Unconventional supersymmetric quantum mechanics in spin systems

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It is shown that the eigenproblem of a two-level Hamiltonian with non-zero off-diagonal terms is involved with a supersymmetry quantum mechanics. This is associated with an intertwining relation between the components of an eigenspinor which is exploited to reduce the spin degrees of freedom in a generic spin model. The scheme is illustrated with examples of spin-boson models including the Jaynes-Cummings model and generalized Rabi models. The generalization of the scheme to a single spin-1/2 is discussed. We also demonstrate how the supersymmetry can reduce the degrees of freedom of a many-spin system. Examples of the Tavis-Cummings model and generalized Dicke models are discussed by utilizing this formalism.

Quantum entanglement is turned out to be a crucial resource in targeting relevant corners of the Hilbert space of a many-body system rather than merely being a puzzle in foundations of quantum mechanics. Entanglement is perceived as a correlation between constituents of the system and can be exploited to reduce degrees of freedom (DOF) which is required to describe the state of the system.

Consider a single spin-1/2 interacting with an external field. If spin is a good quantum number, a unitary transformation can turn the eigenspinor of the system into a product of an eigenstate of the field and an eigenspinor of $\sigma_z$, where $\sigma_x, \sigma_y, \sigma_z$ are Pauli matrices. Otherwise, if spin is not a good quantum number, components of the eigenspinor are intertwined in the associated eigenproblem (EP). The aim of this letter is to show the intertwining relationship indicates an unconventional supersymmetry (USUSY) which can be exploited to diagonalize the Hamiltonian in the spin subspace.

Supersymmetric quantum mechanics (SUSY QM) was initially introduced into non-relativistic QM to study the non-perturbative breaking of supersymmetry (SUSY) and later became a framework on its own. In addition to its utilization in condensed matter systems, SUSY QM is adopted in classifying analytically solvable potentials in a close relation with factorization method. Our focus here is rather on constraints which USUSY offers in reducing DOF of the EP.

We start from a generic two-level Hamiltonian and the associated EP

$$H = \begin{pmatrix} H_+ & F_+ \\ F_- & H_- \end{pmatrix}, \quad H|\Psi\rangle = E|\Psi\rangle,$$

where $H_{\pm} = H_{\pm}^\dagger$, $F_\pm = F_\mp^\dagger$ and the eigenspinor reads as $|\Psi\rangle = (|\psi_+\rangle, |\psi_-\rangle)$. $H_{\pm}$ are restricted to those with discrete eigenvalues $E^{(n)}_{\pm}$, collected in sets $E_{\pm}$. We analyze separately the cases which $E$ is included in or excluded from $E_{\pm}$. If $E \notin E_{\pm}$, the components are connected $|\psi_{\pm}\rangle = G_{\pm} F_{\mp}|\psi_{\mp}\rangle$ through $G_{\pm} \equiv (E - H_{\pm})^{-1}$. This allows to construct the eigensate from a disentangled state, for instance

$$|\Psi\rangle = g_+ \begin{pmatrix} |\psi_-\rangle \\ |\psi_+\rangle \end{pmatrix}, \quad g_+ \equiv \begin{pmatrix} G_+ F_+ & 0 \\ 0 & 1 \end{pmatrix},$$

where the operator $g_+$ returns the entangled state. The EP of $H$ is therefore decoupled into two EPs

$$h_{\pm}|\psi_{\pm}\rangle = E_{\pm}|\psi_{\pm}\rangle, \quad h_{\pm} = H_{\pm} + F_{\pm} G_{\mp} F_{\mp},$$

which show components belong to subsystems governed by $h_{\pm}$ and either carries all information encoded in $|\Psi\rangle$. The fact that $|\psi_{\pm}\rangle$ are degenerate under the action of the hermitian operators $h_{\pm}$ implies a SUSY QM. To make it explicit, we define supercharge operators $Q_{\pm} = G_{\pm} F_{\mp} \sigma_{\pm}$ where $2\sigma_{\pm} = \sigma_x \pm i\sigma_y$. The supercharge operators fulfill $Q_{\pm}^2 = 0$ independent of the nature of the field coupled to the spin. The EP of $H$ can now be recast as $H|\Psi\rangle = |\Psi\rangle$ by the traceless matrix $H = Q_+ + Q_-$. This acts like an idempotent operator $H^2|\Psi\rangle = H|\Psi\rangle$. The superalgebra $sl(1/1)$ between $Q_{\pm}$ and $H^2$ can be constructed

$$\{Q_+, Q_-\} = H^2, \quad [Q_{\pm}, H^2] = 0,$$

where $\{,\}$ and $[,]$ are the anticommutator and the commutator, respectively. We call the SUSY QM characterized in Eq. (4) an unconventional supersymmetric quantum mechanics (USUSY QM) in order to distinguish it from the standard SUSY QM. To contrast the difference between SUSY QM and USUSY QM, we note that if the eigenstate of $H$ is the vacuum of one of the supercharge operators, the other supercharge may not exist. For example, if $Q_+|\Psi\rangle = 0$ and $H_-|\psi_-\rangle = E|\psi_-\rangle$ are satisfied, the eigenstate can be chosen as $|\Psi\rangle = (0 \langle \psi_- |)$, and therefore, $Q_-$ and USUSY QM do not exist. But the standard SUSY QM has a good SUSY if its ground state is the vacuum of all supercharges.

The existence of the USUSY QM, like a symmetry, reduces DOF of the problem as only the EP on one of $|\psi_{\pm}\rangle$ is needed to be dealt. However, the existence of the USUSY is a strong condition for the reducibility of an eigenstate and it can be relegated to existence of only one of the supercharges. Suppose $E = E_{\pm}^{(n)}$ but $E \notin E_{\mp}$, then $h_+$ exists and the EP on $|\Psi\rangle$ is still reducible.
In retrospect, assume we solve two EPs in Eq. (3) instead of the original EP of \( H \). Those eigenvalues of \( H \) which are in \( \mathcal{E}_+ \cap \mathcal{E}_- \) are missing. The possible excluded eigenenergies can be altered by a unitary transformation \( U \in SU(2) \) as the corresponding diagonal terms \( \tilde{H}_\pm \) of \( \tilde{H} = U^\dagger H U \) can have different sets of eigenenergies \( \tilde{E}_\pm \) rather than \( E_\pm \). As a result, any eigenspinor of \( H \) becomes reducible by a unitary transformation given either \( E \notin \tilde{E}_+ \) or \( E \notin \tilde{E}_- \) can be satisfied. Moreover, USUSY QM can be realized for any eigenstate if \( U \) warrants \( E \notin \tilde{E}_\pm \).

We proceed to illustrate the solutions of the reduced EPs in Eq. (3) for some spin-boson models. \( H_\pm \) and \( F_\pm \) are then given in terms of the boson creation (annihilation) operator \( a^\dagger (a) \) with \( [a, a^\dagger] = 1 \). The reduced EPs can be algebraically solved if \( H_\pm \) and \( F_\pm \) close under commutation relations. The celebrated Jaynes-Cummings (JC) model [13, 14], specified by \( h_\pm = a^\dagger a \pm \Delta \) and \( F_\pm = \alpha a \) with \( \Delta \) and \( \alpha \) real numbers, is a suitable example to demonstrate it. The unit of energy is set equal to unity \( \hbar \omega = 1 \) throughout this letter. The conserved operator of the JC Hamiltonian \( C = a^\dagger a + \frac{1}{2} \sigma_z \) induces \( [h_\pm, a^\dagger a] = 0 \) which indicates eigenstates of \( h_\pm \) are the eigenstates of the number operator \( a^\dagger a [n] = n [n] \).

The common eigenenergies of \( h_\pm \) are the solutions of

\[
(E - n - 1 + \Delta)(E - n - \Delta) = \alpha^2 (n + 1), \quad n \in \mathbb{N},
\]

which gives two solutions for a given \( n \). Parity quantum numbers \( \eta = \pm \) are required then to label the eigenenergies \( E^{(n,\eta)} \) and the corresponding eigenstate \( |\Psi^{(n,\eta)}\rangle \). The full eigenstate can be constructed either by an eigenstate of \( h_+ \) or the one of \( h_- \) since the components are superpartners. The only eigenstate with no USUSY QM is the disentangled state \( |\Psi^d\rangle = (0 | 0) \) with \( E = -\Delta \neq 0 \) which is the vacuum of \( Q_+ \), but \( Q_- \) does not exist for this state, and the state has no parity number. It is notable that the normalized spin texture \( \tilde{\rho}_z (r) = \Psi^\dagger(r) \sigma_z \Psi(r) / [\Psi(r)]^2 \) defined by the entangled eigenstates \( \Psi^{(n,\eta)}(r) = \langle r | \Psi^{(n,\eta)} \rangle \) has a topological index [15] [16] defined by \( \tilde{\rho}_z (-|r|) \tilde{\rho}_z (|r|) \rightarrow -1 \) at the limit \( r \rightarrow \infty \) which is absent in \( \Psi^d(r) \). This implies the non-local aspect of the entanglement in the JC model.

If \( H_\pm \) and \( F_\pm \) are not closed algebraically, the exact-diagonalization (ED) routine can be adopted to achieve low-energy solutions of EPs in Eq. (3) by making use of a truncated basis. To illustrate it, we consider a generalization of the Rabi model [17] in the presence of a homogeneous in-plane magnetic field, specified by \( H_\pm = a^\dagger a \pm \Delta \) and \( F_\pm = \alpha a + \beta a^\dagger + \gamma \). Without loss of generality, we suppose \( \alpha, \beta \geq 0 \) while \( \gamma \in \mathbb{C} \).

For \( \gamma = 0 \), the reduced Hamiltonians possess a parity symmetry as \( [h_\pm, e^{i \varphi_0 \sigma_z}] = 0 \) and the intertwining relationship implies two components have different parities \( \langle \psi_+ | \psi_- \rangle = 0 \). The matrix representations of the reduced Hamiltonians become tridiagonal if at least one of \( \alpha, \beta, \gamma \) is zero. Otherwise, a transformation \( U = e^{i \sigma_z \varphi} \) by tan \( \varphi = (\beta/\alpha)^{1/2} \) makes the representation of either \( \tilde{h}_\pm \) tridiagonal (see Supplementary Information). We proceed with \( h_+ \) and assume \( |\tilde{n}\rangle \) are the eigenstates of \( H_\pm \) associated with the eigenenergy \( \tilde{E}_\pm^{(n)} \) after rotating \( H \) with tan \( \varphi = \sqrt{\beta/\alpha} \). We make the matrix out of elements \( \tilde{f}_\pm^{(m,n)} = \langle \tilde{n} | (\tilde{h}_+ - E) | \tilde{n} \rangle \). The \( j \)-th continuant \( \tilde{h}_+^{(j)}(E) \) obeys the recurrence relation [18]

\[
\tilde{h}_+^{(j+1)}(E) = \tilde{j}_+^{(j,j)}(E) \tilde{h}_+^{(j)}(E) - \tilde{j}_+^{(j-1,j-1)} \tilde{h}_+^{(j-1)}(E)
\]

with initial values \( \tilde{h}_+^{(0)}(E) = 0 \) and \( \tilde{h}_+^{(0)}(E) = 1 \). Given the desired convergence is achieved by keeping \( q \) and \( j \) states, the eigenvalues of \( \tilde{h}_+ \) are the roots of the characteristic polynomial \( \tilde{h}_+^{(j)}(E) = 0 \). The possible excluded eigenenergies can be found by diagonalizing the original Hamiltonian \( H(\Psi) = \tilde{E}_\pm^{(n)}(\Psi) \), where the EP constrains the parameters of the model if \( \tilde{E}_\pm^{(n)} \) is an eigenenergy of \( H \). The results for a generalized Rabi model is presented in Fig. 1 as a matter of illustration.

Braak derived analytically the spectrum of the Rabi model, \( \alpha = \beta = \gamma = 0 \), by virtue of the Bargmann-Fock space [19] (some models solved by exploiting the same formalism are reviewed in [17]). The regular eigenenergies (contrasted with isolated solutions including Judd points [20]) are zeros of a transcendental function i.e. the so-called G-function. Each summand in the definition of the G-function is associated with a sequence which needs to be evaluated separately through a three-term recurrence relation which is involved with the tridiagonality of the Rabi model. \( \mathbb{Z}_2 \) symmetry of the Rabi model is invoked through the Fulton-Gouterman transformation [21] [23] to reduce DOF in Braak’s approach. A similar feature in our treatment is endowed with the spin DOF (namely the supercharge operators \( Q_\pm^2 = 0 \)) which can be implemented to any two-level Hamiltonian with non-zero off-diagonal terms and does not relate to symmetries of the field coupled to the spin.

![Graph](image-url)
We generalize the formalism to deal with a spin-$\frac{1}{2}$ system. A Hamiltonian describing coupling between an external field and a single spin-$\frac{1}{2}$ has the form
\[ H_{\frac{1}{2}} = H_0 + \Delta S_z + F_+ S_z + F_- S_z, \]
where $H_0$ does not include spin operators. $S_x,y,z$ are spin-$\frac{1}{2}$ representation of $SU(2)$ and $S_\pm$ are the corresponding ladder operators in the convention $\{S_x, S_z\} = 2S_z$. The scheme of making the Hamiltonian traceless by inverting the diagonal terms in the EP $H_{\frac{1}{2}} |\Psi\rangle = |\Psi\rangle$ and then squaring it $H_{\frac{1}{2}}^2 |\Psi\rangle = |\Psi\rangle$ results as well here in decoupling (almost) half of the components of the eigen-spinor from the rest. This is because $H_{\frac{1}{2}}$ can be written as a sum of two supercharges $Q_\pm = \hat{I}_\pm \mathcal{K}(S_+ + S_-)$ with a fermionic nature $Q_\pm^2 = 0$. $\hat{I}_\pm$ and $\mathcal{K}$ are diagonal $(p + 1) \times (p + 1)$ matrices with entries $(\hat{I}_\pm)_{jj} = \delta_{j,2k+1}$, $(\mathcal{K})_{jj} = \delta_{j,2k}$, with $1 \leq j \leq p + 1$ and $k$ being an integer number, and $(\mathcal{K})_{jj} = 1/\sqrt{|E - H_0 - \Delta (\frac{p}{2} + j - 1)|}$ where $E$ is the eigenenergy of $H_{\frac{1}{2}}$. The scheme can be repeated over and over on the components which are not decoupled in order to achieve ultimately $p + 1$ decoupled EPs (an example is worked out in Supplementary Information).

The eigenstates of the Hamiltonian in Eq. (7) construct irreducible representations of the rotation group [22] of a many-spin system. It is possible to explore directly how the intertwining relation of a single spin can reduce DOF in a many-spin system. We illustrate it for the case of spin-$\frac{1}{2}$. The Hamiltonian of $N$ spin-$\frac{1}{2}$ coupled with an external field
\[ H^{(N)} = H_0 + \sum_{s=1}^{N} \left( \Delta \sigma_z^{(s)} + F_+ \sigma_+^{(s)} + F_- \sigma_-^{(s)} \right) \]
can be represented, for instance, in eigenkets of $\sigma_z^{(1)}$
\[ H^{(N)} = \begin{pmatrix} H_{\frac{1}{2}}^{(N-1)} & F_+ \\ F_- & H_{\frac{1}{2}}^{(N-1)} \end{pmatrix} \]
in order to exercise USUSY of the single spin. $H_{\frac{1}{2}}^{(N-1)}$ and $F_{\pm}$ have a $2^{(N-1)} \times 2^{(N-1)}$ matrix representation ($F_{\pm} \equiv F_{\pm} \mathcal{I}_{N-1}$ where $\mathcal{I}_r$ is a $2^r \times 2^r$ identity matrix). $H_{\frac{1}{2}}^{(N-1)}$ can be shown in the same form of $H^{(N)}$ in Eq. (9) if $N \neq 1$, which attributes a fractal structure to $H^{(N)}$. An eigenspinor of $H^{(N)}$ can be grouped into two components $|\Psi^{(N)}\rangle = (|\Psi^{(N-1)}\rangle |\Phi^{(N-1)}\rangle)$. The same procedure adopted for a single spin-$\frac{1}{2}$ decouples $|\psi^{(N-1)}\rangle$ in the corresponding EP associated with the eigenenergy $E$ and renders two reduced EPs similar to Eq. (9). That is by solving an $(N-1)$-spin subsystem, the system of $N$ spins is solved. Contrary to spin-$\frac{1}{2}$ models, repeating the scheme does not decouple the components down to scalar EPs for $N > 2$. However, the fractal structure of $H^{(N)}$ can be devised to reconstruct $|\Psi^{(N)}\rangle$ as a superposition of eigenstates of the subsystems.

Consider $H_{\frac{1}{2}}^{(r)}$ for $r > 0$ and show its eigenspinor as $|j_r\rangle = (|\Psi^{(r-1)}\rangle |\Theta^{(r-1)}\rangle)$ associated with the eigenenergy $E_j$ where $j_r$ can be a collective index. We illustrate how the intertwining relation can recursively reconstruct $|j_r\rangle$, and then apply the procedure to $|\Psi^{(N)}\rangle$. We assume $|j_r\rangle$ is reducible $|\Phi^{(r-1)}\rangle = G^{(r-1)}_j F_+ |\Theta^{(r-1)}\rangle$ by means of $G^{(r-1)}_j \equiv (E_j - H^{(r-1)}_{\frac{1}{2}})^{-1}$, which leads to
\[ |j_r\rangle = g_{jr} (|\Theta^{(r-1)}\rangle |\Theta^{(r-1)}\rangle), \quad g_{jr} \equiv \text{diag}(G^{(r-1)}_j F_+, 1). \]

Since $H^{(r-1)}_{\frac{1}{2}}$ for $r \neq 1$ has the same structure as $H^{(r)}_{\frac{1}{2}}$, its reducible eigenstates which appear in the expansion (those with $\Omega^{(r)}_{j-1} \neq 0$) can be shown like Eq. (10) (the reducibility here needs to be understood along the same considerations discussed for a single spin). The irreducible eigenstates of $H^{(r-1)}_{\frac{1}{2}}$ with a non-zero coefficient are stuck and cannot be connected to smaller spin subsystems. Similar to the single-spin case, a unitary transformation can alter the irreducible states and remove them from the representation. We call $|j_r\rangle$ a maximally reducible state if no irreducible state comes up in the course of repeating the scheme down to the level where $|j_r\rangle$ finds a representation in terms of eigenstates of $H^{(0)}_{\frac{1}{2}}$. If $|\psi^{(N-1)}\rangle$ is maximally reducible, we can write formally
\[ |\psi^{(N-1)}\rangle = \sum_j \Omega_j^{N-1} |j_{N-1}\rangle, \quad \Omega_j^{N-1} = |j_{N-1}|^{\langle j_{N-1} | \psi^{(N-1)} \rangle}, \]
where $\Omega_j^{N-1} = |j_{N-1}|^{\langle j_{N-1} | \psi^{(N-1)} \rangle}$ and all $j_r$ are summed for $0 \leq r < N$. $|j\rangle$ is
\[ |j\rangle = \prod_{\ell=1}^{N-1} I_{\ell-1} \otimes g_{j_{N-1}} |j_0\rangle |1\rangle, \]
where $|j_0\rangle$ is an eigenstate of $H^{(0)}_{\frac{1}{2}} = H_0 + N\Delta$, and $|1\rangle$ is a spinor with $2^{N-1}$ components and each component is equal to one. The expansion in Eq. (11) can be understood in this way that subsystems of the $N$-spin system provide intrinsically a correlated orthonormal basis to represent the EP of the $N$-spin system. It should be mentioned that a similar representation can be established for a system of many spin-$\frac{1}{2}$ due to the USUSY associated with the single spins.

The correlated basis should be contrasted with a basis constructed out of disentangled states with a dimension of $2^N \times M$ to diagonalize $H^{(N)}$, where $M$ is the number of boson states kept in the truncated basis. If the correlated basis is used to diagonalize $H^{(N)}$, a considerably smaller truncated basis is required to reproduce
The next example is the generalized Dicke model with $H_0 = a^\dagger a$ and $F_+ = \alpha a + \beta a^\dagger + \gamma$. Including $N$ spins $[25, 27]$. In Fig. 2, we show the results of solving the EP of $N$-spin model through diagonalizing the associated reduced Hamiltonian $h^{(N-1)}$. The basis for representing $h^{(N-1)}$ is constructed out of $N$ lowest eigenstates of $H^{(N-1)}_\text{TCC}$. The results are compared with outcomes of a direct ED on $H^{(N)}$ by means of a basis with a dimension of $2^N \times M$. It is the merits of the intrinsic correlated basis that even by shrinking the size of the truncated basis down to $N = 1$, the ground-state energy can be achieved quite accurately in comparison with the direct ED (see also Supplementary Information). Moreover, the results become more accurate by increasing the number of spins $N$. The latter can be attributed to the pattern of correlations in Eq. (12): the higher number of spins induces more correlations into characteristic equations.

We exemplified only spin-boson models in this letter. The USUSY QM and related identities, however, do not rely on the nature of fields coupled with the spin; for instance, $F_\pm$ and $\Delta$ can be spin operators themselves. It can be concluded that the entanglement of the spin and a field provides correlations that can be exploited to reduce DOF. The importance of the entanglement in exploring relevant sectors of Hilbert spaces is elevated in tensor network (TN) methods [13] developed under the influence of the quantum information science. A TN state is a trial wavefunction which allows to control the amount of the entanglement in the state. This aspect is missing in a standard local-basis representation where there is no clue about the structure of the entanglement in the state. Our study can also be of relevance to this realm since it reveals that a system of interacting spins offers its own intrinsic basis with a tractable pattern of entanglement that can be deduced directly from the Hamiltonian. The connection becomes tangible by noticing that the coefficients of the expansion in Eq. (11) have already a matrix form [23]. Moreover, the fractal structure of the states in Eq. (12) mimics the way by which entanglement is implemented in some TN ansatz [12, 29]. It can be subjects of further researches to connect the study presented here and TN methods in order to construct new families of ansatz in the study of spin systems.

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**SUPPLEMENTARY INFORMATION FOR UNCONVENTIONAL SUPERSYMMETRIC QUANTUM MECHANICS IN SPIN SYSTEMS**

**UNITARY TRANSFORMATIONS**

We consider a two-level Hamiltonian and its transformation under a rotation in $SU(2)$

$$H = \begin{pmatrix} H_+ & F_+ \\ F_- & H_- \end{pmatrix}, \quad \tilde{H} = \begin{pmatrix} \tilde{H}_+ & \tilde{F}_+ \\ \tilde{F}_- & \tilde{H}_- \end{pmatrix} = U^\dagger H U,$$

where

$$U^\dagger \equiv U^\dagger(\phi, \theta) = \begin{pmatrix} e^{-i\phi} \cos \frac{\theta}{2} - e^{i\phi} \sin \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} & e^{i\phi} \cos \frac{\theta}{2} \end{pmatrix}.$$  \hspace{1cm} (S2)

Given $H_\pm = H_0 \pm \Delta$, the explicit form of the transformed Hamiltonian is written in terms of the following operators

$$\tilde{H}_\pm = H_0 \pm \Delta \cos \theta \mp \frac{1}{2} (e^{i\phi} F_- + e^{-i\phi} F_+) \sin \theta, \quad \tilde{F}_\pm = \Delta \sin \theta + F_+ e^{-i\phi} \cos^2 \frac{\theta}{2} - F_- e^{i\phi} \sin^2 \frac{\theta}{2}.$$  \hspace{1cm} (S3)

We proceed with the generalized Rabi model specified by $H_0 = a^\dagger a$ and $F_\pm = \alpha a + \beta a^\dagger \pm \gamma$ for $\alpha, \beta \in \mathbb{R}^+$ and $\gamma \in \mathbb{C}$. The transformed Hamiltonian takes the form $\tilde{H}_\pm = a^\dagger a \pm (a^\lambda + a^\dagger \lambda + \tilde{\Delta})$ and $\tilde{F}_\pm = \tilde{\alpha} a + \tilde{\beta} a^\dagger + \tilde{\gamma}$ where

$$\lambda = -\frac{1}{2} \sin \theta (\alpha e^{i\phi} + \beta e^{-i\phi}),$$

$$\tilde{\Delta} = \Delta \cos \theta - \frac{1}{2} \sin \theta (\gamma e^{-i\phi} + \gamma^* e^{i\phi}),$$

$$\tilde{\alpha} = \alpha e^{-i\phi} \cos^2 \frac{\theta}{2} - \beta e^{i\phi} \sin^2 \frac{\theta}{2},$$

$$\tilde{\beta} = \beta e^{-i\phi} \cos^2 \frac{\theta}{2} - \alpha e^{i\phi} \sin^2 \frac{\theta}{2},$$

$$\tilde{\gamma} = \Delta \sin \theta + \gamma e^{-i\phi} \cos^2 \frac{\theta}{2} - \gamma^* e^{i\phi} \sin^2 \frac{\theta}{2}.$$  \hspace{1cm} (S8)

$\tilde{H}_\pm$ satisfy eigenvalue problems $\tilde{H}_\pm |\tilde{n}; \pm \rangle = \tilde{E}_\pm^{(n)} |\tilde{n}; \pm \rangle$, where $|\tilde{n}; \pm \rangle = D^\dagger(\pm \lambda) |n \rangle$ defined by action of the displacement operator $D(\lambda) = e^{\lambda a - \lambda^* a}$ on the eigenket of the number operator $a^\dagger a |n \rangle = n |n \rangle$, and the eigenenergies are $\tilde{E}_\pm^{(n)} = n - |\lambda|^2 \mp \tilde{\Delta}$. The commutation relations between fields of the Hamiltonian change as

$$\begin{align*}
[\tilde{H}_\pm, \tilde{F}_\pm] &= \tilde{\beta}(a^\dagger \pm \lambda^*) - \tilde{\alpha}(a \pm \lambda), \hspace{1cm} (S9) \\
[\tilde{F}_+, \tilde{F}_-] &= |\tilde{\alpha}|^2 - |\tilde{\beta}|^2 = (\alpha^2 - \beta^2) \cos \theta, \hspace{1cm} (S10) \\
[\tilde{H}_+, \tilde{H}_-] &= 2 (\lambda^* a - \lambda a^\dagger). \hspace{1cm} (S11)
\end{align*}$$

**Tridiagonalizing Matrix Representations of generalized Rabi Model**

Given neither of $\alpha, \beta$ and $\gamma$ is zero. Based on the commutation relation in Eq. (S9), setting either $\tilde{\alpha} = 0$ or $\tilde{\beta} = 0$ turns the representation of reduced Hamiltonians

$$\tilde{h}_\pm = \tilde{H}_\pm + \tilde{F}_\pm \tilde{G}_\pm \tilde{F}_+, \quad \tilde{G}_\pm = \frac{1}{E - \tilde{H}_\pm},$$

into a tridiagonal form when represented in the basis of $\tilde{H}_\pm$. To illustrate it, we choose $\tilde{\beta} = 0$ which is satisfied by $\tan \frac{\theta}{2} = \sqrt{\beta/\alpha}$ and $\phi = 0$. Concerning the eigenvalue problem $(\tilde{h}_+ - E) |\psi_+ \rangle = 0$, the matrix elements in the base ket
of $|\tilde{n};-\rangle$ become
\[
\tilde{f}_{+}^{(m,n)} = (\langle \tilde{n};-| (\tilde{\hat{n}} + E)|\tilde{n};-\rangle
= (m + 3|\lambda|^2 + \hat{\Delta} + (m + 1)|\tilde{\alpha}|^2 \hat{\epsilon}_{-}^{(m+1)} + |\tilde{\alpha}|^2 \hat{\epsilon}_{-}^{(m)} - E) \delta_{m,n}
+ (2\hat{\alpha}^* + \tilde{\alpha}^*(\hat{\gamma}^* + \tilde{\alpha}^* \lambda^*) \hat{\epsilon}_{-}^{(m)}) \sqrt{\alpha} \delta_{m+1,n} + (2\lambda + \tilde{\alpha}^*(\hat{\gamma} + \tilde{\alpha} \lambda) \hat{\epsilon}_{-}^{(m)}) \sqrt{\alpha} \delta_{m,n+1},
\]
where $\hat{\epsilon}_{-}^{(m)} = (E - \hat{E}_{-}^{(m)})^{-1}$. The determinant of the tridiagonal matrix can be worked out by means of the three-term recurrence relation in Eq. [1].

**DIAGONALIZING A SPIN-1 MODEL IN THE SPIN SUBSPACE**

Hamiltonian of a single spin-1 coupled with an external field in the associated eigenvalue problem reads
\[
\begin{pmatrix}
H_0 + \Delta & \sqrt{2}F_+ & 0 \\
\sqrt{2}F_- & H_0 & \sqrt{2}F_+ \\
0 & \sqrt{2}F_- & H_0 - \Delta
\end{pmatrix}
\begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix}
= E
\begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix}
= E|\Psi_1\rangle.
\]
We assume the eigenspinor is reducible. This implies the components are not vacuum of the off-diagonal operators $F_{\pm}$ and inverses of the diagonal terms, which appear in the course of decoupling the components, are well-defined. Making the Hamiltonian traceless, we find
\[
\begin{pmatrix}
0 & \sqrt{2}G_1F_+ & 0 \\
\sqrt{2}G_2F_- & 0 & \sqrt{2}G_2F_+ \\
0 & \sqrt{2}G_3F_- & 0
\end{pmatrix}
\begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix}
= \begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix},
\]
where
\[
\begin{pmatrix}
G_1 = (E - H_0 - \Delta)^{-1}, \\
G_2 = (E - H_0)^{-1}, \\
G_3 = (E - H_0 + \Delta)^{-1}.
\end{pmatrix}
\]
Taking the square of the traceless matrix gives
\[
\begin{pmatrix}
2G_1F_+G_2F_- & 0 & 2G_1F_+G_2F_+ \\
2G_2F_-G_1F_+ + 2G_2F_+G_3F_- & 0 & G_3F_-G_2F_+ \\
2G_3F_-G_2F_- & 0 & G_3F_-G_2F_+
\end{pmatrix}
\begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix}
= \begin{pmatrix}
|\psi_1\rangle \\
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix},
\]
which provides a decoupled equation
\[
(H_0 + 2F_-G_1F_+ + 2F_+G_3F_-)|\psi_2\rangle = E|\psi_2\rangle.
\]
Two other components are coupled by a two-level Hamiltonian and can be decoupled by repeating the same scheme to find two extra eigenvalue problems
\[
\begin{pmatrix}
H_0 + \Delta + 2F_+G_2F_- + 4F_+G_2F_+ & 1 & E - H_0 + \Delta - 2F_-G_2F_+ \\
E - H_0 - \Delta - 2F_-G_2F_- & 0 & 1 \\
F_+G_2F_- & F_-G_2F_+ & H_0 - \Delta - 2F_-G_2F_- \\
\end{pmatrix}
|\psi_1\rangle = E|\psi_1\rangle,
\]
\[
\begin{pmatrix}
H_0 - \Delta + 2F_-G_2F_+ + 4F_-G_2F_- & 1 & E - H_0 + \Delta - 2F_-G_2F_- \\
E - H_0 - \Delta - 2F_-G_2F_+ & 0 & 1 \\
F_-G_2F_+ & F_+G_2F_- & H_0 - \Delta - 2F_-G_2F_+
\end{pmatrix}
|\psi_3\rangle = E|\psi_3\rangle.
\]
We note also the full eigenstate can be constructed from a disentangled state
\[
|\Psi_1\rangle = \begin{pmatrix}
\sqrt{2}G_1F_+ & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 \sqrt{2}G_3F_-
\end{pmatrix}
\begin{pmatrix}
|\psi_2\rangle \\
|\psi_3\rangle
\end{pmatrix}.
\]

**EXACT DIAGONALIZATION OF N-SPIN GENERALIZED DICKE MODELS**

The direct exact diagonalization (ED) of the $N$-spin generalized Rabi model $H_0 = a^\dagger a$ and $F_+ = \alpha a + \beta a^\dagger + \gamma$ (see Eq. [8])
\[
H^{(N)}|\Psi^{(N)}\rangle = \begin{pmatrix}
H^{(N-1)}_+ & F_+ \\
F_- & H^{(N-1)}_-
\end{pmatrix}
\begin{pmatrix}
|\psi^{(N)}_+\rangle \\
|\psi^{(N)}_-\rangle
\end{pmatrix} = \begin{pmatrix}
H^{(N-1)}_+ + \Delta & F_+ \\
F_- & H^{(N-1)}_- - \Delta
\end{pmatrix}
\begin{pmatrix}
|\psi^{(N-1)}_+\rangle \\
|\psi^{(N-1)}_-\rangle
\end{pmatrix} = E|\Psi^{(N)}\rangle.
that the eigenstates with error to 2

Particularly, each eigenstate of \( H \) can be diagonalized by means of a truncated basis constructed out of eigenstates of \( H \), having the number of extracted eigenstates of \( H \), having energy errors smaller than 4% in comparison with a direct ED, is shown by \( N_{\text{out}} \). The dashed line corresponds to \( N_{\text{out}}/N_{\text{in}} = 2 \) which is given as a matter of comparison.

is about to diagonalize the matrix representation of \( H \) in the truncated basis \( |n, S_i\rangle \) where \( n \in [0, M - 1] \) is the boson occupation number and \( S_i = (s_1, s_2, \ldots, s_N), i \in [1, 2N] \) is the collective spin index of the N-spin system while \( s_i \) is the state of a single spin. The matrix element of the Hamiltonian is simply given by

\[
(H^{(N)})_{i,j}^{m,n} = \langle n, S_i | H^{(N)} | m, S_j \rangle ,
\]

and the dimension of the matrix is \( 2^N \times M \).

Instead, the reduced Hamiltonian of the N-spin generalized Rabi model in the associated eigenproblem

\[
h_{+}^{(N-1)} |\psi_{+}^{(N-1)}\rangle = \left( H^{(N-1)} + \Delta + F_{+} \frac{1}{E + \Delta - H^{(N-1)} F_{-}} \right) |\psi_{+}^{(N-1)}\rangle = E |\psi_{+}^{(N-1)}\rangle \]

can be diagonalized by means of a truncated basis constructed out of eigenstates of \( H_{-}^{(N-1)} \). The eigenenergies are then given by the roots of the determinant of the matrix

\[
\mathcal{F}^{(N)}_{j,k} = \langle \Psi_j^{(N-1)} | (H^{(N-1)} + \Delta - E + F_{+} \frac{1}{E + \Delta - H^{(N-1)} F_{-}}) | \Psi_k^{(N-1)} \rangle
\]

\[
= \delta_{j,k} \left( E_{j}^{(N-1)} - \Delta - E \right) + \sum_{i=1}^{N} \langle \Psi_j^{(N-1)} | F_{+} | \Psi_i^{(N-1)} \rangle \frac{1}{E + \Delta - E_{i}^{(N-1)}} \langle \Psi_i^{(N-1)} | F_{-} | \Psi_k^{(N-1)} \rangle , \]

where \( |\Psi_i^{(N-1)}\rangle \) is the eigenstate of the \((N-1)\)-spin Hamiltonian with its eigenenergy \( E_{i}^{(N-1)} \). The eigenstate is formally written as

\[
|\Psi_i^{(N-1)}\rangle = \left( \sum_{n=0}^{\infty} c_{n}^{i,1} |n\rangle \right) \approx \left( \sum_{n=0}^{M-1} c_{n}^{i,1} |n\rangle \right) ,
\]

where \( c_{n}^{i,1} \) can be obtained by direct ED of \((N-1)\)-spin system or obtained by solving its reduced eigenproblem. \( h_{+}^{(N-1)} \) is represented in a matrix \((N)\) by means of a \( N \)-dimensional basis. If the truncation is the same for different spins, then \( \max(N) = 2^{N-1}M \). In Fig. S1, it is shown that engaging \( N \) eigenstates of \((N-1)\)-spin system (to diagonalize the reduced Hamiltonian) results in more than \( N \) eigenstates of N-spin system with energy errors < 4%. Particularly, each eigenstate of \( N-1 \) spins leads to two eigenstates of N-spin system when \( N \leq 4 \).

In fact, we can further demonstrate that \( N \) eigenstates of the \((N-1)\)-spin subsystem input in the \( \mathcal{F} \) matrix lead to \( 2N \) eigenstates of the N-spin system. The reason why \( N_{\text{out}} < 2N_{\text{in}} \) with \( N_{\text{in}} > 4 \) in Fig. S1 is due to the fact that the eigenstates with error > 4% are not counted. Note that we just discuss how to use the truncated correlated
basis to recover the eigenstates obtained by the direct ED. The high-energy states of direct ED themselves are not converged because of the truncation of the basis. We here compare the reduced Hamiltonian method with the direct ED method despite the errors of the high-energy states in the direct ED.

We first give a physical argument on the relation between input and output numbers of states in the diagonalization of the reduced Hamiltonian. Assume \( \alpha = \beta = 0 \), then the matrix elements in Eq. (S22) just have diagonal non-zero terms

\[
(F)_{j,j} = \left(E_j^{(N-1)} + \Delta - E\right) + \frac{|\gamma|^2}{E + \Delta - E_j^{(N-1)}}.
\]

The eigenenergies are the roots of \(|F| = \prod_{j=1}^{N} (F)_{j,j} = 0\) which has \(2N\) solutions. Now, turning on \( \alpha \) and \( \beta \) adiabatically just redistribute the eigenenergies and does not generate/annihilate any state. Therefore, exploiting \( N \) states to diagonalize \((N-1)\)-spin system gives rise to \(2N\) eigenstates of \(N\)-spin system. We further analyze a generic spin model in the following.

The roots of the equation \(|F^{(N)}(E)| = 0\) give the eigenenergies of the \(N\)-spin system. The number of the roots is given by the maximum power of \(E\) in this polynomial equation. The difficulty to count the power of \(E\) stems from the fact that \(E\) is contained in the denominators of all the elements of the matrix.

We drop the upper indices of \(F^{(N)}\) and \(E^{(N-1)}\) in the following for convenience, and rewrite its element in short,

\[
(F)_{j,k} = \delta_{j,k} \left(E_j + \Delta - E\right) + \sum_{i=1}^{N} \frac{A_{j,i}B_{i,k}}{\varepsilon_i},
\]

where \(A_{j,i} = \langle \Psi_j^{(N-1)} | F_+ | \Psi_i^{(N-1)} \rangle\), \(B_{i,k} = \langle \Psi_i^{(N-1)} | F_- | \Psi_k^{(N-1)} \rangle = A_{k,i}^{*}\), and \(\varepsilon_i = E + \Delta - E_i\). The determinant of the matrix is given by

\[
|F| = \sum_{\{a_i\}} \varepsilon_{a_1,a_2,\ldots,a_N} \prod_{j=1}^{N} (F)_{j,a_j},
\]

where \(\{a_i\}\) is one of the permutation of the set \(\{a_1,\ldots,a_N\}\), and \(\varepsilon_{a_1,a_2,\ldots,a_N}\) is the levi-civita symbol of this permutation. To figure out the highest power of \(E\) in the equation \(|F(E)| = 0\), we just need to find out the highest power of \(E\) in the denominator, which is shown by \(x\). The term in the determinant \(\prod \left(E_j + \Delta - E\right)\) gives the power of \(E\) already known to be \(N\). Thus the maximum power of \(E\) in the equation \(|F(E)| = 0\) is given by \(x + N\).

First, let us consider the simplest case, \(N = 1\). The determinant equation reads

\[
|F| = (E_1 + \Delta - E) + \frac{A_{1,1}B_{1,1}}{\varepsilon_1} = 0
\]

showing that the maximum power of \(E\) is 2, then there are two roots for this equation, which corresponds to two output eigenstates of \(N\) spins. Second, we consider \(N = 2\),

\[
|F| = (E_1 + \Delta - E) (E_2 + \Delta - E) + (E_1 + \Delta - E) \left(\frac{A_{1,2}B_{1,2}}{\varepsilon_1} + \frac{A_{2,2}B_{2,2}}{\varepsilon_2}\right) + (E_2 + \Delta - E) \left(\frac{A_{1,1}B_{1,1}}{\varepsilon_1} + \frac{A_{1,2}B_{2,1}}{\varepsilon_2}\right) + \frac{A_{1,1}B_{1,1}}{\varepsilon_1} \frac{A_{2,2}B_{2,2}}{\varepsilon_2} + \frac{A_{1,2}B_{2,1}}{\varepsilon_1} \frac{A_{2,1}B_{1,2}}{\varepsilon_2} + \frac{A_{1,1}B_{1,2}B_{2,2}}{\varepsilon_1} + \frac{A_{2,1}B_{1,1}B_{2,2}}{\varepsilon_1} = 0.
\]

The terms with the denominators \(\frac{1}{\varepsilon_1^2},\frac{1}{\varepsilon_2^2}\) are cancelled each other. Hence, the highest power of \(E\) in \(|F| = 0\) is four, which is given by \((E_1 + \Delta - E) (E_2 + \Delta - E) \varepsilon_1 \varepsilon_2\). It means that four roots can be found to correspond to the four eigenstates of the \(N\)-spin system. In the same manner, we can find that there are six roots if \(N = 3\).

We just need to consider terms like

\[
\sum_{\{a_i\}} \varepsilon_{a_1,a_2,\ldots,a_N} \prod_{j=1}^{N} \frac{A_{j,k_j}B_{k_j,a_j}}{\varepsilon_{k_j}}.
\]

in the determinant since it contains the highest power of \(E\) in the denominator. In general, we have

\[
\sum_{\{a_i\}} \varepsilon_{a_1,a_2,\ldots,a_N} \prod_{j=1}^{N} \frac{A_{j,k_j}B_{k_j,a_j}}{\varepsilon_{k_j}} = \sum_{\{a_i\}} \varepsilon_{a_1,a_2,\ldots,a_N} \sum_{\{k_i\}} \frac{A_{1,k_1}B_{k_1,a_1}}{\varepsilon_{k_1}} \frac{A_{2,k_2}B_{k_2,a_2}}{\varepsilon_{k_2}} \prod_{j=3}^{N} \frac{A_{j,k_j}B_{k_j,a_j}}{\varepsilon_{k_j}}.
\]
Using $\epsilon_{a_1,a_2,\ldots,a_N} + \epsilon_{a_2,a_1,\ldots,a_N} = 0$, we obtain that

$$
\epsilon_{a_1,a_2,\ldots,a_N} \sum_{k_1} \sum_{k_2} A_{1,k_1} B_{k_1,a_1} A_{2,k_2} B_{k_2,a_2} \prod_{j=3}^{N} \sum_{k_j \neq k_1, k_j \neq k_2} \frac{A_{j,k_j} B_{k_j,a_j}}{\epsilon_{k_j}} 
$$

$$
+ \epsilon_{a_2,a_1,\ldots,a_N} \sum_{k_1} \sum_{k_2} A_{1,k_1} B_{k_1,a_2} A_{2,k_2} B_{k_2,a_1} \prod_{j=3}^{N} \sum_{k_j \neq k_1, k_j \neq k_2} \frac{A_{j,k_j} B_{k_j,a_j}}{\epsilon_{k_j}} 
$$

$$
= \epsilon_{a_1,a_2,\ldots,a_N} \sum_{k_1 \neq k_2} A_{1,k_1} B_{k_1,a_1} A_{2,k_2} B_{k_2,a_2} - \epsilon_{a_2,a_1,\ldots,a_N} \sum_{k_1 \neq k_2} A_{1,k_1} B_{k_1,a_2} A_{2,k_2} B_{k_2,a_1} \prod_{j=3}^{N} \sum_{k_j \neq k_1, k_j \neq k_2} \frac{A_{j,k_j} B_{k_j,a_j}}{\epsilon_{k_j}} 
$$

by exchanging $a_1$ and $a_2$. It means that for arbitrary two indices $a_1, a_2$, the associated terms with $\frac{1}{\epsilon_{k_1}}$ and $\frac{1}{\epsilon_{k_2}}$ are excluded. For three indices $a_1, a_2, a_3$, by exchanging $a_{1(2)}$ and $a_3$, we also obtain

$$
\sum_{\{a_i\}} \epsilon_{a_1,a_2,a_3} \sum_{k_1 \neq k_2} \sum_{k_3} A_{1,k_1} B_{k_1,a_1} A_{2,k_2} B_{k_2,a_2} A_{3,k_3} B_{k_3,a_3} \frac{A_{j,k_j} B_{k_j,a_j}}{\epsilon_{k_j}} 
$$

$$
= \sum_{\{a_i\}} \epsilon_{a_1,a_2,a_3} \sum_{k_1 \neq k_2, k_3} \frac{(\ldots)}{\epsilon_{k_1} \epsilon_{k_2} \epsilon_{k_3}} 
$$

where $(\ldots)$ only contains $A$ and $B$ and is not related to $\epsilon_{k_i}$. It can be readily generalized

$$
\sum_{\{a_i\}} \epsilon_{a_1,a_2,\ldots,a_N} \prod_{j=1}^{N} \sum_{k_j} A_{j,k_j} B_{k_j,a_j} = \sum_{\{a_i\}} \epsilon_{a_1,a_2,\ldots,a_N} \sum_{k_1 \neq k_2 \ldots \neq k_N} \frac{(\ldots)}{\epsilon_{k_1} \epsilon_{k_2} \ldots \epsilon_{k_N}}, 
$$

due to the fact $\sum_{\{a_i\}} \epsilon_{a_1,a_2,\ldots,a_N} = 0$, where $(\ldots)$ contains $A$ and $B$ and is not related to $E$ at all. Hence, in the summation of all the permutations, only the term with a denominator like $\prod_{k_1 \neq k_2 \ldots \neq k_N} \epsilon_{k_j}$ survives. Then the term of the highest power of $E$ is given by

$$
\prod_{i=1}^{N} \left(E_i^{N-1} + \Delta - E \right) \prod_{k_1 \neq k_2 \ldots \neq k_N} \epsilon_{k_j} 
$$

in the equation $|F| = 0$, so that the number of the roots is $2N$ according to fundamental theorem of algebra.