High-precision evaluation of Wigner’s d-matrix by exact diagonalization

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The precise calculations of the Wigner’s d-matrix are important in various research fields. Due to the presence of large numbers, direct calculations of the matrix using the Wigner’s formula suffer from loss of precision. We present a simple method to avoid this problem by expanding the d-matrix into a complex Fourier series and calculate the Fourier coefficients by exactly diagonalizing the angular-momentum operator $J_z$ in the eigenbasis of $J_z$. This method allows us to compute the d-matrix and its various derivatives for spins up to a few thousand. The precision of the d-matrix from our method is about $10^{-14}$ for spins up to 100.

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I. INTRODUCTION

The spin is a fundamental quantum object and an important candidate for various quantum technologies such as magnetic resonance spectroscopy, quantum metrology, and quantum information processing. An essential requirement in these developments is the precise control of many spins or alternatively a large spin composed of the constituent spins. The simplest case of such control is the rotation around a fixed axis. Accurately describing this process requires high-precision calculations of the Wigner’s d-matrix [1-4] that quantifies the rotation of angle $\theta$ around the y axis: $d_{jm}(\theta) \equiv \langle j, m | \exp(-i \theta J_y) | j, m \rangle \in \mathbb{R}$, where $| j, m \rangle$ is an eigenstate of $J_y$ with eigenvalue $m$, i.e., $J_y | j, m \rangle = m | j, m \rangle$. Hereinafter, $h = 1$ and $i = \sqrt{-1}$.

High-precision calculations of the d-matrix is of interest in quantum metrology [5-7]. For instance, let us consider an atomic Ramsey (or equivalently, Mach-Zehnder) interferometer fed with all spins down as the paradigmatic setup of interferometric phase estimation. These spins then undergo an unknown phase shift $\theta$ via the evolution $\exp(-i \theta J_y)$ inside the interferometer. Finally, by detecting the population imbalance at the output port of the interferometer, i.e., the $J_z$ measurement with respect to the output state $\exp(-i \theta J_y) | j, -j \rangle$, one can record $(2j + 1)$ possible outcomes. The outcome $m$ occurs with probability $P_m(\theta) = \langle j, m | \exp(-i \theta J_y) | j, -j \rangle^2 = [d_{jm^*}(\theta)]^2$ conditioned on the unknown parameter $\theta$, thus $\theta$ can be inferred from appropriate data processing on the outcomes. This process, however, requires accurate evaluation of Wigner’s d-matrix. In addition, the ultimate sensitivity of this estimation is determined by the Fisher information [5-7]: $F(\theta) \equiv \sum_m |\partial P_m(\theta)/\partial \theta|^2/P_m(\theta)$, which requires accurate evaluation of the first-order derivative of Wigner’s d-matrix.

In addition to quantum metrology, the Wigner’s d-matrix is closely related to spherical harmonics and Legendre polynomials and is of interest in many other fields [8-14]. However, the calculation of the d-matrix for large spins ($j \gg 1$) suffers from a serious loss of precision, due to the presence of large numbers that exceed the floating-point precision in Wigner’s original formula [1-4]. To avoid this problem, the d-matrix has been calculated by means of recurrence relations [2]. This method still encounters severe numerical instability in the case of high spin, although a few remedies have been proposed [15-24]. Recently, Gumerov and Duraiswami [24] have developed a new recursion relation for each subspace of spins, which greatly improves the stability. However, the achievable precision (i.e., the maximum absolute error) of their results remains unclear. Most recently, Tajima [25] proposed Fourier-series expansion of the Wigner’s d-matrix and convert the accurate evaluation of the d-matrix to that of the Fourier coefficients. Such a Fourier-series representation has been shown to be more useful in improving the numerical stability and the precision. However, each Fourier coefficient is still a sum of many large numbers that exceed the floating-point precision, so it has to be evaluated with the assistance of a formula-manipulation software [25].

In this paper, we put forward a very simple method to resolve the above large-number problem in evaluating the Fourier coefficients of Wigner’s d-matrix [25]. The essential idea is to express these coefficients via the inner products $(j, m|j, \mu)_s$, where the eigenstates of $J_z$, i.e., $|j, \mu\rangle$, constitute an orthonormalized and completed set. To evaluate such inner products, we write down $J_z$ as a Hermitian matrix in the eigenbasis of $J_z$. Then we numerically diagonalize the $J_z$ matrix to obtain the eigenstates and the inner products. Due to the normalization of $|j, \mu\rangle$, the norm of each Fourier coefficient is not larger than unity, thus we avoid the large-number problem in floating-point calculations. This method allows us to evaluate accurately the d-matrix and its various derivatives for much larger spins up to a few thousands, with an absolute error $O(10^{-14})$ for the d-matrix and $O(j^4 10^{-14})$ for its $k$th-order derivative.

II. FOURIER SERIES OF WIGNER’S D-MATRIX

For large spin $j$, numerical calculation of the Wigner’s formula is subject to intolerable numerical errors because it is a
sum of many large numbers with alternating signs [1–4]:

$$d^j_{m,n}(\theta) = \sum_k w^{(j,m,n)}_k \left( \cos \frac{\theta}{2} \right)^{2j-2k+m-n} \left( \sin \frac{\theta}{2} \right)^{2k+m-n},$$  \hspace{1cm} (1)

where

$$w^{(j,m,n)}_k = \frac{(-1)^{k+m-n} \sqrt{(j+m)!(j-m)!(j+n)!(j-n)!}}{(j-m-k)!(j+n-k)!(k+m-n)! k!}.$$  \hspace{1cm} (2)

and \(k \in [\text{max}(0, n-m), \text{min}(j-m, j+n)].\) Taking \(d^j_{0,0}(\pi/2)\) as an example, the term \(k = j/2\) has a very large magnitude \(|w^{(j,0,0)}_{j/2}|/2^j \propto 2^j/j!\), exceeding the floating-point precision when \(j \gg 1.\)

To avoid this problem, Tajima [25] proposed to expand the Wigner’s d-matrix into a complex Fourier series:

$$d^j_{m,n}(\theta) = \sum_{\mu=-j}^{+j} e^{-i\mu \theta} t^j_{\mu, m,n}.$$  \hspace{1cm} (3)

This representation of the d-matrix is very useful and free from the large-number errors since each Fourier coefficient is less than or equal to 1 (see below). However, an accurate evaluation of the Fourier coefficients \(t^j_{\mu, m,n}\) by means of Eq. (3) remains nontrivial. This is because the large-number problem still exists in the coefficients:

$$t^j_{\mu, m,n} = \frac{1}{2\pi} \int_{0}^{2\pi} d^j_{m,n}(\theta) \left[ e^{-i\mu \theta} \right] d\theta = \sum_{k=\text{max}(0,n-m)} \left[ w^{(j,m,n)}_k \right] t^j_{2j, 2k + m - n},$$  \hspace{1cm} (4)

where we have introduced an integral

$$I^j_{\mu,2j,\lambda} = \frac{1}{2\pi} \int_{0}^{2\pi} \left( \cos \frac{\theta}{2} \right)^{2j-\lambda} \left( \sin \frac{\theta}{2} \right)^{\lambda} e^{i\mu \theta} d\theta = \frac{1}{2^{2j}} \sum_{l=\text{max}(0, j+\mu, j-\lambda)} (-1)^{j-l} \left( \begin{array}{c} 2j - \lambda \cr j + \mu - l \end{array} \right),$$  \hspace{1cm} (5)

with \(\left( \begin{array}{c} a \cr b \end{array} \right) = a!/[b!(a-b)!].\) When \(j \gg 1,\) some terms in the integral are still huge (e.g., the term \(l = j,\) \(\lambda = 0,\) and \(\mu = -j/2).\) Tajima [25] bypassed this problem by employing a symbolic computation software and then reducing the results to double-precision floating numbers.

III. METHOD OF EXACT DIAGONALIZATION

Here, instead of using Eq. (5), we present a very simple method to calculate the Fourier coefficients \(t^j_{\mu, m,n}\) that free from the above mentioned large-number problem. The key observation is that the d-matrix can be rewritten as

$$d^j_{m,n}(\theta) \equiv \langle j, m | e^{-i\theta J_y} | j, n \rangle = \sum_{\mu=-j}^{+j} e^{-i\mu \theta} \langle j, m | j, \mu \rangle \langle j, \mu | j, n \rangle.$$  \hspace{1cm} (6)

where \(|j, \mu\rangle \equiv e^{\pm i j_y} |j, \mu\rangle = e^{-i\theta j_y} e^{i\theta j_y} |j, \mu\rangle\) are eigenstates of \(J_y\) and they constitute an orthonormalized and completed set, i.e., \(\langle j, \mu | j, \mu' \rangle = \delta_{\mu \mu'}\) and \(\sum_{\mu} \langle j, \mu \rangle \langle j, \mu \rangle = 1.\) Here, we use \(|j, m\rangle\) for the eigenstates of \(J_y\) and \(|j, \mu\rangle\) for the eigenstates of \(J_x.\) Comparing Eq. (2) and Eq. (4), we identify the Fourier coefficients in Eq. (2) as

$$t^j_{\mu, m,n} = \langle j, m | j, \mu \rangle \langle j, \mu | j, n \rangle = e^{i\pi m} d^j_{\mu, n}(\pi/2),$$  \hspace{1cm} (7)

which obeys the sum rule \(\sum_{\mu} t^j_{\mu, m,n} = \langle j, m | j, n \rangle = \delta_{mn}.\) From Eq. (7), one can note that all the Fourier coefficients and hence the d-matrix for arbitrary \(\theta\) depend on \(d^j_{\mu, n}(\theta) = \langle j, m | j, \mu \rangle \langle j, \mu | j, n \rangle = \delta_{mn}.\) From Eq. (7), one can easily obtain \(t^j_{\mu, m,n} = (-1)^{m-n} t^j_{\mu, n,m} \) and \(t^j_{\mu, m,n} = (-1)^{n-m} t^j_{\mu, -m,n} \) as observed recently by Tajima [25].

![FIG. 1: (Color online) Computed results of the Wigner’s d-matrix](image)

Most importantly, the first result of Eq. (7) provides a very simple but accurate method to calculate the Fourier coefficients and hence the Wigner’s d-matrix by solving the inner product \(\langle j, m | j, \mu \rangle.\) To this end, we first express \(J_y\) as a \((2j + 1)\)-dimensional Hermitian matrix:

$$J_y = \frac{1}{2i} \begin{pmatrix} 0 & -X_{j+1} & \cdots & \cdots & \cdots \\ X_{j+1} & 0 & -X_{j+2} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & 0 & -X_j \\ X_{j+1} & \cdots & \cdots & X_j & 0 \end{pmatrix}.$$  \hspace{1cm} (8)
where the matrix elements are determined by \( \langle j, m \mid j', m' \rangle = (X_n \theta_{mn+1} - X_n \delta_{mn-1})/(2i) \), with the term \( X_n = \sqrt{(j+m)(j-m+1)} \) satisfying \( X_{jm} = X_{zm+1} \) and \( X_{zj} = 0 \). Next, we diagonalize the Hermitean matrix using standard numerical methods, e.g., the ZHBEV subroutine of LAPACK, or the EVCHF package of the IMSL, to obtain all the eigenvectors \( \{ |j, \mu \rangle \} \) and their probability amplitudes \( \langle j, m \mid j, \mu \rangle \). For the simplest case \( j = 1/2 \), the matrix is indeed the transpose of the Pauli matrix \( \sigma_y \) over two (i.e., \( \sigma_y^2 / 2 \)), which gives two eigenvectors \( |1/2, \pm 1/2 \rangle \), corresponding to the eigenvalues \( \pm 1/2 \). The inner products \( \langle j, m \mid j, \mu \rangle \) for \( j = 1/2 \) are given by \( (1/2, 1/2 \mid 1/2, \pm 1/2) = 1/ \sqrt{2} \) and \( (1/2, -1/2 \mid 1/2, \pm 1/2) = \pm i/ \sqrt{2} \). Inserting them into Eq. (4), one can obtain the Wigner’s d-matrix.

The exact-diagonalization method has two advantages. First, the magnitude of \( \langle j, m \mid j, \mu \rangle \) and hence all the coefficients \( t_j^{(j,m)} \) in Eq. (5) are not larger than unity, since all the eigenvectors \( \{ |j, \mu \rangle \} \) are normalized. This provides a solution to the large-number problem in Eqs. (1) and (3). Second, the matrix in Eq. (6) is tridiagonal and Hermitean, which can be easily diagonalized. By diagonalizing the \( J_y \) matrix only once, all the matrix coefficients and hence all the elements of the d-matrix can be obtained with given \( j \) and \( \theta \) (see the Supplemental Material [28]). This method allows us to calculate Wigner’s d-matrix for \( j \) up to a few thousands. More important, one can compute arbitrary \( k \)-th order derivative of the d-matrix with little additional cost, due to

\[
\frac{\partial^k d_{m,n}(\theta)}{\partial \theta^k} = \langle j, m \mid e^{-i \theta J_y} \rangle (-i J_y)^k \langle j, n \rangle = \sum_{\mu=1}^{+1} (-i \mu)^k e^{-i \theta \sigma_y} f_{j, \mu}^{(j,m,n)}.
\]  

This is indeed a common advantage of the Fourier-series representation. As shown in Fig. 7, the direct evaluation of the first result of Eq. (7) costs double even for the case \( k = 1 \) since \( \langle j, m \mid \exp(-i \theta J_y) \rangle (-i J_y) \langle j, n \rangle \) gives

\[
\frac{\partial d_{m,n}(\theta)}{\partial \theta} = \frac{1}{2} \left[ X_n d_{m,n-1}(\theta) - X_n d_{m,n+1}(\theta) \right],
\]

which depends on two elements of the d-matrix. When \( n = \pm j \), only one of them remains.

**IV. NUMERICAL RESULTS AND ERROR ANALYSIS**

As shown in Fig. 1, we plot the computed results of \( d_{m,n}(\theta) \) in the plane \( (m,n) \), with \( m, n \in [-j, +j] \). For a relatively large spin \( j = 40 \) and a given \( \theta \), \( d_{m,n}(\theta) \) is appreciable only in the central region and tend to zero quickly outside this region. The boundary of this region is determined by (see also the dashed lines of Fig. 2)

\[
m^2 + n^2 - 2mn \cos \theta = j(j+1) \sin^2 \theta,
\]

at which \( \partial^k d_{m,n}(\theta)/\partial \theta^k = 0 \) for \( k = 1, 2 \). This boundary equation follows from the differential equation of the d-matrix [29]. Similar boundary equation has been obtained using the WKB approximation [29].

Given the exact value \( d_{ex} \) and the numerically calculated value \( d_{comp} \) of a matrix element \( d_{m,n}(\theta) \), the absolute error is defined as \( \Delta_{abs} = |d_{comp} - d_{ex}| \) and the relative error is defined as \( \Delta_{rel} = |(d_{comp} - d_{ex})/d_{ex}| \) in the central region (enclosed by the dashed line), but increases rapidly outside this region.

Outside the boundary, the large relative error simply follows from the very small exact values \( d_{ex} \). To illustrate this point, we consider \( d_{m,n}(\theta) \) with \( |m| = |n| = \pm j \). In this case, we have an analytical expression

\[
d_{m,n}(\theta) = (-1)^{|m|} \left( \frac{2j}{j+m} \right)^{1/2} \left( \cos \frac{\theta}{2} \right)^{j+|m|} \left( \sin \frac{\theta}{2} \right)^{-|m|}.
\]

Using the symmetry, one can obtain \( d_{m,n}(\theta) = |\sin(\theta/2)|^{2j} \).

For \( j = 100 \) and \( \theta = \pi/6 \), one can easily obtain the exact values \( d_{m,n}(\pi/6) = 3.974 \times 10^{-118} \), which lie outside the boundary (see the dashed line of Fig. 2(d)). By contrast, although the numerically calculated values \( d_{m,n}(\pi/6) \sim 10^{-17} \) are very close to zero, they are much larger than the exact values, leading to a large relative error \( \Delta_{rel} \).

![Fig. 2: (Color online) The absolute error \( \Delta_{abs} = |(d_{comp} - d_{ex})| \) (the upper panel) and the relative error \( \log_{10} \Delta_{rel} \) (the lower panel) of the Wigner’s d-matrix \( d_{m,n}(\theta) \) with the spin \( j = 100 \), and the rotation angle \( \theta = \pi/6 \) (left), \( \pi/4 \) (middle), \( \pi/2 \) (right), respectively. The computed results are obtained by diagonalizing the matrix in Eq. (6), using the ZHBEV subroutine of LAPACK; While the exact results \( d_{ex} \) are obtained by MATHEMATICA 10.0. The dashed lines are given by Eq. (9).](image-url)
The computed \( d_{m,n}^{j}(\pi/2) \) at \( mn = 0 \) also show large relative error. To see it clearly, we use the exact result \([1]\)

\[
d^{j}_{m,0}(\theta) = (-1)^m \frac{(j-m)!}{(j+m)!} P^m_j(\cos \theta),
\]

where \( P^m_j(x) \) is the associated Legendre polynomial. When \( \theta = \pi/2 \), we obtain the exact results \( d^{j}_{m,0}(\pi/2) = (-1)^m d^{j}_{0,0}(\pi/2) \approx P^m_j(0) = 0 \) for odd \( j \neq m \). In contrast, the computed results are small but nonzero, thus \( \Delta_{\text{rel}} \rightarrow \infty \).

Finally, we discuss the scaling of the error in evaluating the d-matrix and its various derivatives with increasing spin \( j \). For this purpose, we sweep \( m, n, \) and \( \theta \) and calculate the maximum absolute errors \( \Delta_{\text{abs,max}} \) for \( d^{j}_{m,n}(\theta) \) and \( \partial d^{j}_{m,n}(\theta)/\partial \theta \) as functions of \( j \) for \( j \) up to 100. Since the maximum absolute error of the d-matrix almost appears inside the boundary (see the upper panel of Fig. 2), we only sweep \( (m,n) \) within the central region and increase \( \theta \) from 0 to \( \pi/2 \) with an increment \( \pi/36 \) \([25]\). We find that typically the maximum absolute error appears at \( m \sim n \) and \( \theta \sim 0 \) or \( \pi/2 \). As shown in Fig. 3 one can find that numerical results of \( 10^{14} \times \Delta_{\text{abs,max}} \) can be well fitted by \( a j^2 + b \), with \( a \sim 10^{-4} \) and \( b \sim 0.6 \) (see the solid line). This precision is slightly worse than the previous one \( \Delta_{\text{abs,max}} \approx 10^{-4.8(0.006)} \) for the spin \( j \) up to 100 \([25]\). However, if the scaling persists to larger \( j \), our method could provide a smaller error as \( j > 405 \). One can also note that the maximum absolute error of \( \partial d^{j}_{m,n}(\theta)/\partial \theta \) can be approximated by \( j \times \Delta_{\text{abs,max}} \) (the dashed line). More generally, from Eqs. \( 3 \) and \( 7 \), we can deduce that the maximum absolute error in evaluating the \( k \)th-order derivative \( \partial^k d^{j}_{m,n}(\theta)/\partial \theta^k \) is larger than that of the d-matrix by a factor \( O(j^k) \).

V. CONCLUSION

In summary, we have presented a very simple method to evaluate accurately the Wigner’s d-matrix by diagonalizing the angular-momentum operator \( J_z \) in the eigenbasis of \( J_z \). The coefficients of Fourier-series expansion of the d-matrix, closely related to the eigenstates of \( J_z \), are shown to be not larger than unity. This enable us to avoid the large-number problem. The absolute error of \( d^{j}_{m,n}(\theta) \) can reach \( 10^{-14} \) for spin \( j \) up to 100 and the relative error \( 10^{-10} \) within the central region \( m^2 + n^2 - 2mn \cos \theta \leq j(j+1) \sin^2 \theta \), outside which the values of the d-matrix tends to zero quickly. As one of the main advantages, we show that for given \( j \) and \( \theta \), all the elements of Wigner’s d-matrix and their \( k \)-th order derivatives can be obtained by diagonalizing \( J_z \), only once \([28]\). The method presented here is a part of the larger class of algorithms based on the matrix exponents \([30]\). As the matrix exponent of \( J_z \), the Wigner’s d-matrix could be computed even more accurately and efficiently since the matrix in Eq. \( 6 \) is Hermitian and tridiagonal.

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