Projet RGM

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1 Equation

We aim to solve the scattering solutions of the Schrodinger equation having the form

$$(H_0 - E)\ \Psi(\vec{R}) + V(\vec{R})\ \Psi(\vec{R}) + \int d\vec{R}'\ W(\vec{R},\vec{R}';E)\ \Psi(\vec{R}') = 0 \tag{1}$$

where

$$H_0 = -\frac{\hbar^2}{2\mu}\Delta_{\vec{R}}$$

the local potential

$$V(\vec{R}) = \sum_{n=1}^{3} \eta_n e^{-\kappa_n R^2} \tag{2}$$

and a non-local and E-dependent term that we will write in the form

$$W(\vec{R},\vec{R}';E) = -\sum_{i=1}^{4} c_i\ W_i(R,R',\vec{R}\cdot\vec{R}';E)\ e^{-\left(\alpha_i R^2+\beta_i \vec{R}\cdot\vec{R}'+\gamma_i R'^2\right)} \tag{3}$$

In detail

$$\begin{aligned}
W(\vec{R},\vec{R}';E) &= c_1\left[\frac{\hbar^2}{2\mu}\left(4\alpha_1^2R^2+\beta_1^2R'^2+4\alpha_1\beta_1\vec{R}\cdot\vec{R}'-2\alpha_1\right)+E\right]\ e^{-\left(\alpha_1R^2+\beta_1\vec{R}\cdot\vec{R}'+\gamma_iR'^2\right)} && (4)\\
&- c_2 \qquad e^{-\left(\alpha_2R^2+\beta_2R'^2+\gamma_2\vec{R}\cdot\vec{R}'\right)} && (5)\\
&- c_3 \qquad e^{-\left(\alpha_3R^2+\beta_3R'^2+\gamma_3\vec{R}\cdot\vec{R}'\right)} && (6)\\
&- c_4 \qquad e^{-\left(\alpha_4R^2+\beta_4R'^2+\gamma_4\vec{R}\cdot\vec{R}'\right)} && (7)
\end{aligned}$$

That is having a radial dependence $W(\vec{R},\vec{R}';E) \equiv f(R,R',\vec{R}\cdot\vec{R}';E)$

1. It depends on $3\times 2+4\times 4 = 20$ constants and the effective mass μ
2. Usually the RGM equation have the form

   $$E\int dr'\ N(r,r')\chi(r') = \int dr' H(r,r')\chi(r')$$

   that is with a "norm term" $N(r,r')$. Is it absent in your case ?

2 Partial wave solution

After projecting it takes the form

$$-\frac{\hbar^2}{2\mu}u''_L(R) - Eu_L(R) + \left[V(R) + \frac{\hbar^2}{2\mu}\frac{L(L+1)}{R^2}\right]u_L(R) + \int dR' W_L(R,R';E)u_L(R') = 0 \tag{8}$$

with the local potential

$$V(R) = \sum_{n=1}^{3} \eta_n e^{-\kappa_n R^2} \tag{9}$$

and the non-local E-dependent one

$$W_L(R,R';E) = F_L(R,R') + \sum_{n=1}^{4} 4\pi\ i^L\ c_n\ \left\{E\delta_{1n} + \bar{\delta}_{1n}\right\}\ j_L(i\beta_n RR')e^{-(\alpha_n R^2 + \gamma_n R'^2)}\ RR' \tag{10}$$

where

$$\bar{\delta}_{1n} \equiv 1 - \delta_{1n}$$

$$\begin{aligned}
F_L(R,R') &= A(R,R')\left[B_L(R,R') + C_L(R,R') + D_L(R,R')\right]\\
A(R,R') &= -\frac{\hbar^2}{2\mu}4\pi c_1 e^{-(\alpha_1 R^2 + \gamma_1 R'^2)}RR'\\
B_L(R,R') &= \left[-4\alpha_1^2 R^2 - \beta_1^2 R'^2 + 2\alpha_1 + \frac{L(L+1)}{R^2}\right] i^L j_L(i\beta_1 RR')\\
C_L(R,R') &= \delta_{L0}\ 4\alpha_1\beta_1\ i^{L-1} j_{L-1}(i\beta_1 RR')(2L-3)\begin{pmatrix} 1 & L-1 & L\\ 0 & 0 & 0\end{pmatrix}^2 RR'\\
D_L(R,R') &= 4\alpha_1\beta_1\ i^{L+1} j_{L+1}(i\beta_1 RR')(2L-1)\begin{pmatrix} 1 & L+1 & L\\ 0 & 0 & 0\end{pmatrix}^2 RR'
\end{aligned}$$

1. Although not explicit, i think that W_L must be real
2. Since $j_L(z) \approx z^{L+2}$, W_L as well as all the non local kernels vanishes when $R, R \to 0$ and when $R, R' \to \infty$
3. Same remark concerning the absence of "norm term"
4. In practical solutions I prefer multiply equation (8) by $(2\mu/\hbar^2)$, introduce the wave number q driving the assymptotics, and write it in the form

$$\boxed{u''_L(R) + \left[q^2 - v(R) - \frac{L(L+1)}{R^2}\right]u_L(R) - \int dR'\ w_L(R,R';E)\ u_L(R') = 0} \tag{11}$$

   where

$$v = \frac{2\mu}{\hbar^2}V \qquad w = \frac{2\mu}{\hbar^2}W \qquad q^2 = \frac{2\mu}{\hbar^2}E$$

3 3d-solution

We use spherical coordinates $\vec{R} = (r, \theta, \varphi)$ and denote $u = \cos\theta$

$$\vec{R} = \begin{pmatrix} r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{pmatrix} \qquad \vec{R'} = \begin{pmatrix} r'\sin\theta'\cos\varphi' \\ r'\sin\theta'\sin\varphi' \\ r'\cos\theta' \end{pmatrix}$$

$$\vec{R} \cdot \vec{R'} = RR'[\sin\theta\sin\theta'\cos(\varphi - \varphi') + \cos\theta\cos\theta']$$

$$\Psi(R) = \Psi(r, u, \varphi)$$

$$dR = r^2 dr du d\varphi$$

We restrict to a solution in the (r, θ) plane, that is with $\varphi = 0$