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Quantification of Symmetry*

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Abstract *Symmetry is conventionally described in a polarized manner that the system is either completely symmetric or completely asymmetric. Using group theoretical approach to overcome this dichotomous problem, we introduce the degree of symmetry (DoS) as a non-negative continuous number ranging from zero to unity. DoS is defined through an average of the fidelity deviations of Hamiltonian or quantum state over its transformation group G, and thus is computable by making use of the completeness relations of the irreducible representations of G. The monotonicity of DoS can effectively probe the extended group for accidental degeneracy while its multi-valued natures characterize some (spontaneous) symmetry breaking.*

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1 Introduction

Symmetry is a theme of modern physics, which plays a crucial role in the understanding of fundamental interactions of the microscopic world[1] as well as the emergence of macroscopic orders.[2] It has become evident that both the elementary particle structure and the emergent phenomena, e.g., superconductivity and Bose–Einstein condensation, are originated from symmetry and its spontaneous breaking.[3−5] Its applications range from particle physics[6−9] to condensed matter physics,[10−11] and even to biological systems.[12−13]

Conventionally, symmetry is dealt in a dichotomous fashion that a physical system either possesses or not possesses a symmetry. In the group theoretical approach, the symmetry of a quantum system is usually considered by checking that if the system is invariant or not under some transformations, which sometimes form a symmetry group G. The symmetry breaking of the system can be described as a reduction of the symmetry group to its subgroup. Although this conventional approach has succeed in classifying the spectrum structure and even various phases of matters, it is not natural for us because there is not a room for the intermediate circumstance, namely, a continuous measure of symmetry has not been found. Actually, such intermediate issues exist objectively and need to be properly quantified. For example, a charged particle moving in a central potential possesses SO(3) symmetry. When a static magnetic field is applied, no matter how weak it is, the SO(3) symmetry is said to be broken into SO(2). However, SO(3) symmetry can still be approximately used to simplify the equations describing the dynamics and the energy level structure when the magnetic field is weak enough. Another example is the nuclear system that possesses the isospin SU(2) symmetry and thus its energy spectrum of strong interaction can approximately, but effectively, be classified, although the electromagnetic force could break this SU(2) symmetry.

In this regard, it would be of much interest to present a quantitative description of symmetry and its (spontaneous) breaking in this intermediate circumstance, which could determine the extent of approximation for using a given symmetry in practice. To this end, we, in this paper, introduce a continuous measure of symmetry, i.e., the degree of symmetry (DoS), by considering that symmetry is a relative concept: the particular subset G of all physically-allowed transformations needs to be specified for assigning a symmetry to a physical system. More specifically, for a given set G of transformations on the Hamiltonian or the quantum state $F = H$, or ρ, we first define a dual of DoS, the degree $A(G, F)$ of asymmetry (DoAS), by averaging the fidelity deviations (see definition below) over G. Generally, the DoAS ranges from zero to unity, and thus the DoS $S(G, F) = 1 - A(G, F)$ also satisfies $0 \le S(G, F) \le 1$. Evidently, $S(G, F)$ offers sym-

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metry an intermediate description to avoid the dichotomy in the conventional group theoretical analysis.

We will show that, if we choose G as a group, the DoS, bounded with $1/2 \le S(G,F) \le 1$, facilitates a general computable measure of symmetry based on the irreducible representations of G. It is potential in identifying various natures of symmetry that are important to emergent phenomena, such as the spontaneous symmetry breaking (SSB). For example, the thermodynamic SSB corresponds to multi-valued natures of DoS at the low temperature, which is similar to the depiction of the spontaneous magnetization.[14] It is also shown that the multi-level crossing by a proliferation of energy levels brings a peak to the DoS and the extended group can be given to account for the hidden symmetry from accidental degeneracy.

This paper is organized as follows: In Sec. 2, the DoS is introduced and its several properties as well as a computational feasible form are elucidated with the help of group theory. In Sec. 3, the general behavior of DoS under symmetry breaking is investigated, and the discussions are supported with two examples. The next two sections represent the applications of the DoS in identifying accidental level crossings as well as the spontaneous symmetry breaking. The conclusion is given in Sec. 6.

2 Degree of Symmetry

We consider a quantum system with Hamiltonian H, and a set G of n_G transformations on its Hilbert space $\mathcal{H}$. When $OHO^{-1} = H$ for $O \in G$, we say that H (the quantum system) is symmetric with respect to the transformation O. Actually, all symmetric transformations form a group $G'(\subset G)$. It is obvious that, the deviations of OHO^{-1} from H measure the extent of the asymmetry of H with respect to the transformation set. Thus, we use their average over G to define the degree of symmetry breaking (asymmetry) DoAS

$$A(G,H) = \frac{1}{4|\tilde{H}|^2}\overline{|[R(g),H]|^2}\,, \tag{1}$$

where $|O| = \sqrt{\mathrm{Tr}\{O^\dagger O\}}$ indicates the Frobenius norm[15] while $\overline{f(g)}|_G \equiv \overline{f(g)} = n_G^{-1}\sum_{g\in G} f(g)$ is an average of a (group) function $f(g)$ defined on G, and later the subscript G will be occasionally omitted; if G is a group, then $R: g \to R(g) \in \mathrm{End}\,(\mathcal{H})$ is a d-dimensional representation of $g \in G$. Otherwise, $R(g)$ represents a unitary transformation on $\mathcal{H}$. Here, $|[R(g),H]|^2 = |R(g)^\dagger H R(g) - H|^2$ is the fidelity deviation of H under the action of g, and $\tilde{H} = H - d^{-1}\mathrm{Tr}\{H\}$ is a re-biased Hamiltonian such that it is invariant under the zero-point energy shifting $H \to H + \epsilon$ for ϵ being a real number.

It is easy to prove that $0 \le A(G,H) \le 1$, thus the DoS defined by $S(G,H) = 1 - A(G,H)$ or

$$S(G,H) = \frac{1}{4|\tilde{H}|^2}\overline{|\{R(g),\tilde{H}\}|^2} \tag{2}$$

ranges from zero to unity and thus quantifies the extent of the symmetry of H with respect to G. The above definition of DoS is evidently reasonable in physics since it possesses the following properties (for the proofs see Appendix A): (i) Tighter bound when G forms a transformation group $0 \le A(G,H) \le 1/2 \le S(G,H) \le 1$; (ii) Independence of DoS on the basis, i.e., $S(WGW^\dagger, WHW^\dagger) = S(G,H)$, where W is a unitary transformation and $WGW^\dagger = \{WR(g)W^\dagger | g \in G\}$; (iii) Scaling invariance, i.e., $S(G,\lambda H) = S(G,H)$; (iv) Independence of the choice of the zero-point energy, i.e., $S(G,H+\epsilon) = S(G,H)$; (v) Hierarchy property $n_{G'}S(G_s,H) \le n_G S(G,H)$ for a subset $G_s(\subset G)$ with $n_{G'}$ elements.

When G becomes a group, in the spaces $\mathcal{H}^{(l)}$ of its l-th irreducible representations with finite dimensions d_l, the DoS $S = S(G,H)$ is re-expressed as

$$S = \frac{1}{2} + \sum_l \frac{1}{2d_l}\Big(\sum_\alpha \frac{\langle l,\alpha|H|l,\alpha\rangle}{|\tilde{H}|} - \frac{\mathrm{Tr}\{H\}d_l}{d|\tilde{H}|}\Big)^2\,, \tag{3}$$

where $|l,\alpha\rangle$ is a basis vector of $\mathcal{H}^{(l)}$ ($\alpha = 1,2,\ldots,d_l$), and we have used the completeness relations of irreducible representations (see Appendix B). The bisection point 1/2 from property (i) is also reflected in above equation, since each term contributes non-negatively in the summation over l. We point out that, by using Eq. (3), DoS is feasible to be computed based on the measurements with respect to the basis $\{|l,\alpha\rangle\}$. Otherwise, for a continuous group, a straightforward calculation of DoS from Eq. (2) should need to carry out the group integral with the Haar measure, e.g., the sum over SO(3) becomes a Lie group integral (see Eqs. (A44) and (A56)).

3 Symmetry Breaking

Let G be a symmetry group of the quantum system with Hamiltonian H. A perturbation $H' = \lambda V$ breaks the symmetry into the subgroup $G_s(\subset G)$, i.e., $[V,R(g)] \ne 0$ for $g \in G - G_s$ and $[V,R(g')] = 0$ for $g' \in G_s$. For the total Hamiltonian $H(\lambda) = H + \lambda V$, we calculate the DoS under the symmetry breaking (see Appendix C)

$$S(G,H(\lambda)) = 1 - \frac{A(G,V)\lambda^2}{\lambda^2 + \xi\lambda + \eta}\,, \tag{4}$$

where $A(G,V)$ is the DoAS of the Hermitian operator V, the other two coefficients are defined as $\xi = 2\mathrm{Tr}\{\tilde{H}\tilde{V}\}|\tilde{V}|^{-2}$ and $\eta = |\tilde{H}|^2|\tilde{V}|^{-2}$. The above equation exactly reflects the duality between symmetry and asymmetry: the maximal symmetry breaking due to the perturbation corresponds to the minimal symmetry of the considered system. When $|\lambda|$ is increased, there exists a special point $\lambda_A = -2\xi^{-1}\eta$ where the DoS reaches a local minimum $S_{\min} = 1 - A(G,V)\csc^2\varphi$; here φ is the angle between $\tilde{H}$ and $\tilde{V}$ (see Eq. (A35)).

The following two examples are used to illustrate the above conception on quantifying the extent of symmetry and its breaking. First, let us consider a particle residing on a four-site lattice with the following Hamiltonian

$$H = \sum_i \epsilon|i\rangle\langle i| + \sum_{ij} h|i\rangle\langle j|\,, \tag{5}$$

where $|i\rangle$ ($i = 0,1,2,3$) is the single particle state with site i occupied. The site energy ϵ and the hopping strength h are site-independent for the regular tetrahedron geometry (see Fig. 1(a)), and thus H is symmetric to all transformations from the T_d group, which contains (combined) rotations and mirror reflections sending a regular tetrahedron into itself.[16] In this example, we let the symmetry T_d break into C_{3v} through the following perturbation

$$H' = \lambda\Big[\delta_0|0\rangle\langle 0| + \delta_1 \sum_{i=1}^{3}(|i\rangle\langle 0| + \text{h.c.})\Big], \quad (6)$$

where $\lambda\delta_0$ and $\lambda\delta_1$ are the deviations of the energy and the coupling related to the 0-th site. It is well known that C_{3v} has two one-dimensional irreducible representations A_1 and A_2, as well as one two-dimensional irreducible representation E,[16] which correspond to the three kinds of energy levels with one or two-fold degeneracies.

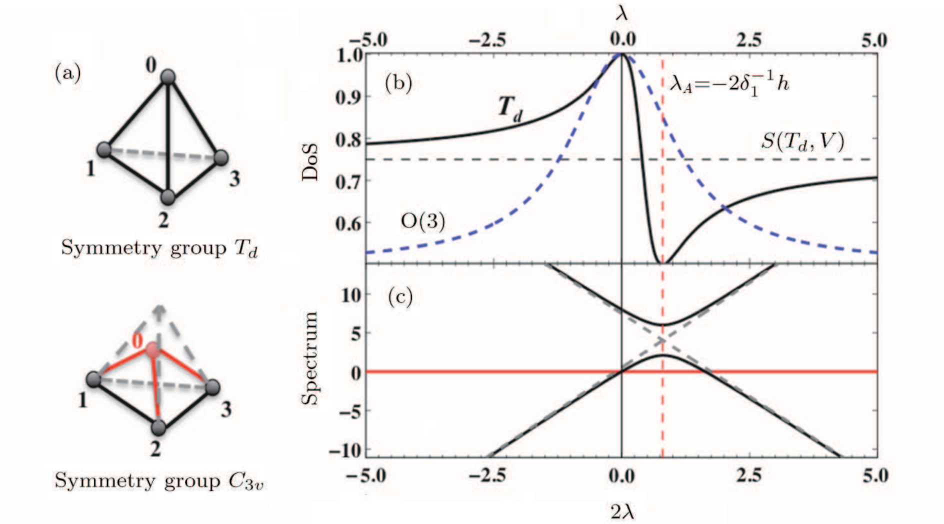

Fig. 1 (Color online) (a) Top: Schematic of a four-site lattice arranged into the regular tetrahedron geometry, with Hamiltonian H and symmetry group T_d. Bottom: The T_d symmetry is broken into C_{3v} upon adding the perturbation $H' = \lambda V$, which changes the hopping strength as well as the site energy relevant for the 0th site. (b) Degree of symmetry (DoS) vs. λ for the four-site model (black solid) and the angular momentum model (blue dashed). The asymptotic value $S(T_d, V)$ (black dashed) and the local minimum λ_A (red vertical line) for the four-site model are also shown. (c) Energy spectrum of the four-site model vs. 2λ. Red line indicates the two degenerate E levels. Avoid level crossing of the two A_1 levels is shown by the grey dashed lines.

The above symmetry breaking from T_d to C_{3v} is quantified by the DoS through Eq. (4) with $G = T_d$. Straightforward calculation shows exact results $A(T_d, V) = (2\gamma^2 + 16)^{-1}(\gamma^2 + 4)$, $\xi = 16(\gamma^2 + 8)^{-1}\delta_1^{-1}h$, and $\eta = \xi\delta_1^{-1}h$. Here, $\gamma = \delta_1^{-1}\delta_0$ is the ratio between the two parameters in H'. As shown in Fig. 1(b), the DoS reaches unity when $\lambda = 0$, indicating the full T_d symmetry that possessed by the original Hamiltonian H. The symmetry breaking perturbation H' suppresses the DoS first quadratically in λ and then, as $|\lambda|$ further increased to approach the strong perturbing limit ($|\lambda| \to \infty$), reaches a γ-dependent asymptotically value $(2\gamma^2 + 16)^{-1}(\gamma^2 + 12)$.

In this model, the special point $\lambda_A = -2\delta_1^{-1}h$, where the DoS reaches the local minimum, indicates an avoid level crossing in the energy spectrum. To see this, we rewrite $H(\lambda)$ in terms of the standard basis of irreducible representations by using the projection operator method.[16–17] The resulting four-dimensional Hilbert space contains two A_1-representations and one E-representation of C_{3v}.[16] The two levels that transform according to the two A_1-representations are coupled and the corresponding avoid level crossing point λ_* is related to λ_A by

$$\lambda_* = \frac{6-\gamma}{12+\gamma^2}\lambda_A\,. \quad (7)$$

Especially, for $\delta_0 \ll \delta_1$ the avoid level crossing happens approximately at $\lambda_A/2$ (see Figs. 1(b) and 1(c)).

Another example demonstrates the DoS of the breaking of the continuous symmetry. The system we considered is a particle with angular momentum j, whose Hamiltonian reads

$$H = \epsilon J^2\,, \quad H' = \lambda J_z\,, \quad (8)$$

where J_i ($i = x, y, z$) are components of the angular momentum operator and $J^2 = J_x^2 + J_y^2 + J_z^2$. In this model, the O(3) symmetry of H is broken by the perturbation, described by H', to O(2). With $G = \mathrm{O}(3)$, the DoS is calculated as $1 - [2\lambda^2 + \epsilon^2 j(j+2)]^{-1}\lambda^2$ (see Appendix D). Unlike the previous model, here the DoS does not show a local minimum and decays monotonically as $|\lambda|$ increasing. Comparison with the generic result Eq. (4) indicates the underlying condition $\mathrm{Tr}\{\tilde{H}\tilde{V}\} = 0$, which is fulfilled by the Hamiltonian Eq. (8).

4 Accidental Degeneracy

Accidental degeneracy of energy levels appears in a quantum system when its parameters are changed to cause a level crossing. It is usually not relevant to the geometric symmetry, but our DoS can reveal the existence of the hidden symmetry. Actually, accidental degeneracy also implies symmetry. The greater the degeneracy, the greater the symmetry.

For the general Hamiltonian $H(\lambda)$ defined above, we introduce the additional transformations: the U(2) operations on the two λ-dependent energy levels of $H(\lambda)$ (or U(N) operations for the more general N levels crossing), which will become degenerate as λ tuned to λ_0. Because $H(\lambda_0)$ is proportional to the identity operator in the degenerate subspace and, as a result, commuted with all U(2) operations, the symmetry group G of $H(\lambda_0)$ is extended to a larger one $G_T = \langle G, \mathrm{U}(2)\rangle$, which is generated by elements in G and U(2). It is expected that the behavior of DoS could manifest the hidden symmetry that implied by the enlarged group G_T: the level crossing at λ_0 could result in a local dip in the DoAS, when the parameter λ is tuned close to λ_0. To see this, we expand the Hamiltonian linearly around λ_0, i.e., $H(\lambda) \approx H(\lambda_0)+\partial_\lambda H(\lambda_0)(\lambda-\lambda_0)$. Since $[R(g), H(\lambda_0)] = 0$ for $g \in G_T$, the DoAS is written as

$$A(G_T, H(\lambda)) \propto A(G_T, \partial_\lambda H(\lambda_0))(\lambda - \lambda_0)^2\,. \qquad (9)$$

Thus, by the duality, the accidental degeneracy indeed manifests itself as a local maximum at λ_0 in DoS.

To illustrate the above idea, we consider the following three-site model whose Hamiltonian is of the same form as Eq. (5) except that $i \in \{1, 2, 3\}$. And the perturbation term

$$H' = \lambda[|1\rangle\langle 1| + |3\rangle\langle 3| - (|1\rangle\langle 3| + \mathrm{h.c.})] \qquad (10)$$

breaks the symmetry from D_3 to $Z_2 = \{e, \sigma\}$. Here, the transformation σ interchanges the basis state $|1\rangle$ with $|3\rangle$. The energy spectrum of $H(\lambda)$ contains two Γ_1 levels $E_{1\pm} = \epsilon+h/2\pm\lambda_{02}$ and one Γ_2 level $E_2 = \epsilon-h+2\lambda$, where $\Gamma_{i=1,2}$ are two irreducible representations of Z_2. The spectrum shows two accidental degeneracies between the Γ_1 and the Γ_2 levels at $\lambda_{01} = 0$ and $\lambda_{02} = 3h/2$, respectively (see Fig. 2(b)).

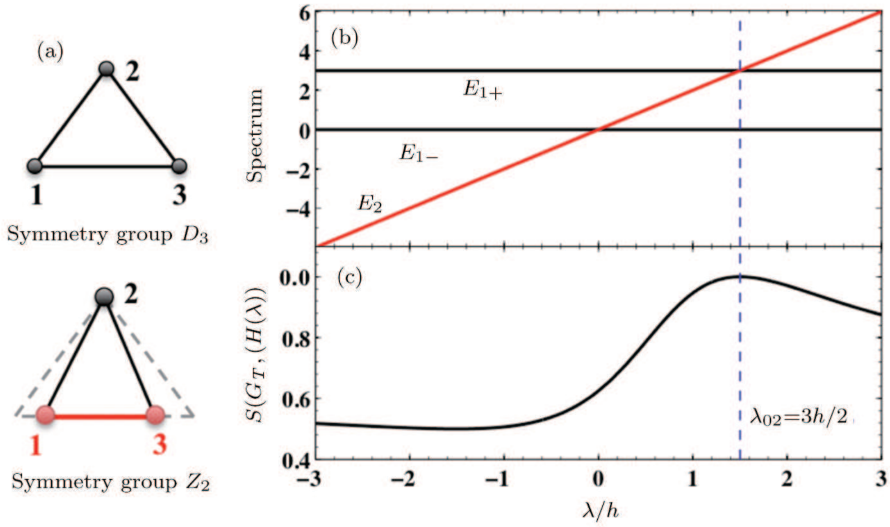

Fig. 2 (Color online) (a) Schematics of the three-site model, with symmetry D_3 breaking into Z_2 by the perturbation Eq. (10). (b) Energy spectrum vs. λ/h for the three-site model, showing two accidental degeneracies at λ_{01} and λ_{02} (blue vertical line). (c) DoS vs. λ/h with respect to G_T, showing that the accidental degeneracy at λ_{02} is identified with the maximum of the DoS.

Indeed, at the accidental degeneracy, $H(\lambda_{02})$ becomes more symmetric since there exists the additional symmetric transformations of U(2): $R(\omega_0; \hat{n}, \omega) = \exp[\mathrm{i}(\omega_0 - \hat{n}\cdot\vec{s}\omega)]$ with pseudo spin-1/2 operators $\vec{s}$ defined by $s_x = (|\psi_{1+}\rangle\langle\psi_2| + |\psi_2\rangle\langle\psi_{1+}|)/2$ *et al.* Here, $|\psi_m\rangle$ is the eigenstate associated with level E_m. The extended symmetry group G_T for $H(\lambda_{02})$ is still U(2) since $Z_2 \subset$ U(2) (see Appendix E). Thus, the two-fold degenerate subspace supports a two-dimensional irreducible representation of G_T. It is shown that the DoS $S(G_T, H(\lambda))=1 - 3[\lambda^2 - \lambda_{02}\lambda + \lambda_{02}^2]^{-1}(\lambda - \lambda_{02})^2/8$ reaches the unity when $\lambda = \lambda_{02}$ (see Fig. 2(c)). Therefore, the DoS indeed signals the hidden symmetry. We notice that, without the geometric symmetry, the above U(2) symmetry defined in the subspace spanned by $|\psi_{1+}\rangle$ and $|\psi_2\rangle$ at the accidental degenerate point is similar to the dynamical symmetry SO(4) of the non-relativistic hydrogen atom.[18]

5 Degree of Symmetry of Quantum State and Spontaneous Symmetry Breaking

In emergent phenomena, the symmetry of the system ground state can be different from that of the underlying Hamiltonian or Lagrangian. This difference is roughly regarded as the spontaneous symmetry breaking (SSB).[2,5,9] For a better depiction of those phenomena, we need to introduce the DoS of quantum state (DoSS) ρ. The similar issue has been investigated through asymmetry measure,[19−21] which was found to give more stringent restrictions to dynamics than Noether's theorem,[22] and was shown to be linked with interesting topics such as finding tighter quantum speed limits;[23] other direct definition through the entropy has also been introduced.[24−26]

Here, we use an analog to the DoS of Hamiltonian Eq. (2) to define the DoSS as

$$S(G,\rho)=\frac{1}{4|\rho|^2}\overline{|\{R(g),\rho\}|^2}\,, \tag{11}$$

where ρ is the density matrix of a quantum state. Advantages of above definition instead of the entropy one is that this definition automatically possesses the similar properties (1)–(5) except for $S(G,\rho)=S(G,\rho+\epsilon)$, which we need not to require for physics.

We now use DoSS to characterize the SSB in thermodynamics. We consider the thermalization of a quantum system with degenerate ground states $\{|G_\alpha\rangle|\alpha=1,2,\ldots,d_G\}$, i.e., $H|G_\alpha\rangle=\varepsilon_0|G_\alpha\rangle$.[27] At the zero temperature such system will have a non-vanishing entropy $S=k_{\rm B}\ln d_G$, known as the modified third law of thermodynamics.[14] By introducing a perturbation $H'=\lambda V$ to break the symmetry so that $|G_{\alpha=0}=G_0\rangle$ becomes the unique ground state, the thermodynamic SSB is described as the following two non-commutative limiting processes: (i) $T\to 0$ and then $\lambda\to 0$; (ii) $\lambda\to 0$ and then $T\to 0$. In these two non-commutative limiting processes, the following state

$$\rho=\frac{1}{Z}\sum\nolimits_{\alpha\neq 0}{\rm e}^{-\varepsilon_\alpha/T}|G_\alpha\rangle\langle G_\alpha| + \frac{1}{Z}{\rm e}^{-\varepsilon_0/T}|G_0\rangle\langle G_0|+\cdots \tag{12}$$

will approach to

$$\rho_{f1}=|G_0\rangle\langle G_0|\,,\quad \rho_{f2}=d_G^{-1}\sum_\alpha|G_\alpha\rangle\langle G_\alpha|$$

respectively (see Fig. 3(a)).

To see the quantitative details of such thermodynamic SSB, we use the DoSS defined by Eq. (11). Let G be a symmetry group of H, and $\{|G_\alpha\rangle\}$ span an irreducible representation of G. Because ρ_{f2} is proportional to the identity operator, thus $[R(g),\rho_{f2}]=0$. This implies that the limiting process (ii) results in a final state with $S(G,\rho_{f2})=1$. On the other hand, from Schur's theorem,[16] in the limiting process (i) there always exists some $g\in G$ such that $[R(g),\rho_{f1}]\neq 0$ and consequently $S(G,\rho_{f1})<1$. This in turn implies an SSB since the final state ρ_{f1} does not retain the full symmetry of the underlying microscopic Hamiltonian H.

The above relation between the DoSS and $\rho_{f1,2}$ suggests the multi-valued natures of DoSS at $(T=0,\ \lambda=0)$ upon different limiting processes as an SSB witness

$$\lim_{\beta\to\infty}\lim_{\lambda\to 0}S(G,\rho)=1\,,\quad \lim_{\lambda\to 0}\lim_{\beta\to\infty}S(G,\rho)<1\,, \tag{13}$$

where $\beta=1/T$ is the inverse temperature.

To illustrate the SSB with an example, let us consider the angular momentum model Eq. (8) again, which shows a spontaneous breaking of O(3) symmetry. In the subspace with $j=1/2$, the ground state is two-fold degenerate without H', i.e., $|1/2,\pm 1/2\rangle$. For a generic thermal state $\rho=Z^{-1}\exp[-\beta H(\lambda)]$, DoSS is shown to be $S({\rm O}(3),\rho)=(3+\cosh^{-1}\beta\lambda)/4$ (see Appendix F), whose multi-valued natures at $(T=0,\ \lambda=0)$ is shown in Fig. 3(b). Specifically, when $\beta\epsilon\gg 1$ while $\lambda\neq 0$ the DoSS is nearly at a constant value $3/4$. Then, by tuning the coupling λ to zero, the DoSS remains fixed at the same constant value (see (i) in Fig. 3(b)). In contrast, if one first fixes the coupling $\lambda=0$ at the high temperature, the DoSS as a function of β from zero to infinity will follow the blue arrowed line (corresponding to the possess (ii)) in Fig. 3(b). In the latter case, the DoSS at large β is unity. In analog to Eq. (13), in this example it is shown that

$$\lim_{\beta\to\infty}\lim_{\lambda\to 0}S(G,\rho)=1\,,\quad \lim_{\lambda\to 0}\lim_{\beta\to\infty}S(G,\rho)=\frac{3}{4}\,. \tag{14}$$

Here, $G={\rm O}(3)$. On the other hand, the difference in DoSS reflected by above equations is also understood through inspecting on the final state, which is $\rho_{f1}=|1/2,-1/2\rangle\langle 1/2,-1/2|$ or $\rho_{f2}=2^{-1}\sum_m|1/2,m\rangle\langle 1/2,m|$ upon limiting processes (i/ii). Clearly, ρ_{f1} is not invariant under the π-rotation that represented by the σ_x operation in the $j=1/2$ subspace, thus results in a DoSS smaller than unity.

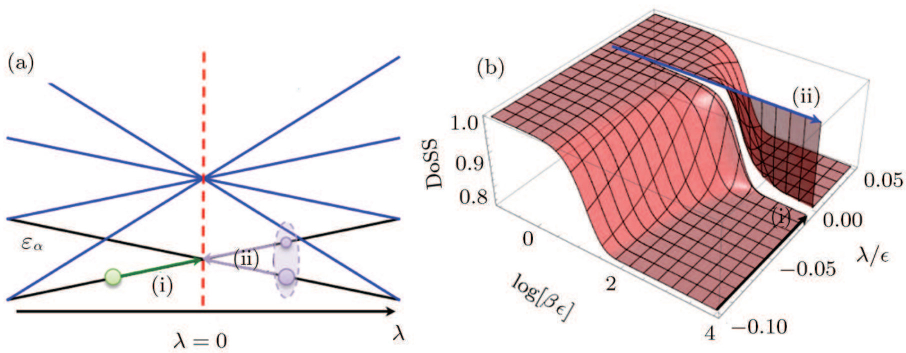

Fig. 3 (Color online) (a) Energy spectrum of a system with degenerate ground states $\{|G_\alpha\rangle\}$ at $\lambda=0$. Upon whether $T\to 0$ (i) before or (ii) after $\lambda\to 0$, the thermal equilibrium state Eq. (12) approaches different final states. (b) DoS of quantum state (DoSS) $S({\rm O}(3),\rho)$ vs. λ/ϵ and $\beta\epsilon$ for the angular momentum model. The multi-valued natures of the DoSS at $T=0$ and $\lambda=0$ are reflected as the two non-commuting limiting processes indicated by (i) and (ii).

6 Conclusion

In this paper, we introduce a continuous measure, the degree of symmetry (DoS), for the symmetry of quantum system, which largely extrapolates the dichotomous approach of symmetry based on group representation theory. It is shown that the DoS possesses some good properties, such as basis-independent, invariant under the zero-point energy shifting as well as the scaling transformation. Since it can be expressed as an average of physical operators under the basis of irreducible representations for transformation groups, this measure is thus computable and detectable based on some quantum measurements.

In contrast to the previous explorations based on the abstract concepts of fuzz set[28] and transform information,[29] our introduced DoS can feasibly open many applications in physics. As illustrated in this paper, the DoS is capable of identifying symmetry relevant phenomena and effects, such as the accidental level crossings and the spontaneous symmetry breaking. This, therefore, implies that the DoS could be a useful measure in related future studies, e.g., in characterizing systems near quantum criticality since it is closely related to the multi-level crossings.[30]

Appendices

Following appendices are organized as follows: In appendix A we provide proofs to several properties of the degree of symmetry (DoS) that have been mentioned in the main text. In appendix B, the DoS is rewritten under the basis of the irreducible representations of transformation group. In appendix C, the generic expression for DoS under symmetry breaking perturbation is derived and the existence of a special point λ_A where the DoS reaches local minimum is discussed. Finally, the calculation details to three examples in the main text are given in appendices D, E, and F, respectively.

Appendix A: Proofs to Properties of the DoS

In the following we present the proofs to five basic properties of DoS $S(G,H)$. To do so, we first show that the degree of asymmetry (DoAS) $A(G,H)$ is bounded, i.e., $0 \leq A(G,H) \leq 1$.

Proof Firstly, for any operator O,

$$|O|^2 = \mathrm{Tr}\{O^\dagger O\} \geq 0\,. \tag{A1}$$

The equality holds if and only if $O=0$. As a consequence,

$$A(G,H) = \frac{1}{4|\tilde{H}|^2}\overline{|[R(g),H]|^2} \geq 0\,. \tag{A2}$$

Then, according to Schwarz inequality $|\mathrm{Tr}\{A^\dagger B\}| \leq \sqrt{\mathrm{Tr}\{A^\dagger A\}\mathrm{Tr}\{B^\dagger B\}}$,

$$\begin{aligned}
A(G,H) =& \frac{1}{4|\tilde{H}|^2}\overline{|[R(g),H]|^2} = \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G}|[R(g),H]|^2 \\
=& \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G}|[R(g),\tilde{H}]|^2 \\
=& \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G}2\mathrm{Tr}\{\tilde{H}\tilde{H}\} - \mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\} \\
&- \mathrm{Tr}\{\tilde{H}R(g)^\dagger\tilde{H}R(g)\} \\
\leq& \frac{1}{2|\tilde{H}|^2 n_G}\sum_{g\in G}\mathrm{Tr}\{\tilde{H}\tilde{H}\} + |\mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\}| \\
\leq& \frac{1}{2|\tilde{H}|^2 n_G}\sum_{g\in G}[\mathrm{Tr}\{\tilde{H}\tilde{H}\} + \sqrt{\mathrm{Tr}\{\tilde{H}^2\}^2}] \\
=& \frac{1}{|\tilde{H}|^2 n_G}\sum_{g\in G}\mathrm{Tr}\{\tilde{H}\tilde{H}\} = 1\,,
\end{aligned} \tag{A3}$$

where $\sqrt{\mathrm{Tr}\{\tilde{H}^2\}^2} = \mathrm{Tr}\{\tilde{H}^2\}$ has been used in above derivation, since the spectrum of $\tilde{H}^2$ is non-negative.

Now let us consider the five properties of DoS $S(G,H)$:

Property 1 Tighter bound when G forms a transformation group

$$0 \leq A(G,H) \leq \frac{1}{2} \leq S(G,H) \leq 1\,. \tag{A4}$$

Proof When G admits a group structure, then the rearrangement theorem is applicable and, consequently, the average of a group function is invariant under the multiplication by a same group element to each one of the summing terms

$$\frac{1}{n_G}\sum_{g\in G}f(g) = \frac{1}{n_G}\sum_{g\in G}f(gg_1)\,, \tag{A5}$$

where $g_1 \in G$ is fixed. By summing over g_1 in Eq. (A5),

$$\sum_{g\in G}f(g) = \frac{1}{n_G}\sum_{g_1\in G}\sum_{g_2\in G}f(g_1g_2)\,. \tag{A6}$$

Furthermore, because both g and g^{-1} contribute in the group function averaging, then it is also essential that $\sum_g f(g) = \sum_g f(g^{-1})$.

Now, one can show that $\sum_g \mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\}$, which appears in Eq. (A3), is actually non-negative. The reasoning is as follows

$$\begin{aligned}
&\sum_{g\in G}\mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\} \\
&= \frac{1}{n_G}\sum_{g_1\in G}\sum_{g_2\in G}\mathrm{Tr}\{R(g_1g_2)^\dagger\tilde{H}R(g_1g_2)\tilde{H}\} \\
&= \frac{1}{n_G}\sum_{g_1\in G}\sum_{g_2\in G}\mathrm{Tr}\{R(g_2)^\dagger R(g_1)^\dagger\tilde{H}R(g_1)R(g_2)\tilde{H}\} \\
&= \frac{1}{n_G}\mathrm{Tr}\Big\{\sum_{g_1\in G}R(g_1)^\dagger\tilde{H}R(g_1)\sum_{g_2\in G}R(g_2)\tilde{H}R(g_2)^\dagger\Big\} \\
&= \frac{1}{n_G}\mathrm{Tr}\Big\{\sum_{g_1\in G}R(g_1)^\dagger\tilde{H}R(g_1)\sum_{g_2\in G}R(g_2)^\dagger\tilde{H}R(g_2)\Big\} \\
&= \mathrm{Tr}\Big\{\Big(\frac{1}{\sqrt{n_G}}\sum_{g\in G}R(g)^\dagger\tilde{H}R(g)\Big)^2\Big\}\,,
\end{aligned} \tag{A7}$$

which is the trace of a squared Hermitian operator, whose eigenvalues are real and non-negative. This implies that

Eq. (A7) is non-negative

$$\sum_{g\in G}\mathrm{Tr}\{R(g)^\dagger \tilde{H} R(g)\tilde{H}\}\geq 0\,. \tag{A8}$$

Then, it follows from the fourth line in Eq. (A3) that

$$\begin{aligned}A(G,H) &= \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G} 2\mathrm{Tr}\{\tilde{H}\tilde{H}\} - 2\mathrm{Tr}\{R(g)^\dagger \tilde{H} R(g)\tilde{H}\}\\ &\leq \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G} 2\mathrm{Tr}\{\tilde{H}\tilde{H}\} = \frac{1}{2}\,.\end{aligned} \tag{A9}$$

Together with Eq. (A2), then it follows that $0 \leq A(G,H) \leq 1/2$. By definition $S(G,H) = 1 - A(G,H)$, thus $1/2 \leq S(G,H) \leq 1$.

Property 2 Independence of DoS on the basis

$$S(WGW^\dagger, WHW^\dagger) = S(G,H)\,, \tag{A10}$$

where $WGW^\dagger$ is understood as performing the unitary transformation W on the representation $R(g)$, to $WR(g)W^\dagger$, with $g \in G$.

Proof Since

$$\begin{aligned}\widetilde{WHW^\dagger} &= WHW^\dagger - \frac{1}{d}\mathrm{Tr}\{WHW^\dagger\}\\ &= WHW^\dagger - \frac{1}{d}\mathrm{Tr}\{H\}\\ &= W\Big(H - \frac{1}{d}\mathrm{Tr}\{H\}\Big)W^\dagger = W\tilde{H}W^\dagger\,,\end{aligned} \tag{A11}$$

thus

$$\begin{aligned}&S(WGW^\dagger, WHW^\dagger)\\ &= \frac{1}{4|\widetilde{WHW^\dagger}|^2}\overline{|\{WR(g)W^\dagger, \widetilde{WHW^\dagger}\}|^2}\\ &= \frac{1}{4|W\tilde{H}W^\dagger|^2}\overline{|\{WR(g)W^\dagger, W\tilde{H}W^\dagger\}|^2}\\ &= \frac{1}{4|W\tilde{H}W^\dagger|^2}\overline{|W\{R(g),\tilde{H}\}W^\dagger|^2}\,,\end{aligned} \tag{A12}$$

but since

$$|WOW^\dagger|^2 = \mathrm{Tr}\{WO^\dagger W^\dagger WOW^\dagger\} = |O|^2\,, \tag{A13}$$

thus Eq. (A12) is written as follows

$$\begin{aligned}&S(WGW^\dagger, WHW^\dagger)\\ &= \frac{1}{4|\tilde{H}|^2}\overline{|\{R(g),\tilde{H}\}|^2} = S(G,H)\,.\end{aligned} \tag{A14}$$

Property 3 Scaling invariance

$$S(G,\lambda H) = S(G,H)\,, \tag{A15}$$

Proof It is easy to prove.

Property 4 Invariance under the zero-point energy shifting

$$S(G, H+\epsilon) = S(G,H)\,. \tag{A16}$$

Proof

$$\begin{aligned}S(G,H+\epsilon) &= \frac{1}{4|\widetilde{H+\epsilon}|^2}\overline{|\{R(g),\widetilde{H+\epsilon}\}|^2}\\ &= \frac{\overline{|\{R(g), H+\epsilon - \frac{1}{d}\mathrm{Tr}\{H+\epsilon\}\}|^2}}{4|H+\epsilon - \mathrm{Tr}\{H+\epsilon\}/d|^2}\\ &= \frac{1}{4|H - \mathrm{Tr}\{H\}/d|^2}\\ &\quad\times \overline{|\{R(g), H+\epsilon - \frac{1}{d}\mathrm{Tr}\{H+\epsilon\}\}|^2}\\ &= \frac{1}{4|\tilde{H}|^2}\overline{|\{R(g), H - \frac{1}{d}\mathrm{Tr}\{H\}\}|^2}\\ &= S(G,H)\,.\end{aligned} \tag{A17}$$

Property 5 Hierarchy property

$$n_{G'}S(G_s,H) \leq n_G S(G,H)\,, \tag{A18}$$

where $G_s(\subset G)$ contains $n_{G'}$ elements.

Proof

$$\begin{aligned}S(G,H) &= \frac{1}{4|\tilde{H}|^2}\overline{|\{R(g),\tilde{H}\}|^2}\\ &= \frac{1}{4|\tilde{H}|^2 n_G}\sum_{g\in G}|\{R(g),\tilde{H}\}|^2\\ &= \frac{n_{G'}}{n_G}\frac{1}{4|\tilde{H}|^2 n_{G'}}\Big[\sum_{g\in G_s}|\{R(g),\tilde{H}\}|^2\\ &\quad + \sum_{g\in G-G_s}|\{R(g),\tilde{H}\}|^2\Big]\\ &\geq \frac{n_{G'}}{n_G}\frac{1}{4|\tilde{H}|^2 n_{G'}}\sum_{g\in G_s}|\{R(g),\tilde{H}\}|^2\\ &= \frac{n_{G'}}{n_G}\frac{1}{4|\tilde{H}|^2}\overline{|\{R(g),\tilde{H}\}|^2}|_{G_s}\\ &= \frac{n_{G'}}{n_G}S(G_s,H)\,,\end{aligned} \tag{A19}$$

thus

$$n_{G'}S(G_s,H) \leq n_G S(G,H)\,. \tag{A20}$$

Appendix B: DoS in Irreducible Representation Space

To carry out the average of the DoS over the transformation group G, we start from Eq. (2) of the main text

$$\begin{aligned}S(G,H) &= \frac{1}{4|\tilde{H}|^2}\overline{|\{R(g),\tilde{H}\}|^2}\\ &= \frac{1}{4|\tilde{H}|^2}\frac{1}{n_G}\sum_{g\in G}|\{R(g),\tilde{H}\}|^2\\ &= \frac{1}{4|\tilde{H}|^2}\frac{1}{n_G}\sum_{g\in G}\mathrm{Tr}\{(R(g)^\dagger\tilde{H} + \tilde{H}R(g)^\dagger)\\ &\quad\times (R(g)\tilde{H} + \tilde{H}R(g))\}\\ &= \frac{1}{4|\tilde{H}|^2}\frac{1}{n_G}\sum_{g\in G}[2\mathrm{Tr}\{H^2\} + 2\mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\}]\\ &= \frac{1}{2} + \frac{1}{2|\tilde{H}|^2}\frac{1}{n_G}\sum_{g\in G}\mathrm{Tr}\{R(g)^\dagger\tilde{H}R(g)\tilde{H}\}\,.\end{aligned} \tag{A21}$$

In the irreducible representation space of G, $R(g)$ has the following direct-sum decomposition

$$R(g) = \sum_l \sum_{\alpha,\beta=1}^{d_l} R_{\alpha\beta}^{(l)} |l,\alpha\rangle\langle l,\beta| \,. \tag{A22}$$

It follows from Eq. (A22) that

$$\begin{aligned}
&\frac{1}{n_G}\sum_{g\in G}\mathrm{Tr}\{R(g)^\dagger \tilde{H} R(g)\tilde{H}\} \\
&= \frac{1}{n_G}\sum_{g\in G}\sum_{ll'}\sum_{\alpha,\beta=1}^{d_l}\sum_{\alpha',\beta'=1}^{d_{l'}} \mathrm{Tr}\{R_{\alpha\beta}^{(l)}(g)^*|l,\beta\rangle\langle l,\alpha| \\
&\quad \times \tilde{H} R_{\alpha'\beta'}^{(l')}(g)|l',\alpha'\rangle\langle l',\beta'|\tilde{H}\} \\
&= \sum_{ll'}\sum_{\alpha\alpha'\beta\beta'} \langle l,\alpha|\tilde{H}|l',\alpha'\rangle\langle l',\beta'|\tilde{H}|l,\beta\rangle \\
&\quad \times \Big[\frac{1}{n_G}\sum_{g\in G} R_{\alpha\beta}^{(l)}(g)^* R_{\alpha'\beta'}^{(l')}(g)\Big] \,.
\end{aligned} \tag{A23}$$

By applying the completeness relations of irreducible representations

$$\frac{d_l}{n_G}\sum_{g\in G} R_{\alpha\beta}^{(l)}(g)^* R_{\alpha'\beta'}^{(l')}(g) = \delta_{ll'}\delta_{\alpha\alpha'}\delta_{\beta\beta'} \,. \tag{A24}$$

Equation (A23) is rewritten as

$$\begin{aligned}
&\sum_{ll'}\sum_{\alpha\alpha'\beta\beta'} \langle l,\alpha|\tilde{H}|l',\alpha'\rangle\langle l',\beta'|\tilde{H}|l,\beta\rangle \frac{1}{d_l}\delta_{ll'}\delta_{\alpha\alpha'}\delta_{\beta\beta'} \\
&= \sum_l \frac{1}{d_l}\sum_{\alpha,\beta=1}^{d_l} \langle l,\alpha|\tilde{H}|l,\alpha\rangle\langle l,\beta|\tilde{H}|l,\beta\rangle \\
&= \sum_l \frac{1}{d_l}\Big(\sum_{\alpha=1}^{d_l}\langle l,\alpha|\tilde{H}|l,\alpha\rangle\Big)^2 \,.
\end{aligned} \tag{A25}$$

Insert Eq. (A25) into Eq. (A21) gives

$$\begin{aligned}
S(G,H) &= \frac{1}{2} + \frac{1}{2|\tilde{H}|^2}\sum_l \frac{1}{d_l}\Big(\sum_{\alpha=1}^{d_l}\langle l,\alpha|\tilde{H}|l,\alpha\rangle\Big)^2 \\
&= \frac{1}{2} + \frac{1}{2|\tilde{H}|^2}\sum_l \frac{1}{d_l}\Big(\sum_{\alpha=1}^{d_l}\langle l,\alpha|H - \frac{1}{d}\mathrm{Tr}\{H\}|l,\alpha\rangle\Big)^2 \\
&= \frac{1}{2} + \frac{1}{2|\tilde{H}|^2}\sum_l \frac{1}{d_l}\Big(\sum_{\alpha=1}^{d_l}\langle l,\alpha|H|l,\alpha\rangle - \frac{d_l}{d}\mathrm{Tr}\{H\}\Big)^2 \\
&= \frac{1}{2} + \sum_l \frac{1}{2d_l}\Big(\sum_{\alpha=1}^{d_l}\frac{\langle l,\alpha|H|l,\alpha\rangle}{|\tilde{H}|} - \frac{\mathrm{Tr}\{H\}d_l}{d|\tilde{H}|}\Big)^2 .
\end{aligned} \tag{A26}$$

Appendix C: Generic Behavior of DoS under Symmetry Breaking Perturbation

The generic expression for the DoS of a Hamiltonian $H(\lambda) = H + \lambda V$ with respect to a symmetry group G of H is written as

$$\begin{aligned}
S(G,H(\lambda)) &= 1 - A(G, H+\lambda V) \\
&= 1 - \frac{1}{4|\tilde{H}(\lambda)|^2}\overline{|[R(g), H+\lambda V]|^2} \\
&= 1 - \frac{1}{4|\tilde{H}(\lambda)|^2}\overline{|[R(g), V]|^2}\lambda^2 \,,
\end{aligned} \tag{A27}$$

where the relation $[R(g), H] = 0$ has been used in above derivation. The denominator is calculated as

$$\begin{aligned}
|\tilde{H}(\lambda)|^2 &= |H(\lambda) - \frac{1}{d}\mathrm{Tr}\{H(\lambda)\}|^2 \\
&= |\tilde{H}|^2 + 2\Big[\mathrm{Tr}\{HV\} - \frac{1}{d}\mathrm{Tr}\{H\}\mathrm{Tr}\{V\}\Big]\lambda + |\tilde{V}|^2\lambda^2 .
\end{aligned} \tag{A28}$$

Thus Eq. (A27) is written as follows

$$\begin{aligned}
S(G,H(\lambda)) &= 1 - \frac{\overline{|[R(g), V]|^2}}{4|\tilde{V}|^2}\frac{\lambda^2}{\lambda^2 + \xi\lambda + \eta} \\
&= 1 - \frac{A(G,V)\lambda^2}{\lambda^2 + \xi\lambda + \eta} \,,
\end{aligned} \tag{A29}$$

where

$$\xi = \frac{2}{|\tilde{V}|^2}\Big[\mathrm{Tr}\{HV\} - \frac{1}{d}\mathrm{Tr}\{H\}\mathrm{Tr}\{V\}\Big] = \frac{2\mathrm{Tr}\{\tilde{H}\tilde{V}\}}{|\tilde{V}|^2}, \tag{A30}$$

$$\eta = \frac{|\tilde{H}|^2}{|\tilde{V}|^2} \,. \tag{A31}$$

Equation (A29) implies that

$$\frac{\partial}{\partial\lambda}S(G,H(\lambda)) = \frac{(2\eta + \xi\lambda)\lambda}{(\lambda^2 + \xi\lambda + \eta)^2}A(G,V) \,. \tag{A32}$$

Thus when $\lambda = \lambda_A = -2\eta/\xi$, the DoS reaches an extreme value (minimum)

$$S_{\min} = S(G, H + \lambda_A V) = 1 - \frac{4\eta}{4\eta - \xi^2}A(G,V) . \tag{A33}$$

It follows from Eqs. (A30) and (A31) that

$$\begin{aligned}
S_{\min} &= 1 + \frac{|\tilde{H}|^2|\tilde{V}|^2}{\mathrm{Tr}\{\tilde{H}\tilde{V}\}^2 - |\tilde{H}|^2|\tilde{V}|^2}A(G,V) \\
&= 1 + \frac{1}{\cos^2\varphi - 1}A(G,V) \\
&= 1 - \csc^2\varphi A(G,V) \,,
\end{aligned} \tag{A34}$$

where

$$\cos\varphi = \frac{\mathrm{Tr}\{\tilde{H}\tilde{V}\}}{|\tilde{H}||\tilde{V}|} \,. \tag{A35}$$

The existence of above non-zero extreme point, i.e., at $\lambda_A = -2\eta/\xi$, is related to $\xi \neq 0$. Especially, the DoS decays monotonically as a function of $|\lambda|$ if $\xi = 0$. Since $\tilde{V}$ differs from V only by a constant term and, in practical case, $\tilde{V} \neq 0$, thus the condition $\xi = 0$ is equivalent to

$$\mathrm{Tr}\{\tilde{H}\tilde{V}\} = 0 \,. \tag{A36}$$

Appendix D: DoS for the Angular Momentum Model

In the following, we give the derivation of the DoS for the model given by Eq. (8) of the main text in detail. As is known,

$$H(\lambda) = \epsilon J^2 + \lambda J_z \,. \tag{A37}$$

We take the angular momentum $J=0,1,2,\ldots,j$ and the dimension of the Hilbert space is $d=(j+1)^2$. It is shown that

$$\begin{aligned}S(\mathrm{O}(3),H(\lambda)) &= 1-\frac{1}{4|\tilde{H}(\lambda)|^2}\overline{|[R(g),H(\lambda))]|^2}|_{\mathrm{O}(3)}\\ &= 1-\frac{\lambda^2}{4|\tilde{H}(\lambda)|^2}\overline{|[R(g),J_z]|^2}|_{\mathrm{O}(3)}\\ &= 1-\frac{\lambda^2}{2|\tilde{H}(\lambda)|^2}\overline{\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_z R(g) J_z\}}|_{\mathrm{O}(3)}\,. \end{aligned}\tag{A38}$$

$$\begin{aligned}|\tilde{H}(\lambda)|^2 &= \mathrm{Tr}\{H(\lambda)-\frac{1}{(j+1)^2}\mathrm{Tr}\{H(\lambda)\}\}^2\\ &= \mathrm{Tr}\{H(\lambda)\}^2-\frac{1}{(j+1)^2}\mathrm{Tr}\{H(\lambda)\}\mathrm{Tr}\{H(\lambda)\}\\ &= \epsilon^2\sum_{i=0}^{j}i^2(i+1)^2(2i+1)+\lambda^2\sum_{i=0}^{j}\frac{1}{3}i(i+1)(2i+1)\\ &\quad -\frac{1}{(j+1)^2}\Big(\epsilon\sum_{i=0}^{j}i(i+1)(2i+1)\Big)^2\\ &= j(j+1)^2(j+2)\Big[\frac{1}{12}\epsilon^2 j(j+2)+\frac{1}{6}\lambda^2\Big]\,.\end{aligned}\tag{A39}$$

Since O(3) can be expressed as a disjoint union of SO(3) and $\hat{\imath}$SO(3), where $\hat{\imath}$ denotes the inversion transformation and it leaves the angular momentum unchanged $[\hat{\imath},J_\alpha]=0$,[31] then it is enough to focus the evaluation of group average on SO(3) at this moment, whose group element provides the following unitary transformation

$$\begin{aligned}R(g) &= R(\theta,\phi,\omega)\\ &= \mathrm{e}^{-\mathrm{i}J_z\phi}\,\mathrm{e}^{-\mathrm{i}J_y\theta}\,\mathrm{e}^{-\mathrm{i}J_z\omega}\,\mathrm{e}^{\mathrm{i}J_y\theta}\,\mathrm{e}^{\mathrm{i}J_z\phi}\,.\end{aligned}\tag{A40}$$

Then for $g\in\mathrm{SO}(3)$

$$\begin{aligned}&\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_z R(g) J_z\}\\ &= \mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{\,\mathrm{e}^{-\mathrm{i}J_z\phi}\,\mathrm{e}^{-\mathrm{i}J_y\theta}\,\mathrm{e}^{\mathrm{i}J_z\omega}\,\mathrm{e}^{\mathrm{i}J_y\theta}\,\mathrm{e}^{\mathrm{i}J_z\phi}J_z\\ &\quad\times\mathrm{e}^{-\mathrm{i}J_z\phi}\,\mathrm{e}^{-\mathrm{i}J_y\theta}\,\mathrm{e}^{-\mathrm{i}J_z\omega}\,\mathrm{e}^{\mathrm{i}J_y\theta}\,\mathrm{e}^{\mathrm{i}J_z\phi}J_z\}\\ &= \mathrm{Tr}\{J_z^2\}-(\cos^2\theta+\sin^2\theta\cos\omega)\mathrm{Tr}\{J_z^2\}\\ &= (\sin^2\theta-\sin^2\theta\cos\omega)\mathrm{Tr}\{J_z^2\}\\ &= (\sin^2\theta-\sin^2\theta\cos\omega)\sum_{i=0}^{j}\frac{1}{3}i(i+1)(2i+1)\\ &= \frac{1}{6}(\sin^2\theta-\sin^2\theta\cos\omega)j(j+1)^2(j+2)\,.\end{aligned}\tag{A41}$$

On the other hand, for $g\in\hat{\imath}\mathrm{SO}(3)$ it follows from $[\hat{\imath},J_\alpha]=0$ that $\hat{\imath}$ commutes with transformations from SO(3) group. Thus a typical term in the average over the transformation set $\hat{\imath}$SO(3) always corresponds with some term in the group average of SO(3)

$$\begin{aligned}&\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{[\hat{\imath}R(g)]^\dagger J_z\hat{\imath}R(g)J_z\}\\ &\quad= \mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger\hat{\imath}J_z\hat{\imath}R(g)J_z\}\\ &\quad= \mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_z\hat{\imath}^2R(g)J_z\}\\ &\quad= \mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_z R(g) J_z\}\,.\end{aligned}\tag{A42}$$

It follows from Eqs. (A38), (A39), (A41), and (A42) that

$$\begin{aligned}&S(\mathrm{O}(3),H(\lambda))\\ &\quad= 1-\frac{\lambda^2}{2|\tilde{H}(\lambda)|^2}\overline{\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_zR(g)J_z\}}|_{\mathrm{O}(3)}\\ &\quad= 1-\frac{\lambda^2}{2|\tilde{H}(\lambda)|^2}\frac{1}{2}[\overline{\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_zR(g)J_z\}}|_{\mathrm{SO}(3)}\\ &\qquad+\overline{\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_zR(g)J_z\}}|_{\hat{\imath}\mathrm{SO}(3)}]\\ &\quad= 1-\frac{\lambda^2}{2|\tilde{H}(\lambda)|^2}\overline{\mathrm{Tr}\{J_z^2\}-\mathrm{Tr}\{R(g)^\dagger J_zR(g)J_z\}}|_{\mathrm{SO}(3)}\\ &\quad= 1-\frac{\lambda^2}{\epsilon^2 j(j+2)+2\lambda^2}\frac{1}{2\pi^2}\int_{-\pi}^{\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{\pi}\mathrm{d}\omega\\ &\qquad\times\sin^2\frac{\omega}{2}(\sin^2\theta-\sin^2\theta\cos\omega)\\ &\quad= 1-\frac{\lambda^2}{\epsilon^2 j(j+2)+2\lambda^2}\,.\end{aligned}\tag{A43}$$

Notice that the average over the group for $G=\mathrm{SO}(3)$ has been replaced by the following Lie group integral[32]

$$\frac{1}{n_G}\sum_{g\in G}\rightarrow\frac{1}{2\pi^2}\int_{-\pi}^{\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{\pi}\mathrm{d}\omega\sin^2\frac{\omega}{2}\,.\tag{A44}$$

Appendix E: Example with Accidental Degeneracy

Here, we show the details on the extended symmetry group G_T of the three-site model at accidental degeneracy, which is a U(2) group defined in a two-dimensional degenerate subspace, as well as the calculation of the corresponding DoS with respect to this extended group.

First let us consider the spectrum and eigenstates of the model Hamiltonian. From Eqs. (5) and (10) of the main text

$$\begin{aligned}H(\lambda) &= H+\lambda V\\ &= \sum_{i=1}^{3}\epsilon|i\rangle\langle i|+\sum_{i\neq j}h|i\rangle\langle j|+\lambda[|1\rangle\langle 1|+|3\rangle\langle 3|\\ &\quad-(|1\rangle\langle 3|+\mathrm{h.c.})]\,.\end{aligned}\tag{A45}$$

The symmetry group of $H(\lambda)$ at $\lambda\neq 0$ is the cyclic group $Z_2=\{e,\sigma\}$, whose representation under the site basis $\{|1\rangle,|2\rangle,|3\rangle\}$ is given by

$$R_{\mathrm{site}}(e)=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix},\quad R_{\mathrm{site}}(\sigma)=\begin{bmatrix}0&0&1\\0&1&0\\1&0&0\end{bmatrix}.\tag{A46}$$

The energy spectrum and corresponding eigenstates are

$$E_{1\pm}=\epsilon+\frac{h}{2}\pm\frac{3}{2}h\,,\quad E_2=\epsilon-h+2\lambda\,,\tag{A47}$$

$$|\psi_{1+}\rangle=\frac{1}{\sqrt{3}}(|1\rangle+|2\rangle+|3\rangle)\,,\tag{A48}$$

$$|\psi_{1-}\rangle = \frac{1}{\sqrt{6}}(|1\rangle - 2|2\rangle + |3\rangle)\,, \tag{A49}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |3\rangle)\,. \tag{A50}$$

When $\lambda = \lambda_{02} = 3h/2$, it follows from Eq. (A47) that E_{1+} and E_2 become degenerate. Because this degeneracy is not guaranteed by the Z_2 symmetry, thus it is accidental. At λ_{02}, the Hamiltonian $H(\lambda_{02})$ is invariant under all U(2) operations within the two-dimensional subspace spanned by $|\psi_{1+}\rangle$ and $|\psi_2\rangle$.[33] Under the eigenbasis $\{|\psi_{1-}\rangle, |\psi_{1+}\rangle, |\psi_2\rangle\}$, where the Hamiltonian diagonalized

$$H_{\rm eig}(\lambda) = \begin{bmatrix} E_{1-} & 0 & 0 \\ 0 & E_{1+} & 0 \\ 0 & 0 & E_2 \end{bmatrix}, \tag{A51}$$

a U(2) transformation parametrized by $\hat{n}$, ω, and ω_0 is written as

$$R_{\rm eig}(\omega_0;\hat{n},\omega) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & {\rm e}^{{\rm i}\omega_0}\Big(\cos\dfrac{\omega}{2} - {\rm i}\cos\theta\sin\dfrac{\omega}{2}\Big) & -{\rm i}\,{\rm e}^{-{\rm i}(\phi-\omega_0)}\sin\theta\sin\dfrac{\omega}{2} \\ 0 & -{\rm i}\,{\rm e}^{{\rm i}(\phi+\omega_0)}\sin\theta\sin\dfrac{\omega}{2} & {\rm e}^{{\rm i}\omega_0}\Big(\cos\dfrac{\omega}{2} + {\rm i}\cos\theta\sin\dfrac{\omega}{2}\Big) \end{bmatrix}, \tag{A52}$$

where ω_0, $\omega \in [0, 2\pi]$; the unit vector

$$\hat{n} = \sin\theta\cos\phi\hat{e}_x + \sin\theta\sin\phi\hat{e}_y + \cos\theta\hat{e}_z\,, \tag{A53}$$

and $[R_{\rm eig}(\omega_0;\hat{n},\omega), H(\lambda_{02})] = 0$.

Because of this U(2) hidden symmetry, the symmetry group of $H(\lambda)$ is extended at λ_{02}. Namely, now $G_T = \langle Z_2, {\rm U}(2)\rangle$ is generated by the original symmetry group Z_2 as well as the U(2) group. For this specific example, however, the group that generated is still the U(2), since all elements in Z_2 could be represented as some U(2) operations. To see how this is achieved, we rewrite the elements of Z_2 Eq. (A46) under the eigenbasis $\{|\psi_{1-}\rangle, |\psi_{1+}\rangle, |\psi_2\rangle\}$

$$R_{\rm eig}(e) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R_{\rm eig}(\sigma) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \tag{A54}$$

Through direct comparison with Eq. (A52), it follows that $R_{\rm eig}(e) = R_{\rm eig}(0;\hat{n},0)$ and $R_{\rm eig}(\sigma) = R_{\rm eig}(\pi/2;\hat{e}_z,\pi)$, hence $Z_2 \subset {\rm U}(2)$ and, therefore, $G_T = {\rm U}(2)$.

The DoS of $H(\lambda)$ with respect to the extended group $G_T = {\rm U}(2)$ is now calculated as follows

$$\begin{aligned} S(G_T, H(\lambda)) &= \frac{1}{4|\tilde{H}(\lambda)|^2}\overline{|\{R(g), \tilde{H}(\lambda)\}|^2}|_{{\rm U}(2)} \\ &= \frac{1}{2} + \frac{1}{2|\tilde{H}(\lambda)|^2} \\ &\quad\times\overline{{\rm Tr}\{R_{\rm eig}(\hat{n},\omega)^\dagger\tilde{H}_{\rm eig}(\lambda)R_{\rm eig}(\hat{n},\omega)\tilde{H}_{\rm eig}(\lambda)\}}|_{{\rm U}(2)}\,. \end{aligned} \tag{A55}$$

The average for the continuous group U(2) is evaluated as a Lie group integral

$$\overline{f(g)}|_{{\rm U}(2)} = \frac{1}{8\pi^3}\int_0^{2\pi}{\rm d}\omega_0\int_{-\pi}^{\pi}{\rm d}\phi\int_0^{\pi}{\rm d}\theta\sin\theta\int_0^{2\pi}{\rm d}\omega\sin^2\frac{\omega}{2}f(g)\,, \tag{A56}$$

which together with Eqs. (A51), (A52) gives that

$$\begin{aligned} &\overline{{\rm Tr}\{R_{\rm eig}(\hat{n},\omega)^\dagger\tilde{H}_{\rm eig}(\lambda)R_{\rm eig}(\hat{n},\omega)\tilde{H}_{\rm eig}(\lambda)\}}|_{{\rm U}(2)} = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}{\rm d}\phi\int_0^{\pi}{\rm d}\theta\int_0^{2\pi}{\rm d}\omega\frac{\sin\theta\sin^2\omega/2}{12} \\ &\quad\times[45h^2 - 12h\lambda + 20\lambda^2 + 3(3h-2\lambda)^2(\cos2\theta + 2\cos\omega\sin^2\theta)] = \frac{1}{6}(3h+2\lambda)^2\,. \end{aligned} \tag{A57}$$

Thus Eq. (A55) is rewritten as

$$S(G_T, H(\lambda)) = 1 - \frac{3}{8}\frac{(\lambda-\lambda_{02})^2}{\lambda^2 - \lambda_{02}\lambda + \lambda_{02}^2}\,. \tag{A58}$$

Appendix F: Example on the Spontaneous Symmetry Breaking

Here, we provide details on the evaluation of the degree of symmetry for quantum state (DoSS) in the angular momentum model. We assume the following state with density matrix

$$\rho = \frac{1}{Z}\,{\rm e}^{-\beta H(\lambda)}\,, \tag{A59}$$

with the partition function $Z = {\rm Tr}\{\exp[-\beta H(\lambda)]\}$ and the Hamiltonian $H(\lambda)$ as given by Eq. (A37).

For $j = 1/2$, Eq. (A59) is explicitly written as

$$\begin{aligned} \rho &= \frac{1}{Z}\,{\rm e}^{-\beta((3/4)\epsilon + (1/2)\lambda\sigma_z)} \\ &= \frac{1}{2\cosh(\beta\lambda/2)}\,{\rm e}^{-(1/2)\beta\lambda\sigma_z}\,. \end{aligned} \tag{A60}$$

The DoSS is calculated based on Eq. (11) of the main text

$$\begin{aligned} S({\rm O}(3), \rho) &= \frac{1}{4|\rho|^2}\overline{|\{R(g),\rho\}|^2}|_{{\rm O}(3)} \\ &= \frac{1}{4|\rho|^2}\frac{1}{2}[\overline{|\{R(g),\rho\}|^2}|_{{\rm SO}(3)} + \overline{|\{R(g),\rho\}|^2}|_{\hat{\imath}{\rm SO}(3)}]\,. \end{aligned} \tag{A61}$$

But since $[\hat{\imath}, \rho] = 0$, then for $g \in \hat{\imath}{\rm SO}(3)$ a typical term in the average over $\hat{\imath}{\rm SO}(3)$ could be rewritten as

$$\begin{aligned} |\{\hat{\imath}R(g),\rho\}|^2 &= {\rm Tr}\{(\hat{\imath}R(g)\rho + \rho\hat{\imath}R(g))^\dagger(\hat{\imath}R(g)\rho + \rho\hat{\imath}R(g))\} \\ &= {\rm Tr}\{(R(g)\rho + \rho R(g))^\dagger(R(g)\rho + \rho R(g))\} \end{aligned}$$

$$=|\{R(g),\rho\}|^2\,, \tag{A62}$$

which is equivalent to a corresponding term in the average over SO(3). Because of this one to one correspondence, it is then concluded that

$$\overline{|\{R(g),\rho\}|^2}|_{\mathrm{SO}(3)} = \overline{|\{R(g),\rho\}|^2}|_{\hat{\imath}\mathrm{SO}(3)}\,, \tag{A63}$$

and Eq. (A65) is rewritten as

$$S(\mathrm{O}(3),\rho) = \frac{1}{4|\rho|^2}\overline{|\{R(g),\rho\}|^2}|_{\mathrm{SO}(3)}$$
$$= \frac{1}{4|\rho|^2}\frac{1}{2\pi^2}\int_{-\pi}^{\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{\pi}\mathrm{d}\omega$$
$$\times \sin^2\frac{\omega}{2}|\{R(\theta,\phi,\omega),\rho\}|^2\,. \tag{A64}$$

The integrand in Eq. (A64) is evaluated as follows

$$|\{R(\theta,\phi,\omega),\rho\}|^2$$
$$= 2[\mathrm{Tr}\{\rho^2\} + \mathrm{Tr}\{R(\theta,\phi,\omega)^\dagger\rho R(\theta,\phi,\omega)\rho\}]\,, \tag{A65}$$

while the first term in Eq. (A65) is just the purity of the quantum state ρ, i.e.,

$$\mathrm{Tr}\{\rho^2\} = |\rho|^2 = \frac{\cosh\beta\lambda}{\cosh\beta\lambda+1}\,, \tag{A66}$$

the second term in Eq. (A65) is evaluated as follows

$$\mathrm{Tr}\{R(\theta,\phi,\omega)^\dagger\rho R(\theta,\phi,\omega)\rho\} = \mathrm{Tr}\{\,\mathrm{e}^{\mathrm{i}(\omega/2)\hat{n}\cdot\vec{\sigma}}\rho\,\mathrm{e}^{-\mathrm{i}(\omega/2)\hat{n}\cdot\vec{\sigma}}\rho\}$$
$$= \frac{1}{4\cosh^2\frac{\beta\lambda}{2}}\mathrm{Tr}\{\,\mathrm{e}^{\mathrm{i}(\omega/2)\hat{n}\cdot\vec{\sigma}}\,\mathrm{e}^{-(1/2)\beta\lambda\sigma_z}\,\mathrm{e}^{-\mathrm{i}(\omega/2)\hat{n}\cdot\vec{\sigma}}\,\mathrm{e}^{-(1/2)\beta\lambda\sigma_z}\} = \frac{1}{4\cosh^2(\beta\lambda/2)}\mathrm{Tr}\Big\{\Big(\cos\frac{\omega}{2}+\mathrm{i}\hat{n}\cdot\vec{\sigma}\sin\frac{\omega}{2}\Big)$$
$$\times\Big(\cosh\frac{\beta\lambda}{2}-\sigma_z\sinh\frac{\beta\lambda}{2}\Big)\Big(\cos\frac{\omega}{2}-\mathrm{i}\hat{n}\cdot\vec{\sigma}\sin\frac{\omega}{2}\Big)\Big(\cosh\frac{\beta\lambda}{2}-\sigma_z\sinh\frac{\beta\lambda}{2}\Big)\Big\}$$
$$= \frac{1}{4\cosh^2(\beta\lambda/2)}\{[1+\cos\theta^2(1-\cos\omega)+\cos\omega]\cosh\beta\lambda+\sin^2\theta(1-\cos\omega)\}\,. \tag{A67}$$

Insert Eqs. (A66), (A67) into Eq. (A64), the DoS is readily calculated

$$S(\mathrm{O}(3),\rho) = \frac{1}{4}\Big(3+\frac{1}{\cosh\beta\lambda}\Big)\,. \tag{A68}$$

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