Distribution of $xp$ in some molecular rotational states

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Developing the analysis of the distribution of the so-called posmom $xp$ to the spherical harmonics that represents some molecular rotational states for such as diatomic molecules and spherical cage molecules, we obtain posmometry (introduced recently by Y. A. Bernard and P. M. W. Gill, Posmom: The Unobserved Observable, J. Phys. Chem. Lett. 1(2010)1254) of the spherical harmonics and demonstrate that it bears a striking resemblance to the momentum distributions of the stationary states for a one-dimensional simple harmonic oscillator.

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I. INTRODUCTION

The quantum mechanics operator of type $xp$ has attracted much attention since the invention of quantum mechanics. In the quantum measurement theory, a frequently quoted pointer’s Hamiltonian that was given by John von Neumann is taken as $H = -\omega xp$ where $\omega$ is some constant, and $x$ is a pointer coordinate and $p$ is the pointer momentum operator. [1–4] Recently, Gill et al. intensively explore the particle’s position-momentum dot product $r \cdot p$, or posmom as they called, and establish a posmometry (the distribution density of the posmom) for some atomic and molecular systems. [5, 6] They consider that the posmom density provides unique insight into types of trajectories electrons may follow, complementing existing spectroscopic techniques that provide information about where electrons are (X-ray crystallography) or where they go (Compton spectroscopy). [5, 6] The posmom operator in one component of the three dimensional Cartesian coordinates, e.g., $Q_1 \equiv (x_p x_1 + p_x r_i)/2$, $(i = 1, 2, 3)$, is an essentially self-adjoint operator, [7, 8] and has already been studied as part of a larger space-time conformal transformation in certain non-relativistic quantum mechanical problems by de Alfaro et al. [9] Jackiw. [10] Currently, the operator $Q_1$ arouses broad interest [8, 11, 12] due to the pioneer work of Berry and Keating who take this operator $Q_1$ to be the Hamiltonian of a system and demonstrate that there are possible connections between the Riemann conjecture and eigenfunctions of the operator. [12] In this paper, we put the operator $Q_1$ on a two-dimensional spherical surface $S^2$ and work out the distribution of $Q_1$ for some molecular rotational states. Precisely, we hope to give the posmometry for spherical harmonics that describes the rotational states for some molecules, such as diatomic molecules, spherical cage molecule $C_{60}$ or $Au_{132}$, etc., of which the vibrational and rotational motions are weakly coupled so that the rotational modes can be independently treated.

Note that with embedding $S^2$ in the three-dimensional flat space $R^3$, there are three operators $Q_i$ $(i = 1, 2, 3)$ that are respectively defined along three axes of coordinate respectively. These three operators are equivalent to each other upon axis rotations or relabeling. [13] Moreover, it is easy to show that there are three pairs of complete set of commuting operators $[Q_i, L_i] = 0$ $(i = 1, 2, 3)$ each of which offers complete description of the states on $S^2$, but they are also equivalent to each other upon axis rotations or relabeling, [13] where $L_i$ is the $i$th components of orbital angular momentum.

This paper is organized as what follows. In section II, we give the complete set of eigenfunctions $\psi_{\lambda_i}$ of the $(Q_1, L_z)$. In section III, we show how to expand spherical harmonics on the bases $\psi_{\lambda_i}$. The section IV briefly concludes this study.

II. COMPLETE SET OF EIGENFUNCTIONS CONSTRUCTED FROM SIMULTANEOUS EIGENFUNCTIONS OF TWO COMMUTING OPERATORS ($Q_1$, $L_z$)

For $S^2$ of fixed radius $r$, parametrized by,

$$x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta,$$



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the preliminary form of the momentum is \( \mathbf{p}' = -i\hbar \nabla_{x^2} \) (\( \nabla_{x^2} \) is the gradient operator on \( S^2 \) [14]), defined by,

\[
\mathbf{p}' = -i\hbar \frac{1}{r} \left( \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi}, \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi}, -\sin \theta \frac{\partial}{\partial \varphi} - \cos \theta \right).
\]

We construct the self-adjoint operators \( Q_i \) in the following symmetric way with noting \( p'_i x_i \neq (x_i p'_i)^\dagger \) because of the presence of the nontrivial metric factor \( 1/\sin \theta \),

\[
Q_i = \frac{1}{2} \left\{ \frac{1}{2} \left[ x_i p'_i + (x_i p'_i)^\dagger \right] + \frac{1}{2} \left[ p'_i x_i + (p'_i x_i)^\dagger \right] \right\}.
\]

The results turn out to be,

\[
Q_i = \frac{1}{2} (x_i p_i + p_i x_i),
\]

where the momenta \( p_i \) (\( i = 1, 2, 3 \)) are the so-called geometric momentum \( \mathbf{p} = -i\hbar (\nabla_{x^2} + M \mathbf{n}) \) [15–21] on \( S^2 \) where \( M \) is the mean curvature \( -1/r \) and \( \mathbf{n} \) is the normal vector, which is proposed for a proper description of momentum in quantum mechanics for a particle constrained on \( S^2 \), and explicitly we have, [15–21]

\[
\begin{align*}
px & = -i\hbar \left( \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi}, \right), \\
yy & = -i\hbar \left( \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi}, \right), \\
zz & = i\hbar \left( \sin \theta \frac{\partial}{\partial \varphi} + \cos \theta \right).
\end{align*}
\]

The following properties of the three operators \( Q_i \) (\( i = 1, 2, 3 \)) are easily verifiable: i) Since the geometric momentum \( \mathbf{p} \) describes the motion constrained on the surface \( S^2 \) and there is no motion along the normal direction \( \mathbf{n} \), which in quantum mechanics is expressed by \( \mathbf{x} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{x} = 2(Q_x + Q_y + Q_z) = 0 \) while it is in classical mechanics expressed by \( \mathbf{x} \cdot \mathbf{p} = 0 \). ii) Three components \( (Q_x, Q_y, Q_z) \) are mutually commuting operators so they have simultaneous eigenfunctions that turn out to be, \( \tan^{-1}(\alpha \pi + a) \cos\alpha \varphi \sin\alpha \varphi/\sqrt{\sin^2 \theta + \cos \theta} \), where the eigenvalues of \( (Q_x, Q_y, Q_z) \) are respectively \( (a_x, a_y, -(a_x + a_y)) \). iii) There are three pairs of complete set of commuting observables \( (Q_i, L_i) \) (\( i = x, y, z \)), and they differ from each other upon a matter of relabelling the axes of coordinate. So, for simplicity, let us study one pair of them \( (Q_z, L_z) \) in detail.

Operators \( Q_z \) and \( L_z \) are essentially independent from each other for they are dependent on variables \( \theta \) and \( \varphi \) respectively,

\[
Q_z = i\hbar (\sin \theta \cos \theta \frac{\partial}{\partial \theta} + \frac{3}{2} \cos^2 \theta - \frac{1}{2}), \quad L_z = -i\hbar \frac{\partial}{\partial \varphi}.
\]

Thus, each of their simultaneous eigenfunctions \( \psi_{\lambda_z, m} \) is a product of two eigenfunctions determined by \( S_z \) and \( L_z \), respectively. The eigenfunctions of \( L_z \) are \( \Phi_m(\varphi) = e^{im\varphi}/\sqrt{2\pi} \) corresponding to the eigenvalues \( mh \). However, finding the eigenfunctions \( \Psi_{\lambda_z} \) of \( Q_z \) in whole full interval of \( \theta \in (0, \pi) \) is in fact a little bit tricky. A direct solution of the following eigenvalue equation

\[
Q_z \Psi_{\lambda_z}(\theta) = h\lambda_z \Psi_{\lambda_z}(\theta)
\]

leads to following two piecewise eigenfunctions,

\[
\Psi_{\lambda_z}^L(\theta) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sin \theta \sqrt{\cos \theta}} \exp(-i\lambda_z \ln \tan \theta), \quad \theta \in (0, \pi/2), \quad \lambda_z \in (-\infty, \infty)
\]

and,

\[
\Psi_{\lambda_z}^{LL}(\theta) = \Psi_{\lambda_z}^L(\pi - \theta), \quad \theta \in (\pi/2, \pi).
\]

Curiously, the functions \( \Psi_{\lambda_z}^L(\theta) \) and \( \Psi_{\lambda_z}^{LL}(\theta) \) are respectively \( \delta \)-function normalizable in half intervals \( \theta \in (0, \pi/2) \) or \( (\pi/2, \pi) \) instead of in full interval of \( \theta \in (0, \pi) \). In order to construct a complete set of the physically satisfactory
eigenstates in the full interval, we need to consider the parity of the eigenstates with respect to the equator $\theta = \pi/2$. Then the complete set of the eigenfunctions in whole interval $\theta \in (0, \pi)$ are,
\[
\Psi_{\lambda z}(\theta) = \{ \Psi^+_{\lambda z}(\theta), \Psi^-_{\lambda z}(\theta) \}
\]  
where $\Psi^+_{\lambda z}(\theta)$ and $\Psi^-_{\lambda z}(\theta)$ are the even (with superscript $+$) and odd (with superscript $-$) parity eigenstates, respectively,
\[
\Psi^+_{\lambda z}(\theta) = \left( \frac{\Psi^+_{\lambda z}(\theta) + \Psi^+_{\lambda z}(\pi - \theta)}{\sqrt{2}} \right), \quad \Psi^-_{\lambda z}(\theta) = \left( \frac{\Psi^+_{\lambda z}(\theta) - \Psi^+_{\lambda z}(\pi - \theta)}{\sqrt{2}} \right), \quad \theta \in (0, \pi).
\]
We have therefore in general the simultaneous eigenstates $\psi_{\lambda z m}(\theta, \varphi)$ of $Q_z$ and $L_z$,
\[
\psi_{\lambda z m}(\theta, \varphi) = \Psi_{\lambda z}(\theta)\Phi_m(\varphi).
\]
A state $\psi(\theta, \varphi)$ on $S^2$ can be expanded in terms of $\psi_{\lambda z m}(\theta, \varphi)$ in the following way,
\[
\psi(\theta, \varphi) = \sum_m \int \left[ c^+_{m}(\lambda z)\Psi^+_{\lambda z}(\theta) + c^-_{m}(\lambda z)\Psi^-_{\lambda z}(\theta) \right] d\lambda z \Phi_m(\varphi),
\]
where the coefficients $c^+_{m}(\lambda z)$ and $c^-_{m}(\lambda z)$ are determined by,
\[
c^+_{m}(\lambda z) = \int \Phi^*_m(\varphi)\Psi^+_{\lambda z}(\theta)\psi(\theta, \varphi) \sin \theta d\theta d\varphi.
\]

### III. Posmometry for Spherical Harmonics

As is well known, the spherical harmonics $Y_{lm}(\theta, \varphi)$ offers a complete Hilbert space for analyzing any state on $S^2$, and also represents the rotational states for some molecules. Explicitly, the spherical harmonics $Y_{lm}(\theta, \varphi)$ takes the following form,
\[
Y_{lm}(\theta, \varphi) \equiv N_{lm} P^m_l(\cos \theta) \frac{1}{\sqrt{2\pi}} e^{im\varphi},
\]
with $P^m_l$ being the associated Legendre polynomial,
\[
P^m_l(x) = \frac{(-1)^m}{2^m l!} (1 - x^2)^{l - m/2} \frac{d^{l+1}}{dx^{l+1}}(x^2 - 1)^l,
\]
and
\[
N_{lm} = \sqrt{\frac{2l + 1 (l - m)!}{(l + m)!}}.
\]
In general, the posmometry for spherical harmonics is given by,
\[
c^\pm_{lm}(\lambda z) = \int \Phi^*_m(\varphi)\Psi^\pm_{\lambda z}(\theta)Y_{lm'}(\theta, \varphi) \sin \theta d\theta d\varphi.
\]
\[= \delta_{m, m'} \int \Psi^\pm_{\lambda z}(\theta)N_{lm'} P^m_l(\cos \theta) \sin \theta d\theta.
\]
From this result, we see that the operator $L_z$ plays a role of identifying the $z$-component of the orbital angular momentum represented by the prior chosen spherical harmonics $Y_{lm}(\theta, \varphi)$, also a choice of the common reference direction in the configuration space.

Now, we calculate the following integral in (20),
\[
I^{\pm}_{lm}(\lambda z) = \int_0^{\pi} \Psi^\pm_{\lambda z}(\theta)N_{lm} P^m_l(\cos \theta) \sin \theta d\theta
\]
\[= \frac{N_{lm}}{2\sqrt{\pi}} \left( \int_0^{\pi/2} \frac{1}{\cos \theta} \exp(i\lambda z \ln \tan \theta) P^m_l(\cos \theta) d\theta \right)
\]
\[\pm \int_{\pi/2}^{\pi} \frac{1}{\sqrt{|\cos \theta|}} \exp(i\lambda z \ln |\tan \theta|) P^m_l(\cos \theta) d\theta \].
With help of the variable transformation \( \theta \to \pi - \theta \) in following integral,

\[
\int_{\pi/2}^{\pi} \frac{1}{\sqrt{\cos \theta}} \exp(i\lambda_z \ln |\tan \theta|) P_l^m(\cos \theta) d\theta = -\int_{\pi/2}^{0} \frac{1}{\sqrt{\cos \theta}} \exp(i\lambda_z \ln \tan \theta) P_l^m(-\cos \theta) d\theta
\]

\[
= \int_{0}^{\pi/2} \frac{1}{\sqrt{\cos \theta}} \exp(i\lambda_z \ln \tan \theta) P_l^m(-\cos \theta) d\theta,
\]

we have therefore for \( I_{lm}^+(\lambda_z) \),

\[
I_{lm}^+(\lambda_z) = \frac{N_{lm}}{2\sqrt{\pi}} \int_{0}^{\pi/2} \exp(i\lambda_z \ln \tan \theta) \left[ \frac{P_l^m(\cos \theta) + P_l^m(-\cos \theta)}{\sqrt{\cos \theta}} \right] d\theta
\]

\[
= \frac{N_{lm}}{2\sqrt{\pi}} \int_{0}^{\pi/2} \exp(i\lambda_z \ln \tan \theta) \left[ P_l^m(\cos \theta) + P_l^m(-\cos \theta) \right] \sqrt{\cos \theta} \sin \theta d\ln \theta
\]

\[
= \left[ 1 \pm (-1)^{l+m} \right] \frac{N_{lm}}{\sqrt{2}} \left( \int_{-\infty}^{\infty} \exp(i\lambda_z u) P_l^m\left( \frac{1}{\sqrt{1+e^{2u}}} \right) \frac{e^u}{(1+e^{2u})^{3/4}} du \right). \tag{24}
\]

In the last line we used a relation \( P_l^m(-x) = (-1)^{l+m} P_l^m(x) \) and introduced the variable transformation

\[
\ln \tan \theta \to u, \text{ or } \theta \to \arctan(e^u), \ (u \in (-\infty, \infty)).
\]

The result (24) is nothing but a Fourier transform of following function,

\[
\frac{N_{lm}}{\sqrt{2}} \left[ 1 \pm (-1)^{l+m} \right] P_l^m\left( \frac{1}{\sqrt{1+e^{2u}}} \right) \frac{e^u}{(1+e^{2u})^{3/4}}. \tag{26}
\]

Since the associated Legendre polynomial \( P_l^m(x) \) (18) are even or odd functions respectively corresponding to \( l + m \) being even or not, the integral \( I_{lm}^+(\lambda_z) = 0 \) with odd \( l + m \) and vice versa. Moreover, since for given quantum numbers \((l, m)\) the \( P_{l}^{-m}(x) \) and \( P_{l}^{m}(x) \) differ by a factor of constant, the pomson distribution densities for the pair of \( P_{l}^{-m}(x) \) and \( P_{l}^{m}(x) \) are the same. The explicit forms \( I_{lm}^+(\lambda_z) \) for the first six nontrivial results for \( P_{l}^{m}(x) \) are with \((l, m) = (0, 0); l = 1, m = 0, 1; \) and \( l = 2, m = 0, 1, 2, \)

\[
I_{00}^+(\lambda_z) = \frac{1}{\sqrt{2\pi}} \left\{ 2i \left\{ \frac{3}{2} \frac{1}{\lambda_z + i} F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{2}(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1 \right) \right. \\
\left. - \frac{i}{\lambda_z + i} F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{2}(\lambda_z + 1); 1/2(\lambda_z + 3); -1 \right) \right\}, \tag{27}
\]

\[
I_{10}^+(\lambda_z) = \frac{1}{4\lambda_z^2 + 2i\lambda_z + 6} \sqrt{\frac{3}{2\pi}} \left\{ -8\lambda_z^2 (2i\lambda_z + 15) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{2}(i\lambda_z + 1); \frac{1}{2}(i\lambda_z + 3); -1 \right) \\
+ (15 + 4\lambda_z(\lambda_z - i)) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{2}(i\lambda_z + 1); \frac{1}{2}(i\lambda_z + 3); -1 \right) \\
+ 4(3 + \lambda_z(\lambda_z + 2i)) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{4}(3 - 2i\lambda_z); \frac{1}{4}(7 - 2i\lambda_z); -1 \right) \\
- 2(7 + \lambda_z(4\lambda_z + 3i)) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{4}(3 - 2i\lambda_z); \frac{1}{4}(7 - 2i\lambda_z); -1 \right) \right\}, \tag{28}
\]

\[
I_{11}^+(\lambda_z) = \frac{1}{8} \sqrt{\frac{3}{\pi}} \left\{ \frac{1}{2\lambda_z + i} 4(4\lambda_z + 3i) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{4}(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1 \right) \\
- \frac{1}{2\lambda_z + i} 8(\lambda_z + 2i) F \left( \frac{3}{4}, \frac{1}{4}; \frac{1}{4}(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1 \right) \\
- e^{\frac{2\pi i}{4}} (9 + 4i\lambda_z) B_{-1} \left( \frac{1}{2}, \frac{3}{4} \right) + e^{\frac{2\pi i}{4}} (7 + 2i\lambda_z) B_{-1} \left( \frac{1}{2}, \frac{7}{4} \right) \right\}, \tag{29}
\]
\[ I_{20}^{+}(\lambda_z) = -\frac{1}{24} \sqrt{\frac{5}{2\pi}} \left\{ \frac{1}{\lambda_z - i} \frac{6(-2\lambda_z + 3i)_{2F1}}{\left(-\frac{1}{4}, \frac{1}{2} \frac{(i\lambda_z + 1); \frac{1}{2}(i\lambda_z + 3); -1} \right) + \frac{1}{\lambda_z - i} \frac{6(4\lambda_z - i)_{2F1}}{\left(-\frac{1}{4}, \frac{1}{2} \frac{(i\lambda_z + 1); \frac{1}{2}(i\lambda_z + 3); -1} \right) + \frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{1}{4}(5 - 2\lambda_z))} \frac{6(1 - i\lambda_z)_{2F1}}{\left(-\frac{1}{4}, \frac{1}{4} \frac{(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1} \right) + \frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{1}{4}(5 - 2\lambda_z))} 3(-1 + 4i\lambda_z)_{2F1}}{\left(-\frac{3}{4}, \frac{1}{4} \frac{(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1} \right) \right\}, \tag{30} \]

\[ I_{21}^{+}(\lambda_z) = \frac{1}{8} \sqrt{\frac{5}{3\pi}} \left\{ \frac{4(4\lambda_z + i)}{2\lambda_z + 3} \frac{3 \frac{1}{4} \frac{3(3 - 2i\lambda_z); \frac{1}{4}(7 - 2i\lambda_z); -1} \right) + 8(\lambda_z + 2i) \frac{\Gamma(\frac{3}{4})}{\Gamma\left(\frac{3}{4}(3 - 2i\lambda_z); \frac{1}{4}(7 - 2i\lambda_z); -1 \right) + e^{\frac{i\pi}{4}} (3 + 4i\lambda_z) B_{-1} \left(\frac{i\lambda_z}{2} + 1, \frac{1}{4}\right) + e^{\frac{i\pi}{4}} (5 + 4i\lambda_z) B_{-1} \left(\frac{i\lambda_z}{2} + 1, \frac{5}{4}\right) \right\}, \tag{31} \]

\[ I_{22}^{+}(\lambda_z) = \frac{1}{8(3 + \lambda_z(2\lambda_z - 5i))} \sqrt{\frac{5}{3\pi}} \left\{ \frac{7 + 4\lambda_z(\lambda_z - 3i)}{3} \frac{\Gamma(\frac{3}{4})}{\Gamma\left(\frac{3}{4}(3 - 2i\lambda_z); \frac{1}{4}(7 - 2i\lambda_z); -1 \right) + 4(3 + \lambda_z(\lambda_z - 2i)) \frac{\Gamma(\frac{3}{4})}{\Gamma\left(\frac{3}{4}(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1 \right) + \frac{(-7 + 2(-4\lambda_z + 5i)\lambda_z)}{3 \frac{1}{4} \frac{(i\lambda_z + 3); \frac{1}{2}(i\lambda_z + 5); -1} \right) + \frac{2(9 + (-4\lambda_z + 15i)\lambda_z)}{3 \frac{1}{4} \frac{(1 - 2i\lambda_z); \frac{1}{4}(5 - 2i\lambda_z); -1} \right) \right\}, \tag{32} \]

where \( F(a, b; c; x) \) is the hypergeometric function, and \( B_z(a, b) \) is incomplete Beta function of rank \( z \): \( B_z(a, b) = z^n \sum_{n=0}^{\infty} z^n \Gamma(n + 1 - b) / \Gamma(1 - b) n!(a + n) \). For an arbitrary \( I_{lm}^{+}(\lambda_z) \) with larger \( l \), \( m \), we observe that the expression has in general four terms but each of the coefficients before the hypergeometric functions becomes a ratio of two polynomials of \( \lambda_z \) with highest terms being not exceeding \( \lambda_z^7 \).

The probability distributions \( |I_{lm}^{+}(\lambda_z)|^2 \) for rotational states represented by spherical harmonics \( Y_{lm}(\theta, \varphi) \) are plotted for cases \( l = 0, \ l = 3, \) and \( l = 20 \) in Figures 1, 2, and 3, respectively. On the whole, they bear a striking resemblance to the momentum distributions of stationary states for the one-dimensional simple harmonic oscillator. It is perfectly understandable that from the force operator \( \hat{p}_z \equiv [\hat{p}_i, \hat{H}]/(\pi \hbar) = -\{x_i/r, \hat{H}\} \sim -x_i \) with \( \hat{H} \) being the rotational Hamiltonian, and \{\( U, V \)\} \equiv UV + VU. In other words, for a classical state, the force is restoring and proportional to the displacement, and the quantity \( x_i \hat{p}_i \) has thus a half period as \( x_i \) or \( p_i \) has.

### IV. CONCLUSIONS

The posmom \( Q_i \) offers a potential new way to understand the quantum motions of an atom and a molecule. This study explores the posmom on two-dimensional surface, and identify that the momentum in it is the geometric momentum that is recently proposed to properly describe the momentum for the constrained motions. From the commutation relations \([Q_i, L_i] = 0, \ (i = 1, 2, 3)\), we have three complete sets of commuting observables, and they are equivalent with each other upon a rotation of coordinates. Thus a novel dynamical representation based on two observables, \( \{Q_z, L_z\} \) in the present paper, is successfully constructed, and any states on the two-dimensional surface can go through a posmometry analysis. Because the free rotation is ubiquitous in microscopic domain, we carry out the posmom distributions of spherical harmonics. Results show that the posmometry bears a striking resemblance to the momentum distributions of stationary states for the one-dimensional simple harmonic oscillators, therefore riches our appreciation of the quantum dynamical behavior.
FIG. 1: Distribution density of \( \frac{x_i p_i + p_i x_i}{2} \) for the ground state of ground rotational state \( Y_{0,0} = \frac{1}{(\sqrt{4\pi})} \) (solid line), and the momentum distribution density for the ground state of one-dimensional simple harmonic oscillator (dashed line). They are almost identical. In all figures, the posmoms and the momenta are made dimensionless.

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FIG. 2: Distribution density of $(x_i p_{x_i} + p_{x_i} x_i)/2$ for the rotational states $Y_{lm}(\theta, \phi)$ with $l = 5$ and $m = 0, 1, 2, 3, 4, 5$, they have number of nodes = 2, 2, 1, 1, 0, 0 respectively. It is worthy of stressing that for a given set $(l, m)$, i.e. each curve in this figure, behaves like a stationary harmonic oscillator state.

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FIG. 3: Distribution density of $(x_ip_{x_i} + p_{x_i}x_i)/2$ for rotational state $Y_{20,0}(\theta, \varphi)$ (solid line), and the momentum distribution density for the 10th excited state of one-dimensional simple harmonic oscillator (dashed line). Since both probabilities in a small interval $\Delta \lambda_z$ are similar, they have the same classical limit: the simple harmonic oscillator.