-1}$ with $\eta = \alpha/2k$.

2.2.2 Projectile States

A second linearly independent solution of Eq. (2.21) is the irregular Coulomb wavefunction, defined by Eq. (A.2). Following from the discussion in Sec. (1.2.2) we

choose the exponential-like solutions

$$X_k^{\pm}(r_1) = H_0^{\pm}(\eta, kr_1) \tag{2.29}$$

$$\underset{r_1\to\infty}{\sim} \exp \pm i(kr_1 - \eta \ln 2kr_1 + \sigma_0) \tag{2.30}$$

so that in open channels ($k^2 > 0$) we have outgoing $(+)$ and incoming $(-)$ distorted plane waves.

For closed channels ($k^2 < 0$) we make the replacement $k \to i\kappa$, $\eta \to \eta/i$. The solutions are then found to be the decaying Whittaker functions

$$X_k(r_1) = W_{\eta,1/2}(kr_1) \tag{2.31}$$

which die off with exponential decay.

2.3 Construction of Physical Solutions

We construct our general wavefunction with asymptotic form (1.11) by building up from the manifold of physically admissible solutions a linear combination of the incident and scattered (reflected) waves given by Eqs. (2.23) and (2.24) summed over the discrete (bound) and continuum (free) states:

$$\psi^S(r_1, r_2) \;=\; u^I_{\epsilon_0}(r_1, r_2) + \sum\!\!\!\!\!\!\int u^R_{\epsilon}(r_1, r_2)\, c^S_{\epsilon\epsilon_0} d\epsilon \tag{2.32}$$

where ϵ_0 is the channel corresponding to the initial state of the atom. In writing down Eq. (2.32) we imply that the generalised summation is over negative bound and continuum (open and closed) target states. Note that the amplitudes $C^S_{\epsilon\epsilon_0}$ are essentially S-matrix elements as we see by comparison of Eq. (2.32) with Eq. (1.11).

Symmetrisation with S needs to be imposed on the general form of the wave function and can be applied in many ways. At first inspection one might question whether

this requirement is indeed satisfied by $\psi(r_1, r_2)$ as given in Eq. (2.32) since it is not explicitly symmetrised with respect to the interchange of r_1 and r_2. Choosing explicit symmetrisation, i.e., by forming

$$\psi_{\mathcal{A}}(r_1, r_2) = \psi(r_1, r_2) + (-1)^S \psi(r_2, r_1) \tag{2.33}$$

as is done in the Close-Coupling equations is one way. However, this form will not satisfy the Temkin-Poet equation in the region $r_1 > r_2$ when ψ is made up from the separable forms. The Temkin-poet equations incorporate the symmetrisation requirement by asking what must happen at the boundary for the final physical scattering solution to be symmetrised. The net result is that symmetrisation is fully included at the expense of having a new set of equations. This feature of the equations was already established and discussed by Temkin in the 1960s. The conditions to be satisfied are given by Eq. (2.15).

Applying the boundary condition (2.15) on the line $r_1 = r_2 = r$ gives us the equation

$$v_\epsilon^{SI}(r) + \sum\!\!\!\!\!\!\int v_\epsilon^{SR}(r)\, c^S_{\epsilon\epsilon_0} d\epsilon = 0 \tag{2.34}$$

where

$$v^0(r) = \left.\frac{\partial u}{\partial r_1}\right|_{r_1=r_2} - \left.\frac{\partial u}{\partial r_2}\right|_{r_1=r_2} \quad \text{(singlet)}$$

$$v^1(r) = u(r, r) \qquad\qquad \text{(triplet).} \tag{2.35}$$

Construction of the v functions is equivalent to generating for each bound and continuum orbital in the expansion of target states in Eq. (2.32) properly symmetrised incoming and outgoing waves if the channel energy is positive and exponentially decaying bound-state solutions if the channel energy is negative.

Following Poet [1] the expansion coefficients $c^S_{\epsilon\epsilon_0}$ in Eq. (2.34) may be determined variationally using a least-squares procedure to yield an integral equation that is

independent of the radial variable r. Let

$$\chi(r) = v_\epsilon^{SI}(r) + \sum\!\!\!\!\!\!\int v_\epsilon^{SR}(r)\, c^S_{\epsilon\epsilon_0} d\epsilon \qquad \text{and} \qquad I = \int_0^\infty |\chi(r)|^2 dr. \tag{2.36}$$

Minimising I by differentiating with respect to $c_{\epsilon\epsilon_0}$ gives

$$\frac{\partial I}{\partial c_{\epsilon\epsilon_0}} = \int_0^\infty dr \left[\sum\!\!\!\!\!\!\int v_\epsilon^{SR}\, v_{\epsilon_0}^{SI^*}\, d\epsilon + \sum\!\!\!\!\!\!\int v_\epsilon^{SR^*}\, v_{\epsilon_0}^{SI}\, d\epsilon + 2\sum\!\!\!\!\!\!\int v_\epsilon^{SR^*}\, v_\epsilon^{SR}\, c^S_{\epsilon\epsilon_0} d\epsilon \right] = 0. \tag{2.37}$$

Since

$$\sum\!\!\!\!\!\!\int v_{\epsilon_0}^{SI^*} v_\epsilon^{SR} d\epsilon = \sum\!\!\!\!\!\!\int v_{\epsilon_0}^{SI} v_\epsilon^{SR^*} d\epsilon \tag{2.38}$$

we obtain the equation

$$\sum\!\!\!\!\!\!\int A^S_{\epsilon\epsilon'} c^S_{\epsilon'\epsilon_0} d\epsilon' = b^S_{\epsilon\epsilon_0} \tag{2.39}$$

where

$$A^S_{\epsilon\epsilon'} = \int_0^\infty v_\epsilon^{SR^*} v_{\epsilon'}^{SR} dr \qquad \text{and} \qquad b^S_{\epsilon\epsilon_0} = -\int_0^\infty v_\epsilon^{SR^*} v_{\epsilon'}^{SI} dr. \tag{2.40}$$

Replacing the integration by a quadrature rule

$$\int_0^\infty f(\epsilon) d\epsilon \approx \sum_j w_j f(\epsilon_j) \tag{2.41}$$

we arrive at

$$\sum_j A_{\epsilon_i \epsilon_j} c^S_{\epsilon_j \epsilon_0} = b^S_{\epsilon_i \epsilon_0}. \tag{2.42}$$

The expansion coefficients $c^S_{\epsilon_j \epsilon_0}$ are determined by solving the system of Eqs. (2.42) by matrix inversion, and then converted to S-matrix elements using the definition

$$S^S_{ij} \;=\; -\left(\frac{k_i}{k_j}\right)^{1/2} c^S_{ij} \tag{2.43}$$

where the indices i and j refer to incoming and outgoing channel states, respectively. The factor $(k_i/k_j)^{1/2}$ is introduced so that the squared modulus of the S matrix gives fluxes and not just probabilities. The cross section for a transition from the state i to j is then obtained through Eq. (1.17).

2.4 Renormalisation of the S-matrix

From the requirement

$$\int_0^\infty |Y_\epsilon(r_2)|^2 \, dr_2 \;=\; N_\epsilon \tag{2.44}$$

and Eqs. (2.26) and (2.28) we obtain the renormalisation factors

$$N_\epsilon \;=\; \frac{1}{2}\left(\frac{2Z}{n}\right)^{3/2} \qquad \text{for bound states} \tag{2.45}$$

$$\;=\; \sqrt{C_0(\eta)\, k} \qquad \text{for continuum states.} \tag{2.46}$$

The total wavefunction, given by Eq. (2.32), is therefore

$$\frac{F}{\sqrt{N}_{\epsilon_0}} \;=\; \frac{u^I_{\epsilon 0}}{\sqrt{N}_{\epsilon 0}} \;+\; \int_0^\infty \frac{u^R_\epsilon}{\sqrt{N}_\epsilon} \left(\sqrt{N}_\epsilon \, c_{\epsilon\epsilon_0} \, \frac{1}{\sqrt{N}_{\epsilon 0}}\right) d\epsilon \tag{2.47}$$

so that the S-matrix now becomes

$$S_{ij} \;=\; -\left(\frac{k_i}{k_j}\right)^{1/2} \left(\frac{N_i}{N_j}\right) c_{ij}. \tag{2.48}$$

This is essentially the form adopted by Poet [1] in his original work.

Having laid down the theoretical foundations of Poet's method, we now discuss the numerical methods used to solve the electron-ion scattering problem for this model.