An effective and efficient algorithm for the Wigner rotation matrix at high angular momenta

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The Wigner rotation matrix (d-function), which appears as a part of the angular-momentum-projection operator, plays a crucial role in modern nuclear-structure models. However, it is a long-standing problem that its numerical evaluation suffers from serious errors and instability, which hinders precise calculations for nuclear high-spin states. Recently, Tajima [Phys. Rev. C 91, 014320 (2015)] has made a significant step toward solving the problem by suggesting the high-precision Fourier method, which however relies on formula-manipulation softwares. In this paper we propose an effective and efficient algorithm for the Wigner d function based on the Jacobi polynomials. We compare our method with the conventional Wigner method and the Tajima Fourier method through some testing calculations, and demonstrate that our algorithm can always give stable results with similar high-precision as the Fourier method, and in some cases (for special sets of \(j, m, k\) and \(\theta\)) ours are even more accurate. Moreover, our method is self-contained and less memory consuming. A related testing code and subroutines are provided as Supplemental Material in the present paper.

I. INTRODUCTION

The microscopic description of collective rotational motion involves quantum-mechanical treatment of angular momentum, in which the three angular-momentum operators, \(j_i\) \((i = x, y, z)\), are generators of the Lie algebra of SU(2) and SO(3). The Wigner D-matrix, a unitary matrix in an irreducible representation of the groups SU(2) and SO(3), enters into the discussion when functions of angular momentum are transformed by the rotation operator \(\hat{R}(\phi, \theta, \psi) = e^{-i\phi \hat{J}_x} e^{-i\theta \hat{J}_y} e^{-i\psi \hat{J}_z}\) with the Euler angles \((\phi, \theta, \psi)\). If the eigenstates of the angular momentum operators are expressed in the spherical basis and labeled by the quantum number \(j\) (with \(j = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots\)) and the projection on the \(z\) axis with \(2j + 1\) quantum numbers labeled as \(m\) or \(k = -j, -j+1, \cdots, j-1, j\), the Wigner D-matrix can be written as,

\[ D^j_{mk}(\phi, \theta, \psi) = \langle jm | e^{-i\phi \hat{J}_x} e^{-i\theta \hat{J}_y} e^{-i\psi \hat{J}_z} | jk \rangle = e^{-i(m\phi + k\psi)} d^j_{mk}(\theta), \tag{1} \]

where

\[ d^j_{mk}(\theta) = \langle jm | e^{-i\theta \hat{J}_x} \rangle | jk \rangle. \tag{2} \]

is the key part in the expression, referred to as Wigner (small) d-matrix. As Eqs. 1 and 2, are functions of the Euler angles for different sets of quantum numbers \(\{j, m, k\}\), they are usually called Wigner D- (d)-functions, respectively 2 3.

As its characteristic feature, \(d^j_{mk}(\theta)\) is known as an oscillation function of \(\theta\). In general, the oscillation frequency of the d-function increases rapidly with the angular momentum \(j\). Figure 1 shows the example for \(j = 30\).

The Wigner D-function plays crucial roles in many discussions of modern physics. As a set of orthogonal functions of the Euler angles, the D-function can be used to expand other functions. The D-function is related to some other well-known functions, for instance, \(\hat{D}^j_{m0}(\phi, \theta, \psi) = Y^j_m(\theta, \phi)\) and \(\hat{D}^j_{00}(\phi, \theta, \psi) = P^j_0(\cos \theta)\), where \(Y^j_m\) \((P^j_0)\) is the spherical harmonic function (Legendre polynomial) 2 4. Furthermore, irreducible tensors can be well defined with the help of the

FIG. 1. (Color online) The highly oscillatory behavior of the Wigner \(d^j_{mk}(\theta)\) function with \(j = 30, m = -2, k = 0\).
II. DIFFERENT METHODS FOR THE WIGNER D-FUNCTION EVALUATION

The conventional method for the $d$-function is based on the following Wigner formula [2], i.e.,

$$d_{mk}^j(\theta) = \sum_{n = n_{\text{min}}}^{n_{\text{max}}} (-1)^n W_n^{jmk}(\theta),$$

where

$$n_{\text{min}} = \max(0, k - m),$$
$$n_{\text{max}} = \min(j - m, j + k),$$

and

$$W_n^{jmk}(\theta) = w_n^{jmk} \left(\cos \frac{\theta}{2}\right)^{2j+k-m-2n} \left(-\sin \frac{\theta}{2}\right)^{m-k+2n}$$

with

$$w_n^{jmk} = \sqrt{(j+m)!(j-m)!(j+k)!(j-k)!} \frac{1}{(j-m-n)!(j+k-n)!(n+m-k)!n!}$$

It can be seen that the Wigner formula involves a summation over many terms, $W_n^{jmk}$, with alternating signs. Each of these terms includes many factorials of large numbers, especially at medium and high spins, as they grow exponentially with $j$. Although cancellation among these terms should finally lead the summation to a normal value for the $d$-function, the procedure would however cause an accumulation of numerical errors. Thus the numerical results from the Wigner formula unavoidably suffers from a serious loss of precision at medium and high spins, except for the neighborhood of $\theta = 0$ and $\pi$.

The problem is the repeated production and cancellation of large numbers. To avoid the problem, Tajima [3] proposed a new method for the Wigner $d$-function based on Fourier-series expansion, in which the $d$-function can be expressed as

$$d_{mk}^j(\theta) = \sum_{\rho = \rho_{\text{min}}}^{j} t_{\rho}^{jmk} f(\rho \theta).$$

In the above formula, $\rho_{\text{min}}$ could be 0, 1/2 or 1 depending on the values of $j$, $m$ and $k$ (see Table I of Ref. [3] for details) and $f$ is $\sin$ ($\cos$) function for $m - k$ being odd (even). In Eq. (7) the Fourier coefficient reads

$$t_{\rho}^{jmk} = 2(-1)^{m-k} \sum_{n=\text{min}}^{\text{max}} \frac{(-1)^n W_n^{jmk} \sum_{r=0}^{\rho-\frac{1}{2}} (-1)^r \left(\frac{2\rho}{2r+p}\right)}{1 + \delta_{\rho 0}}$$

$$\times \frac{1}{2\pi} I_{2(j+\rho-n-r)-m+k-p, 2(n+r)+m-k+p}$$

where $\rho \equiv |m-k|$ (mod 2), the square brackets are the floor function, $|\rho| = \rho/\lfloor\rho\rfloor$, and the floor function [3], $(\rho) = \rho/\lfloor\rho\rfloor$, and the floor function [3], $(\rho) = \rho/\lfloor\rho\rfloor$, and the floor function [3], $(\rho) = \rho/\lfloor\rho\rfloor$, and

$$I_{\lambda\alpha} = \int_{0}^{2\pi} \cos^{\lambda} x \sin^{\alpha} x dx.$$
or Mathematica [3]. On the other hand, in practical applications, one has to read $\tilde{t}_{\rho}^{jmk}$ from files and store into a memory, which consumes about 70 MB (1.2 GB) space for the case of $j \leq 50$ ($j \leq 100$) [3]. Recently, Feng et al. put forward an exact-diagonalization method to calculate the Fourier coefficients, in which the corresponding precision of the $d$-function decreases a little and the requested space doubles to be about 2.4 GB for the case of $j \leq 100$ [11].

It is thus desired to have an efficient algorithm for the $d$-function evaluation, which, while keeps the high precision as of the Tajima Fourier method, is self-contained, and therefore, user-friendly. Towards this goal, we note that the Wigner $d$-function can be expressed in terms of the Jacobi polynomials

$$d_{mk}^j(\theta) = \xi_{mk} \left[ \frac{s!(s+\mu+\nu)!}{(s+\mu)!(s+\nu)!} \right]^{1/2} \times \left( \sin \frac{\theta}{2} \right)^\mu \left( \cos \frac{\theta}{2} \right)^\nu P_s^{(\mu,\nu)}(\cos \theta), \quad (10)$$

where $\mu = |m-k|$, $\nu = |m+k|$, $s = j - \frac{1}{2}(|\mu+\nu|)$ and

$$\xi_{mk} = \begin{cases} 1 & \text{if } k \geq m, \\ (-1)^{k-m} & \text{if } k < m. \end{cases} \quad (11)$$

The Jacobi polynomial in Eq. (10) can be calculated by its explicit expression [45]

$$P_s^{(\mu,\nu)}(z) = \frac{1}{2^s s!} \sum_{n=0}^{s} \binom{s+\mu}{n} \binom{s+\nu}{s-n} (z-1)^{s-n} (z+1)^n, \quad (12)$$

or by the corresponding recurrence relations [45]

$$2s(s+\mu+\nu)(2s+\mu+\nu-2)P_s^{(\mu,\nu)}(z) = (2s+\mu+\nu-1)\left[ (2s+\mu+\nu)(2s+\mu+\nu-2)z + \mu^2 - \nu^2 \right] P_{s-1}^{(\mu,\nu)}(z) - 2(s+\mu-1)(s+\nu-1)(2s+\mu+\nu)P_{s-2}^{(\mu,\nu)}(z), \quad (13)$$

with

$$P_0^{(\mu,\nu)}(z) = 1, \quad (14a)$$
$$P_1^{(\mu,\nu)}(z) = (\mu+1) + (\mu+\nu+2) \frac{z-1}{2}. \quad (14b)$$

It is important to realize that unlike the Wigner method and the Fourier method, the expression in Eq. (10) that leads to the Wigner $d$-function does not involve a summation over many terms with large numbers.

### III. ERROR ANALYSIS OF THE JACOBI METHOD

In this and the next sections we carry out error analysis and discuss precision of the Jacobi method in Eq. (10) by comparing with the conventional Wigner method and the recent Fourier method. In Figs. 2 and 3 the absolute errors for the $d$-function from the three different methods are presented, and in Fig. 4 the errors in an integral calculation involving the $d$-function are illustrated. All these results are obtained by a FORTRAN 90 testing code with standard subroutines for the Wigner, Fourier and Jacobi methods as provided in the Supplemental Material [40], where in all cases floating-point numbers are adopted as double-precision (64-bit) real number.

First in Fig. 2 we show maximum errors of the $d_{mk}^j(\theta)$ calculation as a function of $j$, obtained from the Wigner, Fourier, and Jacobi methods. Results for integer and half-integer $j$’s are illustrated separately. Each error of $d_{mk}^j(\theta)$ is evaluated with respect to the exact value calculated from the formula-manipulation software Mathematica 12.1 where higher than $10^{-25}$ precision is kept. The maximum of the errors is recorded by considering all $\theta$’s from 0° to 180° with an increment of 5°, and for all possible values of $m$ and $k$ with $0 \leq m \leq j$ and $k \leq |m|$ due to the following symmetries,

$$d_{mk}^j(\theta) = (-1)^{m-k} d_{-m-k}^j(\theta), \quad (15a)$$
$$d_{mk}^j(\theta) = (-1)^{m-k} d_{-m-k}^j(\theta), \quad (15b)$$
$$d_{mk}^j(\theta) = d_{-m-k}^j(\theta), \quad (15c)$$
$$d_{mk}^j(-\theta) = (-1)^{m-k} d_{-m-k}^j(\theta), \quad (15d)$$
$$d_{mk}^j(-\theta) = d_{-m-k}^j(\theta), \quad (15e)$$
$$d_{mk}^j(\pi - \theta) = (-1)^{m+k} d_{m-k}^j(\theta). \quad (15f)$$

It can be seen from Fig. 2 that the maximum error from the Wigner method increases exponentially with $j$, in the way similar as that of $W_{n}^{jmk}$ in Eq. (3) of the Wigner formula. Already when $j \geq 25$ the error would exceed $10^{-10}$, which may lead to serious numerical problems in applications such as high-spin calculations in nuclear physics. The origin for loss of precision in the Wigner method is clear. It is caused by the summation over many $W_{n}^{jmk}$ terms in Eq. (3), where numerical errors are accumulated following a power law of $j$.

On the contrary, the maximum error from the Fourier method keeps almost constant in a stable way towards high spins, with the precision as high as about $10^{-14}$ even when $j \approx 100$. Although the Fourier method in Eq. (7) also involves a summation over many terms, each term has very high precision since the corresponding Fourier coefficient $\tilde{t}_{\rho}^{jmk}$ is calculated by means of the formula-manipulation software MAXIMA with very high precision and is stored into a memory [3], so that the accumulation of numerical errors can be avoided.

For the Jacobi method, as seen from Eq. (10), there is no summation over many terms with large numbers and a high-precision evaluation of the $d$-function is then expected. As seen from Fig. 2 when the Jacobi polynomial is calculated directly by its expression of Eq. (12), a very similar loss of precision is found for the Jacobi method as the Wigner formula. This is due to the fact that Eq. (10)
This clearly suggests that it is the recurrence relations in Eqs. (13, 14) that avoid accumulation of numerical errors. Using the recurrence relations to improve numerical precision may be helpful for many other numerical problems. Hereafter, the Jacobi method with the recurrence relations in Eqs. (13, 14) is referred to as the Jacobi method.

The results of the Jacobi algorithm are compared with those of the Wigner, Fourier and Jacobi methods. The exact values of \( d^{(j)}_{m,k}(\theta) \) are obtained by Mathematica 12.1 and the maximum error is taken over all the possible values of \( m, k \) and \( \theta \) for each \( j \). See the text for details.

This involves summation over terms that include factorials of large numbers, which leads to accumulation of numerical errors. However, when the recurrence relations of the Jacobi polynomial in Eqs. (13, 14) are adopted, the Jacobi method provides a similar high-precision and stable behavior of the \( d \) function as the Fourier method.
algorithm for the $d$-function evaluation.

To further carry out precision analysis in details, we take the $j = 40$ case as an example and show in Fig. 3 errors of $a_{mk}^{40}(\theta)$ for different values of $m$, $k$ and $\theta$, with $\theta = 30^\circ$, $60^\circ$, $90^\circ$ and $0 \leqslant m \leqslant j$, $k \leqslant |m|$ due to the symmetries in Eq. (15). The results of the Jacobi algorithm (with the recurrence relations) are compared with those of the Wigner and Fourier methods. It is seen that the Fourier method gives uniformly a $10^{-14} \sim 10^{-15}$ precision nearly irrespective of $m$, $k$ and $\theta$. The Wigner method, however, leads to a rather unstable precision, depending sensitively on $m$, $k$ and $\theta$. The precision from the Wigner method could have errors as large as $\sim 10^{-5}$ when $m \sim k \sim 0$ and $\theta = 90^\circ$ as seen from Fig. 3(g), or it could be very accurate, with the precision as high as $10^{-20}$ when $m \sim j$, $k \sim -j$, $\theta = 30^\circ$ and $60^\circ$ (see Fig. 3(a) and (d)) or $m \sim j$, $|k| \sim j$, $\theta = 90^\circ$ (see Fig. 3(g)), which, for these special cases, is much better than the Fourier method.

Therefore, In Ref. 3, Tajima suggested that if a very high precision is needed for the $d$-function evaluation, one should develop a program to switch between the Wigner and Fourier methods with special values of $j$, $m$, $k$ and $\theta$. It is now very interesting to compare the results of the Jacobi algorithm (with the recurrence relations) in Fig. 3 For each set of $j$, $m$, $k$ and $\theta$, the Jacobi algorithm always reproduces the one with the higher precision between the Wigner and Fourier methods. This pleasant feature in the Jacobi algorithm makes it a natural choice for a switcher as discussed in Ref. 3.

IV. ERROR ANALYSIS WHEN THE WIGNER $d$-FUNCTION IS INTEGRATED

According to the Peter–Weyl theorem, the Wigner $D$-functions, $D_{mk}(\phi, \theta, \psi)$, form a complete set of orthogonal functions of the Euler angles, and are often used to expand functions that are related to rotation. As the Euler angles are continuous variables the expansion takes the form of integrals with $D_{mk}(\phi, \theta, \psi)$ being part of the integrand. Because of the highly oscillatory behavior of the $d$-function, as shown in Fig. 1 especially at high $j$’s, a high precision in numerical calculations for integrals involving the $d$-function becomes an issue.

For discussions, let us take an example from the calculation with angular-momentum projection for the symmetry-violated nuclear wave-functions from mean-field calculations. Assuming axial symmetry for the intrinsic states, $|\Phi_k\rangle$, the $d$-function enters into the calculation through the angular-momentum projector,

$$\hat{P}_{mk}^j = (j + \frac{1}{2}) \int_0^\pi d_{mk}^j(\theta) \hat{R}(\theta) \sin \theta d\theta,$$

where $\hat{R}(\theta) = e^{-i\theta j_y}$ is the rotation operator around the $y$-axis. It can be generally shown that the calculated Hamiltonian matrix elements, for example, takes the form

$$\int_0^\pi d_{kk'}_{mk}^j(\theta) \hat{H} \hat{R}(\theta) |\Phi_{k'}\rangle \sin \theta d\theta,$$

which is an integral over the Euler angle $\theta$ with essentially two functions in the integrand, $d_{kk'}_{mk}^j(\theta)$ and the rotated matrix elements $|\Phi_{k'}\rangle \hat{H} \hat{R}(\theta) |\Phi_{k'}\rangle$ which is expected to be a smooth function of $\theta$. Due to the highly oscillatory behavior of the $d$-function, its precision may be more important for integrals involving the $d$-function as in many potential applications in nuclear physics, quantum metrology and many other fields in the future.

In Fig. 4 we take one such integral for discussions and show the absolute value (error) of the following integral

$$I_{mk}^j = \int_0^\pi d\theta \sin \theta d_{mk}^j(\theta) d_{mk}^{j+1}(\theta) = 0.$$

calculated by the standard Gauss-Legendre quadrature formula with different number of mesh points $N_{\text{mesh}}$. The results of the Jacobi algorithm are compared with those of the Wigner and Fourier methods. It is seen that the error from the Wigner method increases rapidly with $j$ and exceeds $10^{-8}$ at $j \geqslant 35$, irrespective of $N_{\text{mesh}}$, indicating that the error comes mainly from the $d$-function. By comparison, the error from the Jacobi algorithm and Fourier method depends on $N_{\text{mesh}}$ and the precision of the integral could be as high as $10^{-16}$ for $j \leqslant 100$ if $N_{\text{mesh}} = 200$ is taken. This suggests that the Jacobi algorithm for the $d$-function applied in integration calculations can achieve a similar high precision as the Fourier method. The remaining errors in Fig. 4 should then come mainly from the quadrature formula.

Of course, in numerical calculations and practical applications much more complicated integrands generally appear in integrals, for which a large $N_{\text{mesh}}$ is expected, and causes heavier computational burden. Nevertheless, the results in Fig. 4(b) and (c) suggest that one has a choice to use smaller numbers of mesh points if states of only lower angular momenta are studied.

V. SUMMARY

The Wigner $D$- ($d$)-functions serve as indispensable ingredients for many nuclear-structure models and are important for nuclear physics, quantum metrology and many other fields. Numerical evaluation of the Wigner $d$-function, $d_{mk}^j(\theta)$, from the conventional Wigner method suffers from serious errors and instability, especially at medium and high spins. In this paper we present a high-precision and stable algorithm for evaluation of the Wigner $d$-function. The algorithm is based on the Jacobi polynomial and its recurrence relations. Compared with the conventional Wigner method, the loss of precision at medium and high spins is avoided in our Jacobi algorithm, with a very high precision $10^{-14} \sim 10^{-15}$ when $j \leqslant 100$. Compared with the recent Fourier method, our Jacobi algorithm avoids the dependence on
FIG. 4. (Color online) The common logarithm of the maximum error in the numerical value of the integral $I_{mk}^j$ in Eq. (18) by the Gauss-Legendre quadrature formula as a function of $j$. Cases with different number of mesh points $N_{mesh}$ by the Jacobi algorithm are compared with those of the Wigner and Fourier methods. The maximum error is taken over all the possible values of $m$ and $k$ for each $j$. See the text for details.

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[46] See Supplemental Material at for the related testing code and subroutines about the Wigner d function, from which all the results in figures of the paper could be obtained. Note that the Jacobi algorithm is improved by adopting a n! = x_n × 32768^n algorithm for factorials.