

ELASTIC SCATTERING IN A SYSTEM OF THREE HELIUM ATOMS WITHIN A LOCALIZED COMPONENT METHOD

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The investigating of bound states and scattering in a system of He atoms gets complicated by the fact that the binding energy of two-body subsystems is extremely low and two-body wave function is localized in a much wider regions of configuration space than the corresponding two-body potential. Recently developed localized component method allows to get rid of this problem. here we describe the application of the method to a system of three He atoms.

Consider a Faddeev component [1] Φ_i in the asymptotic region $(\mathbf{x}_i, \mathbf{y}_i) \in \Omega \subset \sup V_i$. Obviously, in this region it satisfies a Schroedinger equation with the corresponding channel Hamiltonian

$$(H_0 + V_i(\mathbf{x}_i) - E)\Phi_i(\mathbf{x}_i, \mathbf{y}_i) \approx 0, (\mathbf{x}_i, \mathbf{y}_i) \in \Omega$$

where H_0 is the free three-body Hamiltonian, V_i is the interaction potential in the i -th pair and E is the total energy of the system. This gives us a hint, how to define a new component, which is localized better in configuration space than the original Faddeev component of a wave function

$$\tau_i \equiv (H_0 + V_i(\mathbf{x}_i) - E)\Phi_i(\mathbf{x}_i, \mathbf{y}_i).$$

A set of these components satisfy the following integral equation

$$\tau_i = -V_i \sum_{j \neq i} R_{2j}(E)\tau_j,$$

where $R_{2j}(E)$ are the resolvents of the corresponding channel Hamiltonians. Since $\sup \tau_i \subset \sup V_i$, the components τ_i are more suitable for numerical approximation than the original Faddeev components. On the other hand no explicit representation for integral operators $R_{2j}(E)$ is required, if the equation is being solved using some iterative technique. In this case we only need to calculate the action of the integral operator on a component, what can be done by solving the corresponding differential equation with appropriate boundary conditions numerically. We call the corresponding computational scheme a Localized Component Method (LCM).

The equations for a localized component were successfully applied to investigate bound states and low-energy scattering in a system of three ^4He atoms [2]. The more recent results are obtained for an unsymmetric system of one ^3He and two ^4He atoms. Application of LCM allowed us to produce probably the most accurate nowadays results for such systems. The results of such calculations are provided in the table. The method can be also applied for 4-body calculations, a generalization for Coulomb systems is being investigated.

Potential	$^4\text{He}-^4\text{He}_2$ l_{sc} (Å)	$^3\text{He}-^4\text{He}_2$ l_{sc} (Å)	$^4\text{He}^3\text{He}^4\text{He}_2$ E_0 (mK)
HFD-B	121.9	20.5	-16.03
LM2M2	115.4	20.9	-13.43
TTYPT	115.8	20.9	-13.70
SAPT1	122.4	20.5	-16.23
SAPT2	123.1	20.4	-16.75

Tab. 1. Bound state energies and scattering lengths in a system of three He atoms

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References

- [1] L. D. Faddeev, S. P. Merkuriev, *Quantum scattering theory for several particle systems* Kluwer Academic Publishers, Dordrecht, The Netherlands, 1993
- [2] V.Roudnev, Chem. Phys. Lett. **367**, 95-101 (2003).