Discrete Variable Representation in Studying Few-Body Quantum Systems with Nonzero Angular Momentum

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Abstract—Solving a quantum few-body problem with weak interaction is a complicated task. A procedure for discrete variable representation is developed and applied, allowing the period of calculation to be reduced with no loss of accuracy.

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INTRODUCTION

In this work, we consider systems of Ne₃, He₃, and Li–He₂ particles whose binding energy is low and whose bound state wave function is spread considerably in space. Such systems are of great interest and have been actively studied, especially in [1–7]. Since the interatomic interaction potential of these molecules is weak, the task of finding the binding energies and wave functions is quite difficult. With small changes in the input parameters (e.g., potentials) or with a large calculation errors, the result can differ greatly from the correct one. Substantial computational resources and different ways and means of solving the problem are needed to obtain accurate results.

The aim of this work was to develop and implement discrete variable representation (DVR) [7] and use it to calculate weakly bound molecular systems. Its use allows us to perform calculations with lower computational costs and reduce the period of computation with no loss of accuracy. Due to the properties of the DVR functions, determining the matrix elements of the potential energy operator is greatly simplified.

The procedure was developed initially for the three-body quantum problem with zero orbital momentum [8]. A DVR expansion in Legendre polynomials was constructed. In this work, the algorithm is generalized to nonzero orbital momentum. Features of the DVR expansion in Jacobi polynomials and associated Legendre polynomials are investigated.

Our algorithm is used to calculate the binding energies of the Ne₃, He₃, and Li–He₂ systems. The results are compared to [2–4].

DISCRETE VARIABLE REPRESENTATION FOR NONZERO ORBITAL MOMENTUM

Jacobi coordinates are chosen to represent the Hamiltonian of the three-body quantum system (Fig. 1). Variable \( x \) denotes the distance between particles 2 and 3, \( y \) is the distance between particle 1 and the center of mass of pair (23), and \( \theta \) is the angle between vectors \( \vec{x} \) and \( \vec{y} \). Using the wave function expansion in Wigner \( D \) functions [9], for nonzero orbital momentum \( J \) and its projection \( M \) we can write the Hamiltonian of the three-particle system, which consists of diagonal and off-diagonal blocks [10]:

\[
H_H'_{MM'} = \left( \frac{1}{J+1} \frac{\partial^2}{\partial x^2} + \frac{1}{J+1} \frac{\partial^2}{\partial y^2} + \frac{J(J+1) - M^2}{y^2} + V(x, y, \theta) \right)
\]

(1)

\[
H_H'_{MM'} = \left( \frac{J+1}{J+1} \frac{\partial^2}{\partial \theta^2} + \frac{J+1}{\sin \theta} \right)
\]

(2)

Each block of this matrix Hamiltonian acts on a component of the block vector of the wave function corresponding to projection \( M \). Potential \( V = V(x, y, \theta) \) in (1) is the sum of pairwise potentials, each of which depends only on the distance between particles, and

\[
\lambda_{\pm}(J, M) = \sqrt{J(J+1) - M(M+1)}.
\]

We rewrite the kinetic energy operator for coordinate \( z = \cos \theta \) and apply DVR. Using orthogonal polynomials \( P_n(z) \) and the corresponding quadrature Gaussian formula, DVR functions \( \phi_i(z) \) and their
derivatives $\varphi_i'(z)$ are constructed for the diagonal and off-diagonal parts containing the angular variable:
\begin{equation}
\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} - \frac{M^2}{\sin^2 \theta} = \left(1 - z^2\right) \frac{\partial^2}{\partial z^2} - 2z \frac{\partial}{\partial z} - \frac{M^2}{1 - z^2},
\end{equation}
\begin{equation}
\frac{\partial}{\partial \theta} + (1 \pm M) \cot \theta = -\sqrt{1 - z^2} \frac{\partial}{\partial z} + (1 \pm M) \frac{z}{\sqrt{1 - z^2}}.
\end{equation}

The properties of the DVR function allow us to simplify calculating the potential energy.

$$\varphi_i(z_k) = \frac{P_n(z_k)}{P_n'(z_i)(z_k - z_i)}, \quad \varphi_i(z_k) = \delta_{ik}. \quad (5)$$

Here, points $z_1, \ldots, z_n$ are the zeros of polynomial $P_n(z)$.

To calculate the matrix elements of the kinetic energy operator, we must determine derivatives $\varphi_i'(z)$. By expanding $P_n(z)$ in Taylor series at points $z_i$ and applying to expression (5), we obtain
\begin{equation}
\varphi_i'(z_k) = \frac{P_n'(z_k)}{P_n'(z_i)(z_k - z_i)} \quad \text{when} \quad k \neq i,
\end{equation}
\begin{equation}
\varphi_i'(z_i) = -\frac{P_n''(z_i)}{2P_n'(z_i)}. \quad (6)
\end{equation}

**Jacobi Polynomials**

The integral on interval $[-1; 1]$ can be approximated by the Gauss–Jacobi quadrature formula [11]
\begin{equation}
\int_{-1}^{1} f(z) \, dz = \sum_{i=1}^{n} \frac{w_i}{\rho(z_i)} f(z_i), \quad (7)
\end{equation}
where $\rho = (1-z)^\alpha (1+z)^\beta$ is the weight function, $z_1, \ldots, z_n$ are the zeros of the polynomial $P_n^{(\alpha, \beta)}(z)$.

Choosing DVR functions as basis functions and calculating matrix elements of the potential energy using the Gauss–Jacobi quadrature formula, we obtain the diagonal matrix of the potential energy operator in DVR:
\begin{equation}
V_{ij} = \int \frac{\varphi_i(z)}{w_i} V(x, y, z) \frac{\varphi_j(z)}{w_j} \, dz \approx \sum_k \frac{w_k}{\rho(z_k)} \varphi_i(z_k) \frac{\varphi_j(z_k)}{\rho(z_k)} \delta_{ij}. \quad (8)
\end{equation}

Using the properties of the Jacobi polynomials, we can write explicitly the values of derivatives $\varphi_i'(z)$:
\begin{equation}
\varphi_i'(z_i) = \frac{\beta - \alpha - (\alpha + \beta + 2) z_i}{2(1 - z_i^2)}. \quad (9)
\end{equation}

**Associated Legendre Polynomials**

Associated Legendre polynomials $P_{n}^{(m,m)}(z)$ contain multiplier $\sin^m \theta$, whose explicit consideration can lead to smaller errors in calculations. These polynomials can be expressed through Jacobi polynomials
\begin{equation}
P_{n+m}^{(m,m)}(z) = (-1)^m \frac{(n + 2m)!}{2^m (n + m)!} (1 - z^2)^{m/2} P_n^{(m,m)}(z). \quad (10)
\end{equation}

The zeros of polynomials $P_{n+m}^{(m,m)}(z)$ that differ from $\pm 1$ coincide with the zeros of polynomials $P_n^{(m,m)}(z)$. The DVR functions constructed using the associated Legendre polynomials can therefore be written as
\begin{equation}
\varphi_i(z) = \frac{P_{n+m}^m(z)}{P_{n+m}^m(z_i)} \quad \text{when} \quad z_i \neq \pm 1.
\end{equation}
\begin{equation}
\varphi_i'(z_i) = -\frac{z_i}{1 - z_i^2}. \quad (12)
\end{equation}

**RESULTS AND DISCUSSION**

We developed an algorithm combining finite elements [5] for coordinates $x$ and $y$ and discrete variable representation for angular coordinate $z$. The binding energies of three-particle quantum-mechanical systems were calculated using this algorithm. The energy levels of the weakly bound $^6$Li–$^4$He and $^7$Li–$^4$He molecules were calculated, using DVR based on the Legendre polynomials. With the DVR expansion, we managed to reduce the period of computation consid-
erably with no loss of accuracy. The obtained binding energies, periods of calculation, and relative errors for the He$_3$ system are presented in Table 1. The table shows that the convergence of the calculations without DVR is of a variable character, while the results obtained with DVR approach the exact value from below. Upon an increase in the number of polynomials in the expansion, the energies of both methods converge to the same value.

The calculated values of the binding energies of the $^6$Li–He$_2$ and $^7$Li–He$_2$ systems are given in Table 2. For comparison, the results of other authors [2–4] with the advisory potentials [12–14] of the He–He and He–Li interactions are also given. In the case of the TTY + KTTY and LM2M2 + KTTY potentials, the energy levels we obtained were deeper. Since the way of solving the problem is close to the variational approach, we may assume that our results are closer to the true values.

At the next stage of our study, we constructed DVR functions in Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$ and associated Legendre polynomials $P_n^{(\alpha,\beta)}(z)$. These polynomials allowed us to choose parameters $\alpha$, $\beta$, and $m$, such that weight function $\rho(z)$ smoothed the potential singularity. This approach was tested on the problem of finding the binding energies of the neon trimer for orbital momentum $J = 1$ and positive symmetry. The curve of the error dependence on the number of DVR functions is shown in Fig. 2. The results show that using associated Legendre polynomials improves the convergence of the algorithm, relative to Jacobi polynomials.

![Fig. 2. Convergence of values of two energy levels of Ne$_3$ for DVR functions constructed using Jacobi polynomials and associated Legendre polynomials.](image-url)
CONCLUSIONS

An approach combining discrete variable representation (DVR) and finite elements was used to solve the quantum three-body problem. The energy levels of weakly bound systems consisting of few atoms were calculated. By applying DVR, the period of computation was greatly reduced with no loss of accuracy.

DVR was extended using different types of quadrature formulas to construct DVR functions, particularly formulas based on the Jacobi polynomials and associated Legendre polynomials. These formulas allowed us to consider more accurately features of pairwise potentials at short distances.

The next step of our research is to generalize the proposed method to complex-valued functions to increase the efficiency of the search for resonance states and studies of scattering processes.

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