Parity-symmetry-adapted coherent states and entanglement in quantum phase transitions of vibron models

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Abstract

We propose coherent (‘Schrödinger cat-like’) states adapted to the parity symmetry providing a remarkable variational description of the ground and first excited states of vibron models for finite \(N\)-size molecules. Vibron models undergo a quantum shape phase transition (from linear to bent) at a critical value \(\xi_c\) of a control parameter. These trial cat states reveal a sudden increase in vibration–rotation entanglement linear \((L)\) and von Neumann \((S)\) entropies from zero to \(L(N)_{\text{cat}}(\xi) \approx 1 - 2/\sqrt{\pi N}\) (to be compared with \(L_{\text{max}}(N) = 1 - 1/(N + 1)\)) and \(S(N)_{\text{cat}}(\xi) \approx \frac{1}{\log_2(N + 1)}\), respectively, above the critical point, \(\xi > \xi_c\), in agreement with exact numerical calculations. We also compute inverse participation ratios, for which these cat states capture a sudden delocalization of the ground-state wave packet across the critical point. Analytic expressions for entanglement entropies and inverse participation ratios of variational states, as functions of \(N\) and \(\xi\), are given in terms of hypergeometric functions.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Understanding (zero-temperature) quantum phase transitions (QPTs) [1] has become an important part of quantum many-body theory. On the one hand, quantum fluctuations grow at the QPT and variance and entropic uncertainty measures turn out to give a good description of the QPT. Recently [2–4], uncertainty measures in the (spin-boson) Dicke model [5], which
also undergoes a QPT, have been studied (see also [6–8] for other information theoretical measures of delocalization to study QPTs). On the other hand, large correlations and collective behavior are an intrinsic part of critical systems and, therefore, entanglement measures should also capture the essence of these QPTs (see e.g. [9, 10] for the entanglement properties of the Dicke model and [11] for entanglement and localization of a two-mode Bose–Einstein condensate).

In this paper, we shall focus on the study of entanglement properties of the so-called vibron models [12], which are used to study rotational and vibrational spectra in diatomic and polyatomic molecules and also exhibit a (shape) QPT. They were introduced by Iachello [13] in the 1980s through an algebraic approach, based on the concept of spectrum-generating algebra. We shall restrict ourselves to the two-dimensional $U(3)$ vibron model describing a system containing a dipole degree of freedom constrained to planar motion [14, 15]. The basic example of such a system is a triatomic linear bender molecule, although extensions to more complex molecular systems can also be considered. In these models, one finds different (shape) phases connected to specific geometric configurations of the ground state and related to distinct dynamic symmetries of the Hamiltonian (see e.g. [16]). The QPT occurs as a function of a control parameter $\xi$ that appears in the Hamiltonian $H$ in the form of a convex combination $H(\xi) = (1 - \xi)H_1 + \xi H_2$. At $\xi = 0$, the system is in phase I, characterized by the dynamical symmetry $G_1$ of $H_1$, and at $\xi = 1$, the system is in phase II, characterized by the dynamical symmetry $G_2$ of $H_2$.

The classical, thermodynamic or mean-field limit of these models is studied by using an algorithm introduced by Gilmore [18] which makes use of semi-classical (boson-condensate) coherent states (CS) (see e.g. [19–22] for standard references on CS) as variational states to approximate the ground-state energy. However, these trial states, as such, do not display an intrinsic parity symmetry (see e.g. [23]) present in the Hamiltonian, as they do not have a definite parity. We would like to mention that the key role of parity has also recently been noticed in [24, 25] in the context of QPT (from normal to super-radiant) in the Dicke model for matter–field (spin–boson) interactions. We shall see that disregarding parity leads to wrong results of vibration–rotation entanglement measures for usual variational approximations to the ground state in terms of (non-symmetry-adapted) CS. Then we shall introduce even (resp. odd) CS adapted to the parity symmetry of the Hamiltonian to describe the ground (resp. first-excited) state of the two-dimensional $U(3)$ vibron model. These even and odd CS are ‘Schrodinger’s cat-like-states’ in the sense that they are a quantum superposition of quasi-classical, macroscopically distinguishable (with negligible overlap) states. Schrodinger’s cat states are experimentally generated (see e.g. [26]) and prove to be very useful to study the process of decoherence which limits the development of quantum computing. We shall show that even-cat states provide a finite ($N$)-size approximation to some $N = \infty$ quantities such as the ground-state energy ‘per particle’ and order parameters such as the ‘equilibrium radius’ (see also [27] for other analytical results of finite-size corrections beyond the mean-field limit approximation in vibron models). Even-cat states will also quantitatively and qualitatively capture entanglement and delocalization measures of the exact ground state for finite $N$.

We have to say that finite-size effects have also been discussed in the above-mentioned Dicke model, both numerically [28] and analytically [29], for thermodynamical quantities and in [30] for the entanglement entropy, although the role of parity is not explicit in these studies (see [24, 25] and [2–4] for the relevance of parity in uncertainty measures inside the Dicke model). Finite-size corrections in [29] and in [31] (for two-level boson systems) use a $1/N$ expansion naturally given by the Holstein–Primakoff representation of the angular momentum [32]. For finite-size precursors of QPTs in atomic nuclei models, see for example [33] and references therein. We must stress that, in this paper, we do not make any of these $1/N$ expansions around
$N = \infty$, but we work with finite $N$. Numerical (exact) results of the ground-state energy, entanglement and delocalization measures are already nicely reproduced by even-cat states for finite $N$.

This paper is organized as follows. In section 2, we briefly review the $U(3)$ algebraic approach to two-dimensional (2D) vibron models (more details can be found in [14–16]) and we propose a new kind of variational states by adapting ‘projective’ ('Hartree axial' [31]) CS to the parity symmetry of the Hamiltonian. In section 3, we compute vibration–rotation entanglement measures such as ‘purity’, linear and von Neumann entropy, as a function of the vibron number $N$ (related to the total number of bound states of the molecule) and the control parameter $\xi$, revealing a sudden increase in entanglement from linear to bent phases at the critical point $\xi_c$. The calculation is performed numerically and complemented and compared with two variational approximations (parity-symmetric and non-symmetric), which enrich the study. Finally, we compute the inverse participation ratio (IPR), as a measure of delocalization of the ground-state wave packet across the phase transition, and see that the spreading is captured by the new proposed symmetry-adapted (even-cat) CS, thus revealing the importance of parity symmetry. Section 4 is devoted to conclusions.

2. Vibron model and variational symmetry-adapted coherent states

2D-vibron models describe a system containing a dipole degree of freedom constrained to planar motion. Elementary excitations are (creation and annihilation) 2D vector $\tau$-bosons $\{\tau^+_{i,\ell}, \tau^-_{i,\ell}, \tau_z, \tau_y\}$ and a scalar $\sigma$-boson $\{\sigma^+, \sigma\}$. It is convenient to introduce circular bosons: $\tau_\pm = \mp(i\tau_x + \tau_y)/\sqrt{2}$. The nine generators of the $U(3)$ algebra are bilinear products of creation and annihilation operators, in particular,

$$
\hat{n} = \tau^+_+ \tau_+ - \tau^-_- \tau_-, \quad \hat{l} = \tau^+_+ \tau_+ - \tau^-_- \tau_-, \quad \hat{D}_+ = \sqrt{2}(\tau^+_+ \sigma - \sigma^+ \tau_-), \quad \hat{D}_- = \sqrt{2}(-\tau^+_+ \sigma + \sigma^+ \tau_-)
$$

(1)

denote the number operator of vector $\hat{n}$ and scalar $\hat{n}_s$ bosons, 2D angular momentum $\hat{l}$ and dipole $\hat{D}_\pm$ operators, respectively (see [16] for the remaining four operators $\hat{Q}_\pm, \hat{R}_\pm$, which will not be used here). Assuming the total number of bosons $N = \hat{n} + \hat{n}_s$ and the 2D angular momentum $\hat{l}$ to be conserved, there are only two dynamical symmetry limits, $G_1 = U(2)$ and $G_2 = SO(3)$, associated with two algebraic chains starting from $U(3)$ and ending in $SO(2)$: the so-called cylindrical and displaced oscillator chains. A general Hamiltonian of the $U(3)$ vibron model with only one- and two-body interactions can be expressed in terms of linear and quadratic Casimir operators of all the subalgebras contained in the dynamical symmetry algebra chains. To capture the essentials of the phase transition from the $G_1$-phase (linear) to the $G_2$-phase (bent), it is enough to consider a convex combination of the linear $C_1(U(2)) = \hat{n}$ and quadratic $C_2(SO(3)) = \hat{W}^2 = (\hat{D}_+ \hat{D}_- + \hat{D}_- \hat{D}_+)/2 + \hat{P}$ Casimir operators of the corresponding dynamical symmetries. In particular, we shall consider the essential Hamiltonian [16]

$$
\hat{H} = (1 - \xi)\hat{n} + \xi \frac{N(N + 1) - \hat{W}^2}{N - 1},
$$

(2)

where the (constant) quantum number $N$ is the total number of bound states that labels the totally symmetric $(N + 1)(N + 2)/2$-dimensional representation $[N]$ of $U(3)$. The Hilbert space is spanned by the orthonormal basis vectors

$$
|N; n, l\rangle = \frac{(\sigma^+)^{N-n} (\tau^+_{i,\ell})^n (\tau^-_{i,\ell})^l}{\sqrt{(N-n)! (\frac{n}{2})! (\frac{l}{2})!}} |0\rangle,
$$

(3)
where the bending quantum number $n = N, N - 1, N - 2, \ldots, 0$ and the angular momentum $l = \pm n, \pm (n - 2), \ldots, \pm 1$ or 0 ($n =$ odd or even) are the eigenvalues of $\hat{n}$ and $\hat{l}$, respectively. The matrix elements of $\hat{W}^2$ can be easily derived (see e.g. [16]):

$$\langle N; n', l | \hat{W}^2 | N; n, l \rangle =$$

$$( (N - n)(n + 2) + (N - n + 1)n + l^2 \rangle \delta_{n,n'}$$

$$- ((N - n + 2)(N - n + 1)(n + l)(n - l)) \langle \hat{\delta}_{n,n' - 2}$$

$$- ((N - n)(N - n - 1)(n + l + 2)(n - l + 2)) \langle \hat{\delta}_{n,n' + 2}.$$

From these matrix elements, it is easy to see that time evolution preserves the parity $e^{i\pi n}$ of a given state $|N; n, l\rangle$. That is, the parity operator $\hat{\Pi} = e^{i\pi \hat{n}}$ commutes with $\hat{H}$ and both operators can then be jointly diagonalized. Parity symmetry in the vibron model has been considered in, for instance, [34]. However, this symmetry goes unnoticed when proposing ansätze to approximate the ground-state energy in terms of (non-symmetric) ‘projective’ [16] (or ‘Hartree axial’ [31]) CS,

$$|N; r \rangle = \frac{1}{\sqrt{N!}} (b^+_0)^N |0\rangle, \quad b^+_l = \frac{1}{\sqrt{1 + r^2}} (\sigma^+ + r \tau^+_l),$$

with $r \geq 0$ a free variational parameter and $b^+_l$ the boson condensate. Other rotationally equivalent possibilities can also be considered [35]; moreover, intrinsic excitations can also be constructed by replacing the intrinsic boson $b_l$ with orthogonal excitation bosons, thus defining multi-species CS (see e.g. [36, 37]). In this paper, we shall restrict ourselves to ground-state ansätze.

For future use, we shall provide the explicit expression of the coefficients of the expansion of (4) in terms of the basis vectors (3), which is explicitly given by

$$| N; r \rangle = \sum_{n=0}^{N} \sum_{m=0}^{n} c_{n,m}^{(N)}(r) | N; n, n - 2m \rangle,$$

$$c_{n,m}^{(N)}(r) = \sqrt{\binom{N}{n} \binom{n}{m} \frac{(-r/\sqrt{2})^n (-1)^m}{(1 + r^2)^{N/2}}}.$$
\( \theta \sim r/a_i \), with \( a \) the equilibrium bond length, which reflects the degree of distortion of the molecular framework from linearity \( r = 0 \). The displacement \( r \) is also related to the coordinates of Pöschl–Teller (for the cylindrical oscillator) and Morse (for the displaced cylindrical oscillator) potentials. In (6), we also see that \( r \) provides a measure of the average vibrational \( \langle \hat{\theta} \rangle \) and squared angular momentum \( \langle \hat{W}^2 \rangle \) quantum numbers.

Although \( |N; r_i(\xi)\rangle \) properly describes the ground-state energy density in the thermodynamic limit \( N \to \infty \), we shall show that it does not capture the correct behavior for other ground-state properties sensitive to the parity symmetry \( \Pi \) of the Hamiltonian like, for instance, vibration–rotation entanglement and delocalization measures. This is why we introduce in this paper parity-symmetry-adapted CS. Indeed, a far better variational description of the ground (resp. first-excited) state is given in terms of the even (resp. odd)-parity projected ‘projective’ CS,

\[
|N; r, \pm \rangle = \frac{(1 \pm \hat{\Pi})|N; r\rangle}{\mathcal{N}_\pm(r)} = \frac{|N; r\rangle \pm |N; -r\rangle}{\mathcal{N}_\pm(r)},
\]

where \( \mathcal{N}_\pm(r) = \sqrt{2}(1 \pm |N; -r|N; r\rangle)^{1/2} \) is a normalization constant, with

\[
|N; -r|N; r\rangle = ((1 - r^2)/(1 + r^2))^N,
\]

and we have used that \( \hat{\Pi}^2|\psi\rangle = n^2|\psi\rangle \), and therefore \( \hat{\Pi}|\psi\rangle = (-\hat{\Pi})|\psi\rangle \). Note that the overlap \( \langle N; -r|N; r \rangle \) is negligible for high \( N \) (thermodynamic limit) and any \( r > 0 \); therefore, in this limit, states (8) are a superposition of two non-overlapping (distinguishable) quasi-classical (coherent) wave packets (see [24, 25] and [2–4] for a similar behavior in the Dicke model). This justifies the term ‘Schrödinger cat-like’ for these states. We shall only discuss the even (ground-state ansatz) case here. Expanding \( |N; r, +\rangle \) in basis (3), as we did in (5) for non-symmetric CS, we arrive at the new coefficients

\[
c_{n,m}^{(N,+)}(\xi) = \frac{c_{n,m}^{(N)}(r) + c_{n,m}^{(N)}(-r)}{\mathcal{N}_\pm(r)},
\]

Note that now \( c_{n,m}^{(N,+)}(r) = 0 \) for \( n = \text{odd} \). The variational parameter \( r \) is again computed by minimizing the ground-state energy functional ‘per particle’ \( \mathcal{E}_r^{(N)}(\xi) = \langle \hat{H} \rangle + \mathcal{E}_\xi(\xi) \) as in (6), but now for the symmetric configuration \( |N; r, +\rangle \), given in terms of the new mean values:

\[
\begin{align*}
\langle \hat{n} \rangle_+ &= \frac{r^2((1 + r^2)^N - (1 - r^2)^N)}{(1 + r^2)^N + (1 - r^2)^N}, \\
\langle \hat{W}^2 \rangle_+ &= \frac{2(1 + r^2)^N + (1 - r^2)^N(1 + 2Nr^2 + r^4)}{(1 + r^2)^N + (1 - r^2)^N}.
\end{align*}
\]

Unlike \( \mathcal{E}_\xi(\xi) \), the new energy functional \( \mathcal{E}_r^{(N)}(\xi) \) depends on \( N \). From \( \partial \mathcal{E}_r^{(N)}(\xi)/\partial r = 0 \), we can obtain the new equilibrium radius \( r_e^{(N)}(\xi) \). For example, for \( N = 2 \) and \( N = 3 \), we find analytic explicit expressions for the equilibrium radius and the ground-state energy per particle as a function of the control parameter \( \xi \):

\[
\begin{align*}
r_e^{(2)}(\xi) &= \sqrt{\frac{1}{2} - \frac{1}{2\xi} + \frac{\sqrt{1 - 2\xi + 5\xi^2}}{2\xi}}, \\
\mathcal{E}^{(2)}(\xi) &= \frac{1}{4}(1 + \xi - \sqrt{1 + \xi (-2 + 5\xi)}), \\
r_e^{(3)}(\xi) &= \sqrt{\frac{1}{2} - \frac{1}{2\xi} + \frac{\sqrt{1 - 4\xi + 16\xi^2}}{2\xi}}, \\
\mathcal{E}^{(3)}(\xi) &= \frac{1}{2}(1 + \xi - \sqrt{1 + \xi (-4 + 7\xi)}).
\end{align*}
\]

For higher values of \( N \), we can compute \( r_e^{(N)}(\xi) \) numerically. Figure 1 compares \( r_e(\xi) \) in (7) with \( r_e^{(N)}(\xi) \) for \( N = 2, 3, 8, 32 \). We observe that the equilibrium radius \( r_e^{(N)}(\xi) \) of the even-cat
state |N; r, +⟩ approaches the equilibrium radius \( r_e(\xi) \) of the CS |N; r⟩ in the thermodynamic limit, that is, \( r_e^{(N)}(\xi) \to r_e(\xi) \) for \( N \to \infty \). Moreover, one can also see (figure 2) that the energy density \( \mathcal{E}_e^{(N)}(r_e^{(N)}(\xi)) \) of the even-cat state is a increasing function of \( N \) and that it approaches the energy density \( \mathcal{E}_e(r_e(\xi)) \) of the CS in the thermodynamic limit, that is, \( \mathcal{E}_e^{(N)}(r_e^{(N)}(\xi)) \to \mathcal{E}_e(r_e(\xi)) \) for \( N \to \infty \) too. This behavior is displayed in figure 2 and it is also shared by the exact (numerical) density energy. Therefore, even-cat states provide a ground-state energy description of the finite-size \( (N < \infty) \) regime. For future use, let us finish the description of variational states by providing the explicit expression of the basis wavefunctions
The ‘purity’ of matrix \( RDM \) for vibrational modes by integrating out the rotational degrees of freedom:

\[
\langle q | N; n, l \rangle = \frac{2^{-N/2} \pi^{-3/4} e^{-\left(q_0^2 + q_1^2 + q_2^2\right)/2}}{\sqrt{(N - n)! \left(\frac{n + 1}{2}\right)! \left(\frac{n + 2}{2}\right)!}} \times H_{N-n}(q_0) H_{\frac{n+1}{2}}(q_1) H_{\frac{n+2}{2}}(q_2). \tag{13}
\]

3. Vibration–rotation entanglement and delocalization measures

Let us denote by

\[
|\psi^{(N)}(\xi)\rangle = \sum_{n=0}^{N} \sum_{m=0}^{n} c_{n,m}^{(N)}(\xi)|N; n, l = n - 2m\rangle \tag{14}
\]

the exact ground state of our system obtained by numerical diagonalization of Hamiltonian (2) in terms of the basis vectors (3) with coefficients \( c_{n,m}^{(N)}(\xi) \), and by \( \psi_\xi^{(N)}(q) = \langle q | N; \, r_\xi(\xi) \rangle \) the corresponding wavefunction in the position representation \( q = (q_0, q_1, q_2) \), written in terms of Hermite polynomials (13). Let us consider the bipartite system given by vibrational \( (q_0) \) and 2D-rotational \( \vec{q} = (q_1, q_2) \) degrees of freedom. Then, we can compute the reduced density matrix (RDM) for vibrational modes by integrating out the rotational degrees of freedom:

\[
\rho_\xi^{(N)}(q_0, q_0') = \int \int \psi^{(N)}(\xi)(q_0, \vec{q}) \psi^{(N)*}(\xi)(q_0', \vec{q'}). \tag{15}
\]

The ‘purity’ of \( \rho_\xi^{(N)} \) is given by

\[
\text{Tr} \left( \rho_\xi^{(N)} \right)^2 = \int \int \psi^{(N)}(q_0, \vec{q}) \rho_\xi^{(N)}(q_0, q_0') \psi^{(N)*}(q_0, q_0') \tag{16}
\]

where we have used the orthogonality properties of the basis vectors (3) and the coefficients of expansion (14). Actually, the RDM \( \rho_\xi^{(N)} \) is an \( (N + 1) \times (N + 1) \) diagonal matrix:

\[
(\rho_\xi^{(N)})_{n,n'} = \lambda_n^{(N)}(\xi) \delta_{n,n'}, \tag{17}
\]

with the eigenvalues

\[
\lambda_n^{(N)}(\xi) = \sum_{m=0}^{n} \left(c_{n,m}^{(N)}(\xi)\right)^2, \tag{18}
\]

and the vibrational quantum number \( n \) running from 0 to \( N \). Using coefficients (5) and (10) for the (non-symmetric) CS and even-parity-adapted CS (cat) (4) and (8), respectively, one can explicitly compute

\[
\begin{align*}
\lambda_n^{(N)}(\xi)_{\text{CS}} &= \binom{N}{n} \frac{r_\xi(\xi)^{2n}}{(1 + r_\xi(\xi)^2)^N}, \\
\lambda_n^{(N)}(\xi)_{\text{cat}} &= \binom{N}{n} \frac{(1 + (-1)^n) r_\xi(\xi)^{2n}}{(1 + r_\xi(\xi)^2)^N + (1 - r_\xi(\xi)^2)^N}.
\end{align*} \tag{19}
\]

The purity is then given in terms of hypergeometric functions as

\[
\text{Tr}(\rho_\xi^{(N)})^2_{\text{CS}} = \frac{2F_1(-N, -N; 1; r_\xi(\xi)^2)}{(1 + r_\xi(\xi)^2)^{2N}}, \tag{20}
\]

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Figure 3. Comparison of the exact linear entropy $L^{(N)}$ with the coherent state (top) and even-cat (bottom) variational approximations as a function of $\xi$ for $N = 20, 32, 60$.

Instead of $\text{Tr} (\rho^{(N)}_{\xi})^2$, we shall use, for instance, the linear entropy

$$L^{(N)}(\xi) \equiv 1 - \text{Tr} (\rho^{(N)}_{\xi})^2,$$

as a measure of entanglement. Since the size of $\rho^{(N)}_{\xi}$ is $N + 1$, the linear entropy $L^{(N)}(\xi)$ then ranges between 0 (pure state) and $N/(N + 1)$ (completely mixed state). Figure 3 compares the exact (numerical) linear entropy with that of the CS and cat states (5) and (8), respectively. One can see that linear entropy for the CS configuration gives wrong results in both phases. In particular, in the second (bent) phase for the maximal value at $\xi = 1$, we have

$$L^{(N)}_{\text{CS}}(1) = 1 - 4^{1-N} \binom{2N}{N},$$

(23)
which can be computed by taking into account that \( r_\varepsilon(1) = 1 \). Much better agreement (remarkably for high \( N \)) is reached through the even-cat configuration, with linear entropy at \( \xi = 1 \) given by

\[
L_{\text{cat}}^{(N)}(1) \simeq 1 - 2^{1-2N} \left( \frac{2N}{N} \right),
\]

(24)

where we have also used that \( r_\varepsilon^{(N)}(1) = 1, \forall N \). Here we have made the approximation

\[
\sum_{i=0}^{[N/2]} \left( \frac{N}{2i} \right)^2 \simeq 1 \sum_{n=0}^{N} \left( \frac{N}{n} \right)^2 = \frac{1}{2} \left( \frac{2N}{N} \right),
\]

(25)

with \([N/2] = \text{Floor}(N/2)\), which is quite accurate even for relatively small values of \( N \). Thus, we have that the purity of the RDM for the even-cat is essentially half the purity for the CS at \( \xi = 1 \), a simple correction with important consequences that makes (24) a very good estimate for the entanglement linear entropy as a function of \( N \) in the rigidly bent phase [15]. Moreover, \( L_{\text{cat}}^{(N)}(\xi) = 1 \) (maximal entanglement) for the rigidly bent phase \( (\xi = 1) \) in the thermodynamic limit. For rigidly linear molecules [15], \( \xi = 0 \), the vibration–rotation entanglement linear entropy is zero.

For completeness, we also provide in figure 4 a comparative plot for the von Neumann entropy,

\[
S^{(N)}(\xi) = -\text{Tr}(\rho_\xi^{(N)} \log_2(\rho_\xi^{(N)})) = -\sum_{n=0}^{N} \lambda_n^{(N)}(\xi) \log_2(\lambda_n^{(N)}(\xi)).
\]

(27)

The qualitative behavior of \( S^{(N)}(\xi) \) is quite similar to that of \( L^{(N)}(\xi) \). Actually, one can see again that von Neumann entropy for the CS configuration gives wrong results in both phases. In particular, for high \( N \) and rigidly bent molecules, \( \xi = 1 \), von Neumann entropy behaves like

\[
S_{\text{cat}}^{(N)}(1) \simeq \frac{1}{2} \log_2(N+1), \quad S_{\text{CS}}^{(N)}(1) \simeq 1 + \frac{1}{2} \log_2(N+1),
\]

(28)

denoting a von Neumann entropy excess of 1 of the CS with respect to the cat and exact configurations.

At this point, one could still think that the CS approximation, albeit wrong for finite \( N \), still captures the essence of the growth of entanglement. Therefore, one could ask himself/herself whether parity is really essential to properly describe the ground state of vibron models in the thermodynamic limit or not. To answer this question positively, we need to provide a quantity from the ground state which is strongly sensitive to parity. This quantity turns out to be the ‘inverse participation ratio’ (IPR):

\[
P^{(N)}(\xi) = \int \int \int \int_{-\infty}^{\infty} dq_0 dq_1 dq_2 |\psi^{(N)}_\xi(q_0, q_1, q_2)|^4.
\]

(29)
We can interpret the IPR as a measure of the spread or delocalization of a wavefunction $\psi$ over a particular basis (here the position eigenfunctions $|q\rangle$); much in the same way, the von Neumann entropy is a measure of the spread of a density matrix $\rho$ over its diagonal basis. From figure 5 we see that the exact (numerical) ground-state wavefunction exhibits a sudden delocalization across the phase transition, a spread that is also captured by the even-cat (8) but goes unnoticed in the case of the CS ansatz (4), (5), for which the IPR remains constant with the control parameter $\xi$. This kind of behavior is also shared by the ground state in the Dicke model [5], where the wave packet in the normal phase splits up into two (almost) non-overlapping sub-packets in the super-radiant phase (see e.g. [24, 25] and [2–4]). Here too, overlap (9) goes to zero for $\xi > \xi_c (r > 0)$ in the thermodynamic limit $N \to \infty$, so that the ground-state wavefunction (8) is a linear superposition of two (almost) non-overlapping sub-packets in the bent phase.

For completeness, we also provide the IPR

$$\tilde{\Pi}^{(N)}(\xi) = \sum_{n=0}^{N} \sum_{m=0}^{n} (\epsilon_{n,m}^{(N)}(\xi))^4; \quad (30)$$
Figure 5. Comparison of the exact IPR \( P^{(N)}(\xi) \) with the coherent state (dashed-constant) and even-cat (dotted) variational approximations as a function of \( \xi \) for \( N = 8 \) and \( N = 20 \).

over basis (3) for the CS and cat ansatzs in terms of hypergeometric functions:

\[
\tilde{P}_{\text{CS}}^{(N)}(\xi) = \frac{\frac{3}{2}F_2\left(\frac{1}{2}, -N, -N; 1, 1; r_c(\xi)\right)}{(1 + r_c(\xi)^2)^{2N}}, \tag{31}
\]

\[
\tilde{P}_{\text{cat}}^{(N)}(\xi) = 2((1 + r_e^{(N)}(\xi)^2)^N + (1 - r_e^{(N)}(\xi)^2)^N)^{-2} \times \left(3F_2\left(\frac{1}{2}, -N, -N; 1, 1; r_e^{(N)}(\xi)^4\right)\right)
+ 3F_2\left(\frac{1}{2}, -N, -N; 1, 1; -r_e^{(N)}(\xi)^4\right). \tag{32}
\]

4. Conclusions

We have obtained exact (numerical) results of entanglement and delocalization of the ground state in 2D vibron models for finite \((N)\)-size molecules. These two features provide sharp indicators of the shape QPT present in this model, denoting an abrupt change in the structure of the ground state at the critical point \( \xi_c \).

This result has been complemented and compared with two variational approximations (parity-symmetric and non-symmetric) which enrich the study. Even-parity (cat) configurations turn out to give a remarkably good variational description of entanglement measures (linear and von Neumann entropies), quantitatively reproducing the exact values for the entanglement entropy in the rigidly (linear and bent) phases and qualitatively capturing the entanglement entropy behavior in the ‘floppy’ (intermediate) region.

Results reveal the emergence of vibration–rotation entanglement in the bent phase of vibron models, where vibrational and rotational modes are entangled but not maximally entangled.

Unlike other ansätze in the literature, these Schrödinger’s cat states do capture a delocalization of the ground-state wave packet through the IPR \( P^{(N)}(\xi) \) across the phase transition, thus proving the relevance of parity symmetry for a proper description of the ground state in vibron models.
As a general comment, we know that entanglement is a crucial resource for information processing, being at the heart of quantum communication protocols and quantum computing efficient algorithms. Although the work we present here is theoretical, there arises the natural question about an eventual experimental feasibility of the obtained vibration–rotation entanglement for quantum information processes. We know that phonon–roton scattering, emission and absorption have been extensively studied in helium superfluid and we think that it is worth exploring this new possibility in molecules.

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