A new method of description of three-particle Coulomb systems

V.B. Belyaev, A.A. Naumkin

BLTP JINR, Dubna, Russia

Introduction

Method of intermediate hamiltonians for lower bounds of eigenvalues [1]

$$H = H^0 + H'$$

H^0 – solvable,

H' – positive definite

Intermediate hamiltonians

$$H^k = H^0 + H' P^k$$

where P^k – finite rank operator:

$$P^k|\varphi\rangle = \sum_{k=1}^{K} \alpha_i |p_i\rangle$$

p_i – linearly independent states

$$H^0 \leq H^k \leq H^{k+1} \leq H$$

if $|\varphi\rangle = |p_m\rangle \longrightarrow H^k|\varphi\rangle = H|p_m\rangle$

3-body system hamiltonian

$$\hat{H} = -\sum_{i=1}^{3} \frac{1}{2m_i} \nabla_i^2 + \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

Introducing Jackobi coordinates

$$\mathbf{x}_i = \left[\frac{m_j m_k}{m_j + m_k}\right]^{1/2} (\mathbf{r}_j - \mathbf{r}_k) = \sqrt{\mu_{j,k}} (\mathbf{r}_j - \mathbf{r}_k)$$

$$\mathbf{y}_i = \left[\frac{m_i(m_j + m_k)}{m_1 + m_2 + m_3}\right]^{1/2} \left(-\mathbf{r}_i + \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k}\right)$$

$$\hat{H} = -\frac{1}{2}\nabla_{\mathbf{x}}^2 - \frac{1}{2}\nabla_{\mathbf{y}}^2 + V$$

$V(\mathbf{x}, \mathbf{y}) = \frac{b_1}{x_1} + \frac{b_2}{x_2} + \frac{b_3}{x_3}$, where $\quad b_i = \sqrt{\frac{m_j m_k}{m_j + m_k}} z_j z_k$

Hyperspherical coordinates

$$x = \rho \cos \alpha, \quad y = \rho \sin \alpha$$

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho}\frac{\partial}{\partial \rho}\right) - \frac{1}{2\rho^2}\hat{K} + V$$

$$\hat{K} = \frac{\partial^2}{\partial \alpha^2} + 4 \cot 2\alpha \frac{\partial}{\partial \alpha} + \frac{1}{\cos^2 \alpha}\Delta_{\Omega_1} + \frac{1}{\sin^2 \alpha}\Delta_{\Omega_2}$$

$$V(\rho, \Omega) = \frac{1}{\rho} f(\Omega)$$

$f(\Omega)$ – angular part of the Coulomb potential

$$f(\Omega) = \frac{b_1}{\cos \alpha_1} + \frac{b_2}{\cos \alpha_2} + \frac{b_3}{\cos \alpha_3}$$

α_i are hyperangles in different sets of Jacobi coordinates

Lipmann-Schwinger equation

$$(E - H_0)|\Psi\rangle = V|\Psi\rangle$$

$$|\Psi\rangle = (E - H_0)^{-1}V|\Psi\rangle$$

Here

$(H_0 - E)^{-1} = \hat{G}_0(E)$ – free Green function

Coordinate representation:

$$\Psi(\mathbf{R}) = -\int d\mathbf{R}' G_0(E;\mathbf{R},\mathbf{R}')V(\mathbf{R}')\Psi(\mathbf{R}')$$

Finite rank approximation

$$\hat{f}^N = \sum_{i,j}^{N} f|\varphi_i\rangle d_{ij} \langle\varphi_j| f$$

Here $|\varphi_i\rangle$ – auxilliary functions in angular space

$$d_{ij}^{-1} = \langle\varphi_i| f |\varphi_j\rangle$$

For $i = 1 \ldots N$ $\quad \hat{f}^N |\varphi_i\rangle = f|\varphi_i\rangle$

We use the finite rank operator f^N instead of f in the Lipmann-Schwinger equation.

We obtain representation for solution

$$\Psi(\rho,\Omega) = -\sum_{i,j}^{N} \int \rho'^4 d\rho' d\Omega' G_0(E,\rho,\rho';\Omega,\Omega') f(\Omega') \varphi_i(\Omega')\, d_{ij}\, C_j(\rho')$$

where $$C_j(\rho') = \int d\Omega'' \varphi_j(\Omega'') f(\Omega'') \Psi(\rho,\Omega'')$$

Integrating over angular variables

$$\int d\Omega\, \varphi_k(\Omega) f(\Omega) \ldots$$

results in a system of one-dimensional integral equations

Integral equations

$$C_k(\rho) = -\sum_{i,j} \int d\rho' \, \tilde{M}_{ki}(\rho,\rho') d_{ij} \, C_j(\rho')$$

$$\tilde{M}_{ki}(\rho,\rho') = {\rho'}^4 \int d\Omega \, d\Omega' \, \varphi_k(\Omega) f(\Omega) G_0(E;\rho,\rho';\Omega,\Omega') f(\Omega') \varphi_i(\Omega')$$

Let us introduce 3-body radial free Green functions

$$G_0^K(E;\rho,\rho') = \iint \mathcal{Y}^{l_1 l_2}_{KLM}(\Omega) \, G_0(E,\mathbf{R},\mathbf{R}') \, \mathcal{Y}^{l_1 l_2}_{KLM}(\Omega_\kappa) d\Omega \, d\Omega' =$$

$$= \int_0^\infty \frac{\kappa \, d\kappa}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 J_{K+2}(\kappa\rho) \, J_{K+2}(\kappa\rho') \frac{1}{\kappa^2 + 2mE} =$$

$$= \frac{1}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 \begin{cases} I_{K+2}(\kappa_0\rho) K_{K+2}(\kappa_0\rho'), & 0 \le \rho \le \rho' \\ K_{K+2}(\kappa_0\rho) I_{K+2}(\kappa_0\rho'), & 0 \le \rho' \le \rho \end{cases}$$

Let us insert

full sets of hyperspherical functions $|\mathcal{Y}^{l_1 l_2}_{KLM}\rangle\langle\mathcal{Y}^{l_1 l_2}_{KLM}|$

$$\tilde{M}_{ki}(\rho,\rho') = \rho'^4 \int d\Omega\, d\Omega'\, \varphi_k(\Omega) f(\Omega) G_0(E;\rho,\rho';\Omega,\Omega') f(\Omega')\varphi_i(\Omega')$$

and we obtain

Summation in the kernel is limited by K_{max}

$$\tilde{M}_{ki}(\rho,\rho') = \rho'^4 \sum_{KLMl_1l_2} G_0^K(E;\rho,\rho')\langle\varphi_k|f|\mathcal{Y}^{l_1l_2}_{KLM}\rangle\langle\mathcal{Y}^{l_1l_2}_{KLM}|f|\varphi_i\rangle$$

$$C_k(\rho) = -\sum_{i,j}\int d\rho'\, \tilde{M}_{ki}(\rho,\rho') d_{ij}\, C_j(\rho')$$

The integral equations are transformed into matrix ones using discretisation by ρ, and the values of E are calculated as its eigenvalues.

Details of calculation

- Total angular momentum L = 0
- The ground state energy is calculated
- Auxiliary functions φ_i are hyperspherical functions
- Calculations are performed with 100 discretizing points.

Binding energies

E, eV	Exp.	FRA	E_N, eV (theory)		
			$K_{max} = 6$	$K_{max} = 10$	$K_{max} = 14$
H^-	14,34	N=1	25	20	18,2
		N=3	20	18,5	17,1
		N=6	18	16,2	15,6
He	79,0	N=1	102	98	95
		N=3	99	91	89
		N=6	95	87	85
H_2^+	16,25	N=1	7,3	10	11
		N=3	8,5	12	13,7
		N=6	10,1	13,5	15,1
$pp\mu$	2782	N=1	1050	1700	1850
		N=3	1360	2044	2101
		N=6	1690	2290	2332
$dd\mu$	2988	N=1	1200	1820	1990
		N=3	1540	2072	2480
		N=6	1845	2195	2654

Numerical convergency

E, eV	Exp.	E, eV (theory)			
		D = 40	60	80	100
H–	14,34	20,1	17,5	16	15,6
He	79,0	121	90,1	87	85

D is a number of discretizing points

Here $N = 6$, $K_{max} = 14$

This method was used in [2] to calculate binding energies of three-body systems in adiabatic approach

Conclusion

- The method proposed simplifies treatment of 3-body Coulomb systems
- Reasonable values of 3-body systems binding energies are obtained

References

1. N.W. Bazley, D.W. Fox, Phys.Rev. 124 (1961) 483
2. V.B. Belyaev, I.I. Shlyk, Nucl.Phys. A 790 (2007) 792c