Quantum-mechanical rotation of linear rigid body: (0)general properties of rigid bodies

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Abstract. Quantum-mechanical rotation of a linear rigid body is theoretically investigated in the context of the two-alpha-particle system of ^{8}Be. It is widely known that rigid rotors normally have six dynamical degrees of freedom, except for linear rigid bodies, i.e., a solid line connecting two particles, which have five degrees of freedom. As a result, the wave functions of the linear rigid body are reduced to the spherical harmonics rather than Wigner's D-function. A brief review is presented about the quantum-mechanical treatments of rigid rotors, and their general properties are discussed for the preparations of the study of the excited spectrum of ^{8}Be in terms of the the linear rigid body.

1. Introduction

Two-body systems are the simplest many-body system, but the study of these systems can provide us with plenty of insights about the genuine many-body problem. For instance, the Bohr model applied to the hydrogen atom is one of such examples resulting a success. A hydrogen atom consists of a proton and an electron, which is a two-body system interacting via the Coulomb force. With this model, one can understand why the spectrum is discrete and how atomic spectra follow such particular patterns of the level spacing, and so on. The new concepts such as the atomic shell structure induced from the model motivated physicists to make extended applications of the theory to more complicated atomic systems.

In the case of the nuclear many-body problem, deuterons should be regarded as the "basic" two-body system corresponding to hydrogen atoms in the atomic many-body problem. Deuteron is a nuclear system of a proton and a neutron[1] interacting through the bare nuclear two-body interaction including the tensor force, which breaks the angular momentum conservation. The system is stable but weakly bound. As a consequence, no excited states are observed so far, whereas a hydrogen atom presents a variety of excited states known as the Balmer series, Lyman series and Paschen series. Deuterons can be fragile against external influences that may cause rotations and vibrations.

[1] For unknown reasons yet, it is known that nuclear two-body systems of two protons, and of two neutrons do not exist in this universe, although such two-body correlations are anticipated to play a role in unbound and resonant states.

This nuclear two-body system can easily break up, so that they are dismissed for a consideration if such collective excitations are concerned.

Beryllium 8 (^{8}Be) contains eight nucleons (four protons and four neutrons). However, it is believed to be well approximated as a two-body system of the alpha particles. The alpha particle is a nucleus of Helium 4 (^{4}He), which is the second lightest element in the universe. Its constituent particles are two protons and two neutrons. The binding energy of the alpha particle is exceptionally large (about 28 MeV) in comparison with other nuclei (the average nuclear binding energy is roughly 8 MeV). This tightly-bound many-body system can be hence regarded as a "particle", as Rutherford anticipated in the first place when they discovered the alpha rays emitted from radioactive materials. In terms of the alpha particles, one can consider that ^{8}Be consists of two alpha particles, or the two-alpha system. If such an approximation is admitted to be valid, then ^{8}Be can be viewed as the basic system possessing excited states, which may enable further and more profound understanding of the structure of nuclear many-body systems.

However, one may feel unfortunate to hear that ^{8}Be has no bound state, although it is "just" unbound. The total mass of two alpha particles are only 92 keV smaller than the ground state of ^{8}Be, so that one can say that these two states are almost "degenerate" in energy. The half-life time is estimated to be of the order of 10^{-2} fs [2], which is significantly longer than the elapse time for two alpha particles to pass by at the relative velocity equal to the speed of light, that is, $4R_\alpha/c \simeq 2.2 \times 10^{-8}$ fs (R_α is the radius of the alpha particle and it was recently measured to be 1.68 fm[1]. The speed of light is denoted as c). With this near-stability, ^{8}Be shows rich excited spectra in the continuum on top of its "just-unbound" ground state, which can attract interests of many physicists with their delight. A special attention may be made here that in such unbound excited spectrum one can find a rotational-like band connected through E2 (i.e., electric quadrupole) transitions. There are arguments whether this spectrum can be really interpreted as a rotational band or not[2].

There are varieties of criteria for judging if a given series of spectra can be interpreted as a rotational band. When a nucleus of interest can "rotate", at least, from a theoretical point of view, the nuclear many-body Hamiltonian must be approximated well to the following form

$$H \simeq H_{\mathrm{intr}} + H_{\mathrm{coll}}, \tag{1}$$

where H_{intr} and H_{coll} are part of the Hamiltonian depending on the intrinsic (single-particle) and

[2] A way of estimation is presented in Appendix.

collective degrees of freedom, respectively. In general, these two types of degrees of freedom are coupled through the interaction term V. The smaller V is, the better the interpretation of nuclear rotation is. The decoupling limit can also be understood as the adiabatic approximation to the dynamics of the single-particle motions against the collective motions. In the adiabatic approximation, the collective and intrinsic dynamics can be separately handled. The collective part can be treated as a "rigid rotor", while the intrinsic part can be described in terms of the mean-field theory. The direct products of the collective and intrinsic states can be assigned as the members in the rotational band.

In the case of ^{8}Be, the intrinsic states should be expressed as an interacting system of two alpha particles, which can be easily solved once the effective interaction among the alpha particle is given. The Buck potential is one of such phenomenological interactions aimed at the approximation to the inter-alpha-particle force. Whereas, the collective states can be represented as a quantisation of a rigid rotor, which is normally expressed in terms of Wigner's D-function. However, the mass distribution of ^{8}Be allows one to employ the spherical harmonics in descriptions of the collective part of ^{8}Be, because the shape of the nucleus can be regarded as a linear rigid body, the special case of the rigid bodies.

The investigation of the "rotational" band of ^{8}Be thus needs to be divided into two parts: one for the collective motions and the other for the intrinsic motions. The former is taken into consideration in the present paper while the latter will be presented elsewhere to follow.

2. Physics of rigid bodies as a collective dynamics

If the decoupling between the collective and intrinsic degrees of freedom is justified to a good approximation, the collective dynamics can be described by means of rotations of a rigid body[3].

The number of degrees of freedom is six in total for a rigid body[4]. Due to the Galilean symmetry, the effective degrees of freedom can be reduced to be three, which correspond to rotational angles of the rigid body. Through time dependency of these angles, the dynamics of the rigid body is expressed in classical mechanics through the Euler equations. The angular momentum vector is then introduced as the canonical variables to the angles. In quantum mechanics, energy rather than time is chosen for the description of rotational motions, so that Hamiltonian corresponding to the

[3] On the contrary, if the coupling is expected, not only rotations but also surface vibrations need to be taken into account. This is because the intrinsic motions may cause the structure or "shape" of the mean field.

[4] Details are given in Appendix why only six degrees of freedom can describe the motions of a rigid body.

kinetic energy of the rigid body are considered in the following form

$$H_{\mathrm{coll}} = \sum_{i=1}^{3} \frac{I_k^2}{2\mathcal{J}_k}, \tag{2}$$

where I_k and $\mathcal{J}_k$ are the k-th component of angular momentum and moment of inertia. This expression is obtained after the principal axes are chosen to be the axes of the body-fixed coordinates, which can be always done for the quadratic form.

Quantisation of this collective Hamiltonian was achieved independently by Casimir and Wigner[3]. They chose the first non-trivial situation where collective rotation is possible, which means rigid bodies with deformation into the axial symmetry.

3. Quantum mechanical rotations

Rotational motions in classical mechanics are literally "motions", that is, one can observe objects of interests moving around and changing their positions in time. This means that dynamical variables are functions of time. In quantum mechanics where energy is chosen for the description of quantum states, the relevant dynamics is not described as a function of time. In other words, if one looks at quantum rotation, it does not "move". Instead, it is represented as a superposition of states pointing at different "directions". However, it is angular momenta rather than orientation angles that is used for dynamical variables in quantum mechanical rotations. The Heisenberg uncertainty principle does not allow to specify the accurate directions at which the rigid body points, so that angular momentum is more convenient theoretically. In addition, the Hamiltonian commutes with the angular momentum operators, so that it is natural to employ a set of basis associated with angular momentum.

Angular momentum operators I_x, I_y, I_z do not commute with each other, but follows the following commutations relations

$$[I_x, I_y] = i\hbar I_z \quad \text{(with cyclic permutations for indices).} \tag{3}$$

On the contrary, the total angular momentum operators $I^2 = I_x^2 + I_y^2 + I_z^2$ commutes with any of the components of angular momentum

$$\left[I^2, I_x\right] = \left[I^2, I_y\right] = \left[I^2, I_z\right] = 0 \tag{4}$$

Therefore, the angular momentum basis can be specified by the eigenvalues of the total angular momentum I^2 and one of the components (normally chosen for I_z), hence

$$I^2|IM\rangle = I(I+1)\hbar^2|IM\rangle, \quad I_z|IM\rangle = M\hbar|IM\rangle. \tag{5}$$

It is possible to demonstrate [5]that the Hamiltonian commutes with the total angular momentum

$$\left[H_{\text{coll}}, I^2\right] = 0. \tag{6}$$

The eigenstates of the collective Hamiltonian are thus the simultaneous eigenstates with those of the total angular momentum.

As for the commutation relation with the angular momentum for the quantisation axis (it is I_z in the present case), it is calculated as [6]

$$[H_{\text{coll}}, I_3] = \frac{1}{2}\left(\frac{1}{\mathcal{J}_2} - \frac{1}{\mathcal{J}_1}\right)(2I_1 I_2 - i\hbar I_3), \tag{7}$$

so that a mixture is expected in general with respect to the M quantum number (an exception is the case when $\mathcal{J}_1 = \mathcal{J}_2$, which corresponds to the axially-symmetric deformation).

In this way, the collective eigenstates can have a general form

$$|\Psi^I_{\text{coll}}\rangle = \sum_{M=-I}^{I} C_M |IM\rangle, \tag{8}$$

and the following eigenvalue equations are satisfied.

$$H_{\text{coll}}|\Psi^I\rangle = E^I|\Psi^I\rangle, \tag{9}$$

$$I^2|\Psi^I\rangle = I(I+1)\hbar^2|\Psi^I\rangle. \tag{10}$$

"Quantum rotations" are produced with the rotational operator

$$R(\theta\phi\chi) = \exp\left(-i\chi\boldsymbol{n}(\theta\phi)\cdot\boldsymbol{I}\right), \tag{11}$$

as

$$|\Psi^I_{\text{coll}}(\theta\phi\chi)\rangle = R(\theta\phi\chi)|\Psi^I_{\text{coll}}\rangle. \tag{12}$$

One should note that this "rotation" is not a type of "rotation" seen in classical mechanics, that is, the time-dependent motions described by the angle variables. The quantum rotation introduced above should be understood as mathematical properties of quantum states with respect to the rotational transformation.

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[5] A proof is given in Appendix.
[6] See Appendix for details.

3.1 Collective states with spherical symmetry

Let us consider the rotation of the spherical collective state. For an infinitesimal rotation $|\chi| \ll 1$, we have

$$R(\theta\phi\chi)|\Psi^I_{\mathrm{coll}}\rangle \simeq \{1 - i\chi\boldsymbol{n}(\theta\phi)\cdot\boldsymbol{I}\}\,|\Psi^I_{\mathrm{coll}}\rangle. \tag{13}$$

If $|\Psi^I_{\mathrm{coll}}\rangle$ has the spherical symmetry, then the second term in the right of the above equation needs to vanish whatever χ is.

First of all, the raising and lowering operators $I_\pm = I_x \pm iI_y$ are introduced here, which satisfy

$$I_\pm|IM\rangle = \sqrt{(I \mp M)(I \pm M + 1)}\hbar|IM \pm 1\rangle. \tag{14}$$

Then, let us rewrite the second term in terms of the raising and lowering operators. Using

$$n_xI_x + n_yI_y = n_x\frac{I_+ + I_-}{2} + n_y\frac{I_+ - I_-}{2i} = \frac{n_x - in_y}{2}I_+ + \frac{n_x + in_y}{2}I_-, \tag{15}$$

we have

$$\begin{aligned}\boldsymbol{n}\cdot\boldsymbol{I}|IM\rangle =& \frac{n_x - in_y}{2}\sqrt{(I-M)(I+M+1)}\hbar|IM+1\rangle + \frac{n_x + in_y}{2}\sqrt{(I+M)(I-M+1)}\hbar|IM-1\rangle \\ &+ n_zM\hbar|IM\rangle.\end{aligned} \tag{16}$$

When $M = I$, we have

$$\boldsymbol{n}\cdot\boldsymbol{I}|II\rangle = \frac{n_x + in_y}{2}\sqrt{2I}\hbar|II-1\rangle + n_zI\hbar|II\rangle. \tag{17}$$

When $M = I - 1$, we have

$$\boldsymbol{n}\cdot\boldsymbol{I}|II-1\rangle = \frac{n_x - in_y}{2}\sqrt{2I}\hbar|II\rangle + \frac{n_x + in_y}{2}\sqrt{2(2I-1)}\hbar|II-2\rangle + n_z(I-1)\hbar|II-1\rangle. \tag{18}$$

The $|II\rangle$ component in $|\Psi^I_{\mathrm{coll}}(\theta\phi\chi)\rangle$ has its coefficient as

$$\hbar\left(C_In_zI + C_{I-1}\frac{n_x - in_y}{2}\sqrt{2I}\right) \tag{19}$$

which needs to be zero whatever values (n_x, n_y, n_z) are. This condition is satisfied only for $I = 0$, and $M = 0$ is automatically determined in this case. In other words, the collective state with the spherical symmetry must have only one component $(I, M) = (0, 0)$. This result implies that a quantum state with the rotational symmetry cannot "rotate" (i.e., has no angular momentum).

One cannot thus specify the orientation of the spherical states, or fluctuations of the orientation is extremely large. From the viewpoint of the Heisenberg uncertainty principle, the fluctuation in angular momentum is expected to be zero instead, hence the collective states with the spherical symmetry results in an eigenstate $|00\rangle$.

3.2 Collective Hamiltonian with spherical symmetry

When all the moments of inertia are equal, the collective Hamiltonian has the rotational symmetry (i.e., spherical symmetry). Putting $\mathcal{J}_0 = \mathcal{J}_x = \mathcal{J}_y = \mathcal{J}_z$, the Hamiltonian reads

$$H_{\rm coll} = \frac{I^2}{2\mathcal{J}_0} \to \frac{I(I+1)\hbar^2}{2\mathcal{J}_0}. \tag{20}$$

The last expression is a C-number, or an eigenvalue, which can be obtained when the angular momentum eigenstates are operated to the Hamiltonian. Because the collective Hamiltonian commutes with the total angular momentum, the collective Hamiltonian can be always treated as a C-number in the presence of the spherical symmetry. Note that the M quantum number does not appear in the Hamiltonian, which means that all the $2I+1$ states of $|IM\rangle$ for $M = I, I-1, \cdots, -I+1, -I$ are energetically degenerate.

It is obvious, but the ground state is $|00\rangle$, which has the spherical symmetry. This state does not "rotate" as discussed above. Excited states have non-zero values for angular momentum ($I \neq 0$) and there are $2I+1$ degeneracy for a given states labelled with I.

Let us estimate the energy scale for rotation asociated with the *spherical* rigid body. The moment of inertia for a spherical rigid body is given as $\mathcal{J}_0 = \frac{2}{5}mr^2$, where m and r is the mass and radius of the sphere. Because the nuclear mass is roughly $m = m_N A$ (m_N is the nucleon mass) and the nuclear radius is given phenomenologically as $r = r_0 A^{1/3}$ where $r_0 = 1.2$ fm, the moment of inertia is estimated

$$\mathcal{J}_0 = \frac{2}{5}(m_N A)\cdot(r_0 A^{1/3})^2 = \frac{2}{5}m_N r_0^2 A^{5/3}. \tag{21}$$

The scale for the rotational energy is then evaluated as

$$\frac{\hbar^2}{2\mathcal{J}_0} = \frac{5}{4}\frac{(\hbar c)^2}{m_N c^2 r_0^2}A^{-5/3} \simeq \frac{5}{4}\frac{(197)^2}{(1.0\times 10^3)(1.2)^2}A^{-5/3} \sim 34A^{-5/3} \quad \text{(MeV)}, \tag{22}$$

where the mass energy for a nucleon is assumed to be $m_N c^2 = O(1\text{GeV})$.

For the alpha particle ($A = 4$), the rotational energy scale is calculated to be about 15 MeV, which is far larger than the typical rotational excitations. For instance, $I = 2$ states are expected to be found at $E = 6 \times 15 = 90$ MeV. These states should be interpreted as "highly excited states", rather than "low-lying collective states", which are normally regarded as "rotational" states.

3.3 Collective states with axial symmetry

Because the spherically symmetric rigid bodies produce "no rotation" in their ground state $|00\rangle$ and are not placed in the low-energy regions where typical rotational bands are seen, deformed rigid bodies need to be taken into account for nuclear collective rotation.

The simplest deformed case can be obtained by imposing $\mathcal{J}_x = \mathcal{J}_y$, or axial symmetry (for the z axis in this choice). Now, the collective Hamiltonian is expressed as

$$H_{\rm coll} = \frac{I_x^2 + I_y^2}{2\mathcal{J}_x} + \frac{I_z^2}{2\mathcal{J}_z} = \frac{I^2}{2\mathcal{J}_x} + \frac{1}{2}\left(\frac{1}{\mathcal{J}_z} - \frac{1}{\mathcal{J}_x}\right) I_z^2 \rightarrow \frac{I(I+1)\hbar^2}{2\mathcal{J}_x} + \frac{\hbar^2}{2}\left(\frac{1}{\mathcal{J}_z} - \frac{1}{\mathcal{J}_x}\right) M^2. \quad (23)$$

The energy spectrum for given I will splits into $M+1$, and the degeneracy due to the spherical symmetry is broken by the axial deformation. However, still two-fold degeneracy $(M, -M)$ remains. In manu cases, the rotational energy around the axes perpendicular to the axial-symmetry axis is lower than the symmetry axis, that is, $\mathcal{J}_z < \mathcal{J}_x$, so that the second term in the collective Hamiltonian has the positive sign. This means that the lowest state for given I is $|I0\rangle$, which can be interpreted that the collective rotation is possible around the axes perpendicular to the symmetry axis.

Now, it is clear that the collective Hamiltonian with the axial symmetry commutes not only with the total angular momentum but also with the component of the symmetry axis (I_z in the present case). The quantum states for a rigid body with the axial symmetry is thus expressed as

$$|\Psi^{I,K}_{\rm coll}\rangle = |IK\rangle. \quad (24)$$

This states can be "rotated" with the rotational operator

$$|\Psi^{I}_{\rm coll}(\theta\phi\chi)\rangle = R(\theta\phi\chi)|\Psi^{I,K}_{\rm coll}\rangle = R(\theta\phi\chi)|IK\rangle. \quad (25)$$

Because rotation mixes the K quantum number, the rotated collective state are not the eigenstate of $|IK\rangle$. With the completeness of the angular momentum basis,

$$\begin{aligned} |\Psi^{I}_{\rm coll}(\theta\phi\chi)\rangle &= \sum_{M=-I}^{I} |IM\rangle\langle IM|R(\theta\phi\chi)|IK\rangle \\ &= \sum_{M} D^{I}_{MK}(\theta\phi\chi)|IM\rangle, \end{aligned} \quad (26)$$

where the expansion coefficient $D^{I}_{MK}(\theta\phi\chi)$ is called "Wigner's D function".

4. ^{8}Be and the linear rigid body

As mentioned earlier, ^{8}Be is a nucleus consisting of eight nucleons, but can be considered as a two-alpha system. In the limit that the alpha particle is a point particle, the collective part of ^{8}Be can be regarded as a linear rigid body carrying only five degrees of freedom. However, we should keep in mind that the radius of the alpha particle is recently measured to be 1.68 fm [1], so that it is not a point particle. In addition, recent calculations by means of the alpha-cluster model numerically show that there is a spatial overlap between the two alpha particle in the ground state of ^{8}Be. The distance between the centres of mass of the alpha particles is about 3 fm, so that the spatial overlap is estimated to be 1.38 fm. The actual shape of ^{8}Be cannot be well approximated by a linear rigid body, as a matter of fact. Nonetheless, what is aimed at here is a qualitative and intuitive understanding of the possible rotation of ^{8}Be. We thus stick with the linear rigid-body collective model in this paper.

Out of the five degrees of freedom possessed by the linear rigid body, three are assigned for the centre-of-mass coordinates as seen in the general cases of rigid bodies. The angular variables thus have only two degrees of freedom. The rod-like shape of the linear rigid body provides only two angles to specify the orientation. In comparison with the general rigid body, one angle becomes redundant, which must be the rotation around the axis of the "rod".

Wigner converted his D function with the orientation representation from $(\theta\phi\chi)$ to the Euler angles $(\alpha\beta\gamma)$, together with the conversion of the rotational operator

$$R(\alpha\beta\gamma) = \exp(-i\alpha I_z)\exp(-i\beta I_y)\exp(-i\gamma I_z), \tag{27}$$

as

$$D^I_{M'M}(\alpha\beta\gamma) = \langle IM'|R(\alpha\beta\gamma)|IM\rangle. \tag{28}$$

Corresponding to the redundancy in the linear rigid body, one may fix γ to be zero, to have the following relation between Wigner's D function and the spherical harmonics

$$Y_{lm}(\beta\alpha) = \sqrt{\frac{2l+1}{4\pi}}D^{l*}_{m0}(\alpha,\beta,0). \tag{29}$$

This relation means that the quantum-mechanical rotation of the linear rigid body can be expressed in terms of the spherical harmonics.

When the two-body problem is considered, the Schrödinger equation can be separated into the Centre-of-mass and relative coordinates. As a result, the equation is reduced to be the one-body problem in three-dimensional space. The one-body Schrödinger equation in three-dimensional space can be then separated further into the radial and angular coordinates. It is known that the angular part of the wave function is nothing but the spherical harmonics. As seen in the hydrogen atom, the wave function describes the "shape" of the system and the spherical harmonics carries the information about the "deformation" of the system.

It is very interesting to know that the quantum rotation of the linear rigid body can be expressed as a product of the collective wave function, which is the spherical harmonics, and the intrinsic wave function, which is also the spherical harmonics. In other words, the nuclear deformation and rotation are described with the same mathematical functions. Nuclear deformation is related closely to the mean field, which can be a reflection of the intrinsic degrees of freedom. From this mathematical properties, it can be theoretically anticipated that these two types of degrees of freedom can be "mathematically" mixed even if they are well decoupled from a physical viewpoint.

5. Conclusion

A theoretical consideration is given for the eight-nucleon system of Beryllium 8 (^{8}Be) by assuming that the system can be approximated as a two-alpha system, at least, from a qualitative point of view. The decoupling limit is employed so as to allow the adiabatic rotation of ^{8}Be. As a consequence, the collective and intrinsic parts can be taken into account separately, and the former is exclusively studied in this paper. In association with the possible rotational band in ^{8}Be, the physical meaning of quantum rotations is reviewed briefly from a rigid-body perspective. It is learned that Wigner's D function and the spherical harmonics are related with each other when the linear rigid body is concerned.

A possible superposition or mixing between the intrinsic and collective degrees of freedom is expected "by chance" through a mathematical similarity, rather than physical processes and consequences. An investigation whether such a new type of "mixing" is possible or not will be carried out in the next study, which will be planned in the near future.

Appendix

1. A way to estimate the half-life time of unbound states

Nuclear resonances, which are unbound but have a finite life time, have an energy width Γ, which is related to the half life $\tau_{1/2}$ through the uncertainty principle, $\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$. This inequality can be interpreted as $\Gamma \cdot \tau_{1/2} \simeq \frac{\hbar}{2}$, so that the half life can be estimated to be

$$\tau_{1/2} \simeq \frac{1}{2}\frac{\hbar}{\Gamma}. \quad \text{(A1)}$$

In nuclear physics, the Planck constant $\hbar$ should be expressed in the unit of MeV·fs, which results in

$$\tau_{1/2} = 0.5 \times \frac{6.58 \times 10^{-7}}{\Gamma} \quad \text{(fs)}, \quad \text{(A2)}$$

if Γ is provided in the unit of MeV.

The ground state (0^+) of ^{8}Be has a very narrow width $\Gamma = 5.57$ eV ($= 5.57 \times 10^{-6}$ MeV), which gives rise to an estimation $\tau_{1/2} \simeq 6.0 \times 10^{-2}$ fs. On the contrary, the other members in the "rotational" band have larger widths, $\Gamma = 1.513$ MeV and 3.5 MeV respectively for the 2^+ and 4^+ states. The corresponding estimates are calculated to be $\tau_{1/2} \simeq 2.2 \times 10^{-7}$ fs and $\tau_{1/2} \simeq 9.4 \times 10^{-8}$ fs, respectively. The half lives of the excited states are only slightly longer than the "passing-by time", which is given in the main text as $4R_\alpha/c = 2.2 \times 10^{-8}$ fs, and are far shorter than the estimated half life of the ground state.

2. The number of degrees of freedom of a rigid body

Rigid bodies in classical mechanics are supposed to be a special case of classical many-body systems. Consider N particles in which the mutual distances are all fixed to certain values, $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. With this constraints, it can be demonstrated that this N-body system has only six degrees of freedom in general, which is the number of degrees of freedom for a rigid body. The number of degrees of freedom for a rigid body can be counted with a method of induction applied to N-particle systems.

When $N = 1$, the corresponding system is a particle in the three-dimensional space, hence the total number of degrees of freedom is three. The $N = 2$ case is the simplest rigid body. Two particles carry six degrees of freedom ($6 = 3 \times 2$), but their distance r_{12} is fixed. This condition reduces the effective degrees of freedom by one, therefore the total number of degrees freedom is five ($5 = 6 - 1$). In the same way, the number of degrees of freedom for $N = 3$ can be evaluated to be six ($6 = 3 \times 3 - 3$) because the constraints are imposed for r_{12}, r_{23} and r_{31}. With these three particles, a triangular plane is formed in general (except the case when the three particles are placed along a line). The plane can be considered as the body-fixed xy plane and the normal vector to the plane can be regarded as the z axis in the body-fixed frame. In this way, an intrinsic Cartesian coordinate system can be set as the body-fixed frame. At $N = 4$, the fourth particle's position must be fixed with respect to the body-fixed frame formed by the other three particles. Hence the three constraints for x, y and z in the intrinsic coordinates are imposed. Therefore, an addition of a particle to the $N = 3$ rigid body produces three more degrees of freedom due a presence of a particle, but these degrees of freedom are cancelled by the three constraints. As a result, we have $6 = 6 + 3 - 3$ for the $N = 4$ rigid body. For $N \geq 4$, the same argument can be applied repeatedly, hence the number of degrees of freedom remains to be fixed to 6. This result should be interpreted as the general cases for the number of degrees of freedom for the finite N. Finally, the continuum rigid body can be obtained as the limit $N \to \infty$, so that it is concluded that a rigid body has six dynamical degrees of freedom.

The six degrees of freedom of a rigid body can be decomposed into $3+3$. The first three degrees of freedom are for the centre-of-mass coordinates, but they can be neglected as a dynamical variables, thanks to the Galilean invariance in the non-relativistic equation of motion. The remaining three describe the genuine dynamics of the rigid body. They corresponds to three angles to specify which direction the rigid body faces. For example, the Euler angles can be employed as the dynamical variables for the motion of a rigid body.

The linear rigid body corresponds to the $N = 2$ case, where the total degrees of freedom is five. The five degrees of freedom are decomposed into $3 + 2$. The first three are for the centre-of-mass variables, while the remaining two corresponds to the rotational angles of the linear rigid body. Even if there are more than three particles to form a rigid body, it can be a linear rigid body when all the particles are placed along a line. In other words, a rod-shaped rigid body can be classified as a linear rigid body.

3. Commutation relation between the rigid-rotor Hamiltonian and the total angular momentum

First of all, we have

$$\left[H_{\rm coll}, I^2\right] = \left[\sum_{k=1}^{3} \frac{I_k^2}{2\mathcal{J}_k}, I^2\right] = \sum_k \frac{1}{2\mathcal{J}_k}\left[I_k^2, I^2\right] \tag{C1}$$

With an identity $[AB, C] = A[B, C] + [A, C]B$, we have

$$\left[I_k^2, I^2\right] = I_k\left[I_k, I^2\right] + [I_k, I^2]I_k, \tag{C2}$$

which turns to be zero because I_k and I^2 commute with each other.

4. Commutation relation between the rigid-rotor Hamiltonian and the angular momentum component

$$[H_{\rm coll}, I_k] = \left[\sum_{k'=1}^{3} \frac{I_{k'}^2}{2\mathcal{J}_{k'}}, I_k\right] = \sum_{k'} \frac{1}{2\mathcal{J}_{k'}}\left[I_{k'}^2, I_k\right] \tag{D1}$$

With the identity above, we have

$$\begin{aligned}\left[I_{k'}^2, I_k\right] =& I_{k'}\left[I_{k'}, I_k\right] + [I_{k'}, I_k]I_{k'} \\ =& i\hbar\sum_q \epsilon_{k'kq}\left(I_{k'}I_q + I_qI_{k'}\right) \\ =& i\hbar\sum_q \epsilon_{k'kq}\left(2I_{k'}I_q - i\hbar\sum_{q'}\epsilon_{k'qq'}I_{q'}\right)\end{aligned} \tag{D2}$$

When $k=3(=z)$, we have

$$
\begin{aligned}
\left[I_{k'}^2, I_3\right] =& i\hbar\sum_q \epsilon_{k'3q}\left(2I_{k'}I_q - i\hbar\sum_{q'}\epsilon_{k'qq'}I_{q'}\right) \\
=& i\hbar\epsilon_{k'31}\left(2I_{k'}I_1 - i\hbar\sum_{q'}(\epsilon_{k'1q'}I_{q'})\right) + i\hbar\epsilon_{k'32}\left(2I_{k'}I_2 - i\hbar\sum_{q'}(\epsilon_{k'2q'}I_{q'})\right) \\
=& i\hbar\epsilon_{1k'3}\left(2I_{k'}I_1 + i\hbar\sum_{q'}(\epsilon_{1k'q'}I_{q'})\right) - i\hbar\epsilon_{k'23}\left(2I_{k'}I_2 - i\hbar\sum_{q'}(\epsilon_{k'2q'}I_{q'})\right) \\
=& \begin{cases} -i\hbar\left(2I_1I_2 - i\hbar I_3\right) \quad (k'=1) \\ i\hbar\left(2I_2I_1 + i\hbar I_3\right) = i\hbar(2I_1I_2 - i\hbar I_3) \quad (k'=2) \\ 0 \quad (k'=3) \end{cases} .
\end{aligned}
\tag{D3}
$$

Therefore,

$$
[H_{\rm coll}, I_3] = \frac{1}{2}\left(\frac{1}{\mathcal{J}_2} - \frac{1}{\mathcal{J}_1}\right)\left(2I_1I_2 - i\hbar I_3\right). \tag{D4}
$$

In the similar way, we have

$$
[H_{\rm coll}, I_1] = \frac{1}{2}\left(\frac{1}{\mathcal{J}_3} - \frac{1}{\mathcal{J}_2}\right)\left(2I_2I_3 - i\hbar I_1\right). \tag{D5}
$$

$$
[H_{\rm coll}, I_2] = \frac{1}{2}\left(\frac{1}{\mathcal{J}_1} - \frac{1}{\mathcal{J}_3}\right)\left(2I_3I_1 - i\hbar I_2\right), \tag{D6}
$$

or we can summarise the above result as

$$
[H_{\rm coll}, I_i] = \frac{1}{2}\left(\frac{1}{\mathcal{J}_j} - \frac{1}{\mathcal{J}_k}\right)\left(i\hbar I_i - 2I_jI_k\right), \tag{D7}
$$

where the indices (i, j, k) can be re-ordered in a cyclic permutation.

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