Collapse-induced Orientational Localization of Rigid Rotors

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We show how the ro-translational motion of anisotropic particles is affected by the model of Continuous Spontaneous Localization (CSL), the most prominent hypothetical modification of the Schrödinger equation restoring realism on the macroscale. We derive the master equation describing collapse-induced spatio-orientational decoherence, and demonstrate how it leads to linear- and angular-momentum diffusion. Since the associated heating rates scale differently with the CSL parameters, the latter can be determined individually by measuring the random motion of a single levitated nanorotor.

I. INTRODUCTION

It is an open question whether the quantum superposition principle holds at arbitrary length and mass scales. Its validity has been confirmed for increasingly large particles and distances by interference experiments involving single neutrons and atoms [11,14], Bose-Einstein condensates [5,10], and massive molecules [11,15]. By direct verification of quantum superpositions [17,18] provide a dynamical description of the wave function collapse through an objective modification of the Schrödinger equation. One of the most prominent collapse theories is the continuous spontaneous localization (CSL) model [19–21]. By adding a nonlinear and stochastic term to the Schrödinger equation it describes the random localization of the wave function of a delocalized particle. The modification involves two parameters, the random localization of the wave function of a delocalized particle. The modification is motivated by recent advances in optical trapping and control of the nanoparticle [27,28]. Motivated for bodies with cylindrical and spheroidal shape.

Specifically, we present the master equation describing the impact of CSL on the ro-translational quantum dynamics of a rigid nanoparticle. The associated localization rate for orientational superpositions is then evaluated for bodies with cylindrical and spheroidal shape. We determine the resulting linear momentum and angular momentum diffusion constants quantifying the rate of motional heating. Their dependence on the CSL parameters implies that the anisotropic shape of a nanoparticle can be exploited in future CSL tests. Finally, by solving the master equation for planar rotations we show how CSL leads to an enhanced spread of the orientational wave packet dynamics.

II. SPATIO-ORIENTATIONAL LOCALIZATION

All observable effects of CSL are accounted for by considering the modified time evolution of the state operator, \( \partial_t \rho = -i[H, \rho]/\hbar + \mathcal{L} \rho \). The modification \( \mathcal{L} \rho \) to the von Neumann equation can be cast in Lindblad form as

\[
\mathcal{L} \rho = -\frac{\lambda_{\text{C}}}{2r_{\text{C}}^2} \int d^3s \left[ M(s), [M(s), \rho] \right].
\]

The mass operators \( M(s) \) depend on the position operators \( r_n \) and masses \( m_n \) of the constituent atoms,

\[
M(s) = \sum_n m_n e^{-(s-r_n)^2/2r_{\text{C}}^2}.
\]

A. Master equation for a rigid body

The position of the individual atoms can be specified by the center-of-mass position \( R_{\text{cm}} \), the orientation \( \Omega \) (parameterized e.g. with Euler angles) and the displacements \( \Delta r_n \) from the orientation-dependent equilibrium position \( R(\Omega)r_n^{(0)} \), i.e., \( r_n = R_{\text{cm}} + R(\Omega)r_n^{(0)} + \Delta r_n \). Here, the matrix \( R(\Omega) \) rotates from the body-fixed frame to the space-fixed frame \( \{ e_1, e_2, e_3 \} \). If the displacements \( \Delta r_n \)
of the individual atoms around their equilibrium position are small compared to \( r_c \) it is admissible to describe the particle as a rigid body with position \( \mathbf{R}_{cm} \) and orientation \( \Omega \).

Denoting the mass density by \( \varrho[\mathbf{R}^T(\Omega)] = \sum_n m_n \delta[\mathbf{R}^T(\Omega) - \mathbf{r}_n(0)] \), and the position and orientation operators as \( \mathbf{R}_{cm} \) and \( \Omega \), one can rewrite the mass operator \( \mathbf{M}(\mathbf{s}) \) as

\[
\mathbf{M}(\mathbf{s}) \approx \int d^3 \mathbf{r} \varrho[\mathbf{R}^T(\Omega)] e^{-(\mathbf{s} - \mathbf{R}_{cm})^2/2}.
\]

\[
= \frac{r^3_c}{(2\pi)^{3/2}} \int d^3 k e^{-r^2_c k^2/2} \mathbf{L} \mathbf{k} e^{ik \mathbf{R}_{cm}}.
\]

The Fourier transform of the mass density \( \tilde{\varrho}(\mathbf{k}) \), often referred to as form factor, is normalized to the total mass of the particle, \( \tilde{\varrho}(0) = M \).

The re-translational master equation is obtained by inserting the mass operators (3) into Eq. (1). Its incoherent part takes the form

\[
\mathbf{L} \rho = \frac{r^2_c \lambda C}{\pi^{3/2} m_0} \int d^3 \mathbf{k} e^{-r^2_c k^2} 
\times \left[ e^{-ik \mathbf{R}_{cm}} \tilde{\varrho}[\mathbf{R}^T(\Omega) \mathbf{k}] \rho \tilde{\varrho}^*[\mathbf{R}^T(\Omega) \mathbf{k}] e^{ik \mathbf{R}_{cm}} 
- \frac{1}{2} \left\{ |\tilde{\varrho}[\mathbf{R}^T(\Omega) \mathbf{k}]|^2 , \rho \right\} \right].
\]

(4)

Being diagonal in position and orientation it describes spatio-orientational decoherence. Evaluating the matrix elements \( \langle \mathbf{R}_{cm} | \mathbf{L} | \mathbf{R}_{cm}' \rangle \Omega' \) one finds that the decay of the spatial off-diagonal elements depends not only on the distance \( |\mathbf{R}_{cm} - \mathbf{R}_{cm}'| \) but also on the direction of displacement. We will see next that the decay of orientational coherences depends only on the relative orientation \( \Omega(\Omega', \Omega) \) defined by \( \mathbf{R}(\Omega') = \mathbf{R}(\Omega') \mathbf{R}(\Omega) \).

### B. Orientational Localization

Tracing out the center-of-mass degrees of freedom in Eq. (4) shows how pure orientational superpositions decay under the CSL modification. Specifically, the localization rate \( F(\Omega, \Omega') \), defined as

\[
\langle \Omega | \mathbf{L} \mathbf{R}_{cm} | \Omega' \rangle = - F(\Omega, \Omega') \langle \Omega | \mathbf{L} | \mathbf{R}_{cm} | \Omega' \rangle \ , \quad (5)
\]

is given by

\[
F(\Omega, \Omega') = \frac{r^3_c \lambda C}{2\pi^{3/2} m_0^{3/2}} \int d^3 \mathbf{k} e^{-r^2_c k^2} 
\times |\tilde{\varrho}[\mathbf{R}^T(\Omega) \mathbf{k}] - \tilde{\varrho}[\mathbf{R}^T(\Omega') \mathbf{k}]|^2 .
\]

(6)

Its imaginary part vanishes even for complex form factors, \( \tilde{\varrho}(\mathbf{k}) = \tilde{\varrho}^*(-\mathbf{k}) \), due to the odd symmetry of the integrand. As anticipated, the localization rate depends on the relative orientation \( \mathbf{R}(\Omega) \), as follows from rotating \( \mathbf{k} \).

For azimuthally symmetric bodies the localization rate (6) is only a function of the angle between the symmetry axes \( \mathbf{m}(\Omega) \) and \( \mathbf{m}(\Omega') \). It is depicted in Fig. 1 for the case of a cylindrically and a spheroidally shaped homogeneous mass density of radius \( R \) and length \( L \). The respective form factors \( \tilde{\varrho}(\mathbf{k}) \)

\[
\tilde{\varrho}_{cyl}(\mathbf{k}) = \frac{2M}{R |e_3 \times k|} J_1(R|e_3 \times k|) \text{sinc} \left( \frac{L}{2} e_3 \cdot k \right) ,
\]

(7)

\[
\tilde{\varrho}_{sph}(\mathbf{k}) = M \sqrt{\frac{2\pi}{2}} \left( \frac{R^2 |e_3 \times k|^2 + L^2 |e_3 \times k|^2/4}{\sqrt{R^2 |e_3 \times k|^2 + L^2 |e_3 \times k|^2/4}} \right)^{3/2} ,
\]

(8)

where we chose the symmetry axis along \( e_3 \); \( J_n(\cdot) \) are Bessel functions.

If the maximum extension of the nanoparticle is well below the localization length \( r_c \), (6) takes on the form

\[
F(\Omega, \Omega') \approx \frac{\lambda C M^2}{8\pi m_0 r^4_c} \left( \frac{R^2}{a} - \frac{L^2}{b} \right)^2 |\mathbf{m}(\Omega) \times \mathbf{m}(\Omega')|^2 ,
\]

where \( a, b \) are numerical constants, \( a_{cyl} = 4, b_{cyl} = 12 \) and \( a_{sph} = 5, b_{sph} = 20 \).

This rate increases with \( \sin \alpha = |\mathbf{m}(\Omega) \times \mathbf{m}(\Omega')|^2 \), as also observed for environmentally induced orientational decoherence of small particles [43, 44]. Note that Eq. (9) vanishes if the spheroid is deformed into a sphere, \( R = L/2 \); the same holds for cylinders with isotropic tensor of inertia, i.e. \( R = L/\sqrt{3} \). Remarkably, the localization rate (6) scales with the tenth power of the particle size (at fixed density). This holds for arbitrarily shaped small particles, as follows from dimensional analysis of (6).
III. LINEAR- AND ANGULAR-MOMENTUM
DIFFUSION

The exact master equation (1) of spatio-orientational
decoherence can be simplified for states which are sufficiently well localized in position and orientation (around \(\Omega_0\)) implying that \(\langle R_{cm}\Omega|\rho|R'_{cm}\Omega'\rangle \approx 0\) unless \(\{R_{cm} - R'_{cm} + \mathcal{L}(R_0)\mathcal{R} | R_0 - 1\}\) \(\ll r_C\) for all \(n\). This requirement demands that the relative orientation is small, \(R_0(\Omega) \approx 1 + \epsilon_{ijk} d\Omega_i e_k \otimes e_j\) with \(d\Omega_i\) the angle of rotation around the \(e_i\) axis.

Expanding the CSL modification \(\mathcal{L}\rho\) into lowest order of \(|R_{cm} - R'_{cm}|\) and \(d\Omega\), shows that the total localization is given by a sum of pure center-of-mass and pure orientational localization,

\[
\langle R_{cm}\Omega|\mathcal{L}\rho|R'_{cm}\Omega'\rangle \approx -\langle R_{cm}\Omega|\rho|R'_{cm}\Omega'\rangle \\
\times \left[F_{cm}(R_{cm} - R'_{cm}, \Omega_0) + F_{rot}(\Omega, \Omega')\right].
\]

The respective rates can be expressed as

\[
F_{cm}(R, \Omega_0) = \frac{\lambda_C}{2\pi} R \cdot \mathcal{R}(\Omega_0) A_{cm} R^T(\Omega_0) R
\]

\[
F_{rot}(\Omega, \Omega') = \frac{\lambda_C}{2} d\Omega A_{rot} d\Omega',
\]

where \(d\Omega = (d\Omega_1, d\Omega_2, d\Omega_3)\). Here the geometry tensors

\[
A_{cm} = \frac{r_C^5}{\pi^{3/2} m_0^2} \int d^3k e^{-i\mathbf{r}_C \cdot \mathbf{k}} |\hat{\rho}(\mathbf{k})|^2 \mathbf{k} \otimes \mathbf{k} ,
\]

\[
A_{rot} = \frac{r_C^3}{\pi^{3/2} m_0^2} \int d^3k e^{-i\mathbf{r}_C \cdot \mathbf{k}} [\mathbf{k} \otimes \nabla_{\mathbf{k}} \hat{\rho}(\mathbf{k})] \otimes [\mathbf{k} \times \nabla_{\mathbf{k}} \hat{\rho}(\mathbf{k})],
\]

account for the nonspherical shape of the matter density. They naturally generalize the geometry factor for momentum diffusion in a single spatial direction as defined in Ref. [24].

A. Azimuthally symmetric bodies

The tensors \(A_{cm}\) and \(A_{rot}\) share the symmetries of the mass density \(\rho(\mathbf{r})\). In particular, for an azimuthally symmetric body also invariant under spatial inversion, like a cylinder or a spheroid, the geometry tensors have the general form

\[
A_{cm} = \frac{2r_C^2}{\lambda_C \hbar^2} \left[ D_{\parallel} \mathbb{I} + (D_\perp - D_{\parallel}) e_3 \otimes e_3 \right]
\]

\[
A_{rot} = \frac{2D_{rot}}{\lambda_C \hbar^2} (e_1 \otimes e_1 + e_2 \otimes e_2),
\]

where we chose the symmetry axis to point into direction \(e_3\). As demonstrated below, the constants \(D_{\parallel}\), \(D_{\perp}\) and \(D_{rot}\) are diffusion coefficients. For cylindrical bodies they are specified in the appendix.

Plugging relations (13) into (11) leads to the localization rates

\[
F_{cm}(R, \Omega_0) = \frac{D_{\parallel}}{\hbar^2} R^2 + \frac{D_{\perp} - D_{\parallel}}{\hbar^2} [\mathbf{R} \cdot \mathbf{m}(\Omega_0)]^2
\]

\[
F_{rot}(\Omega, \Omega') = \frac{D_{rot}}{\hbar^2} |\mathbf{m}(\Omega) \times \mathbf{m}(\Omega')|^2.
\]

The corresponding master equation reads

\[
\partial_t \rho = -\frac{i}{\hbar} [\mathbf{H}, \rho] - \frac{D_{\parallel}}{\hbar^2} \sum_{i=1}^{3} [R_{i,c.m}, [R_{i,c.m}, \rho]]
\]

\[
- \frac{D_{\parallel} - D_{\perp}}{\hbar^2} [R_{cm} \cdot \mathbf{m}(\Omega_0), [R_{cm} \cdot \mathbf{m}(\Omega_0), \rho]]
\]

\[
- \frac{15D_{rot}}{4\hbar^2} \int_{S_2} d^2\mathbf{n} \left[[\mathbf{n} \cdot \mathbf{m}(\Omega)]^2, [\mathbf{n} \cdot \mathbf{m}(\Omega)]^2, \rho\right].
\]

It describes linear- and angular momentum diffusion [48] as discussed next.
B. Heating rates

In order to demonstrate that the master equation (15) indeed describes linear and angular momentum diffusion, we note that the expectation values of the linear momentum operator \( P_{cm} \) and of the angular momentum operator \( J \) are conserved,

\[
\partial_t \langle P_{cm} \rangle = 0, \quad \partial_t \langle J \rangle = 0, \quad \text{(16a)}
\]

while the second moments increase linearly with time,

\[
\partial_t \langle P_{cm}^2 \rangle = 2D_{\|} + 4D_{\perp}, \quad \partial_t \langle J^2 \rangle = 4D_{\text{rot}}. \quad \text{(16b)}
\]

This follows with the canonical commutation relations by direct calculation. The linear- and angular-momentum heating rates are thus fully determined by the diffusion coefficients.

In Fig. 2 we show the diffusion coefficients of cylindrical bodies as a function of the localization length \( r_C \). Remarkably, angular momentum diffusion is stronger for long rods than for flat discs of the same volume, since the diffusion coefficient of disks is bounded, \( D = \lambda_C \hbar^2 M^2/4m_0^2 \) as \( R/r_C \rightarrow \infty \), while for long rods we find the asymptotic behavior \( D_{\text{rot}} \sim \sqrt{\pi} \lambda_C \hbar^2 M^2/24 \rho \cdot m_0^2 \) as \( L/r_C \rightarrow \infty \). We note that the diffusion constants of spheroidal particles agree qualitatively with those of cylinders.

An important feature of the spatio-orientational localization, as compared to pure center-of-mass localization, is that the linear and the angular momentum diffusion coefficients depend differently on the CSL parameters \( \lambda_C \) and \( r_C \) even for small particles \( L/r_C \ll 1 \). Specifically, for small nanoparticles we have \( D_{\text{rot}} \propto \lambda_C/r_C^2 \), while \( D_{cm} \propto \lambda_C/r_C^2 \). Thus, simultaneously measuring the linear- and angular-momentum diffusion coefficients of a levitated nanorotor would allow one to determine both CSL parameters in a single experiment (provided that environmental decoherence can be controlled). This is illustrated in Fig. 3 where we show how the CSL location rate \( \lambda_C \) and the CSL length \( r_C \) would be extracted from a hypothetical measurement of the heating rates \( \Gamma_{cm} = 2D_{\|}/M = 10^{-8} \text{K/s} \) and \( \Gamma_{\text{rot}} = 2D_{\text{rot}}/I = 10^{-10} \text{K/s} \) of a silicon spheroid.

IV. PLANAR ROTATIONS

As a simple and exactly solvable application, we study the impact of the CSL modification on the rotational dynamics of the planar rotor with inversion symmetry and a single orientational degree of freedom \( \alpha \in [-\pi, \pi] \). The respective master equation can be obtained from (15) by tracing out the center-of-mass degrees of freedom and

\[ \partial_t w(\alpha, m) + \frac{\hbar m}{I} \partial_\alpha w(\alpha, m) = D_{\text{rot}} \left[ w(\alpha, m - 2) - 2w(\alpha, m) + w(\alpha, m + 2) \right] / (2\hbar)^2. \quad \text{(19)} \]

The CSL modification thus enters in the discretized form of a second order angular momentum derivative. The fact
that only next-to-nearest angular momentum quantum number \( m \) are coupled is due to the inversion symmetry of the rotor.

The solution of Eq. (19) with the initial condition \( w_0(\alpha, m) \) can be explicitly given as

\[
w(\alpha, m; t) = \sum_{\ell \in \mathbb{Z}} \int_{-\pi}^{\pi} d\alpha' \, w_0 \left( \alpha - \alpha' - \frac{\hbar mt}{I}, m - 2\ell \right) T_t(\alpha', \ell).
\]  

(20)

The kernel

\[
T_t(\alpha', \ell) = \frac{e^{-D_{\text{rot}} t/2h^2}}{2\pi} \sum_{k \in \mathbb{Z}} e^{ik(\alpha' + \ell t)/t} I_\ell \left[ \frac{D_{\text{rot}} t}{2h^2} \sin \left( \frac{\hbar kt}{I} \right) \right]
\]

(21)

which involves the modified Bessel functions \( I_\ell(\cdot) \), preserves the normalization of \( w(\alpha, m; t) \). In the limit of vanishing diffusion, \( D_{\text{rot}} \approx 0 \), (20) describes the classical shearing of the Wigner function, \( T_t(\alpha', \ell) \approx \delta(\alpha') \delta_{\ell 0} \).

Angular momentum diffusion broadens the momentum distribution since the energy increases linearly with time, \( \partial_t \langle p_\ell^2/2I \rangle = D_{\text{rot}}/I \), which in turn enhances the orientational spread. This is demonstrated in Fig. 4 for the initial superposition state \( \psi_0(\alpha) \propto \exp[-\cos^2 \alpha/4\sigma_0^2] \) with Wigner function

\[
w_0(\alpha, m) = \frac{(-1)^m}{N} I_m \left[ \frac{\cos(2\alpha)}{4\sigma_0^2} \right],
\]

(22)

where the normalization is \( N = 2\pi I_0(1/4\sigma_0^2) \).

In order to quantify how the orientational spread increases due to the CSL modification, we evaluate the variance \( \sigma^2_0(t) = 1 - \langle \cos(\alpha) \rangle^2_t \), with \( \cos(\alpha) = \cos(\alpha, \sin \alpha) \) the unit vector in the plane. Equation (20) yields

\[
\sigma^2_0(t) = 1 - (1 - \sigma^2_0(t)) \exp \left\{ -\frac{D_{\text{rot}} t}{2h^2} \left[ 1 - \sin \left( \frac{2\hbar t}{I} \right) \right] \right\}.
\]

(23)

The unperturbed variance

\[
\sigma^2_0(t) = 1 - \left[ \langle \cos \left( \alpha + \frac{\hbar t}{I} \right) \rangle_0 \right]^2 + \left[ \sin \left( \alpha + \frac{\hbar t}{I} \right) \right]^2_0
\]

(24)

is here evaluated with respect to the initial state.

One observes from (24) that in the absence of CSL, \( D_{\text{rot}} = 0 \), the initial variance recurs at integer multiples of the revival time \( \pi I/h \). Equation (23) shows that the CSL modification suppresses these revivals on the time scale \( 2h^2/D_{\text{rot}} \). As evident from (23), the CSL modification enhances the orientational spread at all times.

V. CONCLUSION

The master equation derived in this article shows how the orientational localization induced by the CSL model leads to a heating of the center-of-mass and the rotational motion. The associated diffusion of the linear and the angular momentum can be conveniently expressed in terms...
of geometry tensors involving the form factor. For the special case of planar rotations we illustrated how the CSL modification can suppress quantum behavior and lead to an appreciable enhancement of the orientational motion. Remarkably, we find that the combined measurement of translational and rotational heating of a single particle would allow one to determine the individual CSL parameters even if the particle is small compared to the CSL localization length.

Acknowledgment

We thank Stefan Nimmrichter for helpful discussions.

Appendix A: Diffusion coefficients for Cylinders

A calculation of the diffusion coefficients $D_\perp, D_\parallel$ and $D_{\text{rot}}$ as defined in Eq. (13) for a cylinder of length $L$ and radius $R$ yields

\begin{align}
D_\parallel &= \frac{\lambda_\parallel h^2}{2R_C^2} \frac{M^2}{m^2 R_C^4 L_C^2} h_1(L_C) \left\{ 1 - e^{-R_C^2} \left[ I_0 \left( R_C^2 \right) + I_1 \left( R_C^2 \right) \right] \right\}, \\
D_\perp &= \frac{\lambda_\perp h^2}{2R_C^2} \frac{M^2}{m^2 R_C^4 L_C^2} h_2(L_C) e^{-R_C^2} I_1 \left( R_C^2 \right), \\
D_{\text{rot}} &= \frac{\lambda_{\text{rot}} h^2}{2} \frac{M^2}{m^2 R_C^4 L_C^2} \left( \frac{R_C^2}{2} h_1(L_C) \left\{ 1 - 2e^{-R_C^2} \left[ I_0 \left( R_C^2 \right) + \left( 1 - \frac{5}{3R_C^2} \right) I_1 \left( R_C^2 \right) \right] \right\} \right) + \frac{L_C^2}{3} e^{-R_C^2} I_1 \left( R_C^2 \right) [h_2(L_C) - 2] \\
&\quad \quad \quad \quad \quad + \left\{ 1 - e^{-R_C^2} \left[ I_0 \left( R_C^2 \right) + 2I_1 \left( R_C^2 \right) \right] \right\} [h_1(L_C) - h_2(L_C)],
\end{align}

where $I_0(\cdot), I_1(\cdot)$ denote modified Bessel functions. We abbreviated $R_C = R/\sqrt{2}r_C$, $L_C = L/2r_C$, $h_1(L_C) = 1 - e^{-L_C^2}$, and $h_2(L_C) = \sqrt{\pi L_C} \text{erf} \left( L_C \right) - h_1(L_C)$.

with $\text{erf}(\cdot)$ the error function. In the limit of thin disks, $R/r_C \to \infty$, at constant volume $\pi R^2 L$, the rotational diffusion coefficient approaches $D_{\text{rot}} \to \lambda_{\text{rot}} h^2 M^2/4m^2$, while in the case of long rods we have $D_{\text{rot}} \sim \sqrt{\pi \lambda_{\text{rot}} h^2 M^2 L/24m^2 r_C}$ as $L/r_C \to \infty$. Note that the spatial diffusion coefficient along the cylinder’s symmetry axis $\text{A1a}$ was already derived in Ref. [24].

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