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LETTER TO THE EDITOR

Canonical decoupling of different degrees of freedom for a two-level system coupled to phonons

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Abstract. We consider the quantum model of a two-level system linearly coupled to M harmonic oscillators. Using symmetry arguments we show the existence of new constants of motion for this physical system. Starting with this knowledge, we develop a systematic treatment by which an effective canonical decoupling of different degrees of freedom is obtained.

The problem of diagonalization of the Hamiltonian model

$$H_{\rm SB} = \sum_{k=1}^{M} [\hbar\omega_k \alpha_k^\dagger \alpha_k + \varepsilon_k(\alpha_k + \alpha_k^\dagger)\sigma_x] + \tfrac{1}{2}\hbar\omega_0\sigma_z \tag{1}$$

which is a finitely many modes version of the well known spin-boson Hamiltonian model, is of current interest in many areas of physics. $H_{\rm SB}$ describes the linear coupling between a two-level object and a M-mode bosonic field. The two-level system is represented, as usual, by Pauli operators σ_x, σ_y, σ_z; α_k and $\alpha_k^\dagger$ are the Bose operators for the kth quantized field mode with frequency ω_k and fulfil canonical commutation relations:

$$[\alpha_k, \alpha_{k'}] = 0 \qquad [\alpha_k, \alpha_{k'}^\dagger] = \delta_{kk'}. \tag{2}$$

The spin-boson Hamiltonian is one of the few Hamiltonian models describing the coupling of small systems to its environment [1]. It arises in various contexts as a description of quantum tunnelling of a macrosystem between two minima of a double well potential [2], the coupling of an isolated defect in a crystal to phonons [3], or the coupling of a molecule to the radiation field [4].

The aim of this letter is twofold: (a) to provide evidence of the existence of some symmetry properties of $H_{\rm SB}$ connected to new constants of motion; (b) to show the way to take advantage of this knowledge to make relatively simpler the search of eigenstates and eigenvalues of $H_{\rm SB}$. For simplicity we take $M = 2$, pointing out, however, that all the conclusions achieved in this case can be generalized to the case $M > 2$. Thus $H_{\rm SB}$ assumes the form

$$H_{\rm SB} = \hbar\omega_1\alpha_1^\dagger\alpha_1 + \hbar\omega_2\alpha_2^\dagger\alpha_2 + \varepsilon_1(\alpha_1 + \alpha_1^\dagger)\sigma_x + \varepsilon_2(\alpha_2 + \alpha_2^\dagger)\sigma_x + \tfrac{1}{2}\hbar\omega_0\sigma_z. \tag{3}$$

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It is immediately verified that the canonical transformation which changes the sign of α_1, $\alpha_1^\dagger$, α_2, $\alpha_2^\dagger$, σ_x, σ_y, leaving σ_z unmodified, is a symmetry transformation for $H_{\rm SB}$ [5–6]. A unitary operator G that accomplishes such a transformation may be taken in the form [6]

$$G = \exp\{\mathrm{i}\pi[N + \tfrac{1}{2}\sigma_z + \tfrac{1}{2}]\} = -\sigma_z \cos\pi N = G^\dagger \tag{4}$$

where

$$N = \alpha_1^\dagger\alpha_1 + \alpha_2^\dagger\alpha_2. \tag{5}$$

This is easily seen considering the anticommutation properties of the Pauli operators and the fact that the operator $\cos(\pi N)$ anticommute with the four operators α_1, $\alpha_1^\dagger$, α_2, $\alpha_2^\dagger$.

Of course $[H_{\rm SB}, G] = 0$, that is G is a constant of motion. In addition G is a Hermitian operator whose eigenvalues are only $+1$ and -1. These properties suggest looking for a unitary operator T such that $T^\dagger G T = -\sigma_z$. In this way, submitting $H_{\rm SB}$ to the canonical transformation realized by T, we get a new Hamiltonian operator which commutes with σ_z and therefore can depend on the pseudo-spin variables only through σ_z if we take into account that the Casimir operator for the group $SU(2)$ is a multiple of the unit operator. As a consequence pseudo-spin and bosonic variables can be easily and exactly separated in the diagonalization problem of the transformed Hamiltonian. It has been shown [6] that T may be chosen inside a class of unitary operators, a representant of which is

$$T = \exp\left\{-\mathrm{i}\frac{\pi}{2}(\sigma_x - 1)(\alpha_1^\dagger\alpha_1 + \alpha_2^\dagger\alpha_2)\right\}. \tag{6}$$

Observing that

$$T = \cos^2\left(\frac{\pi}{2}N\right) + \sigma_x \sin^2\left(\frac{\pi}{2}N\right) = T^\dagger \tag{7}$$

we easily get

$$T^\dagger G T = -\sigma_z \qquad T^\dagger \alpha_i T = \alpha_i \sigma_x \qquad \text{with } i = 1, 2 \tag{8}$$

and

$$H_{\rm B} = \hbar\omega_1\alpha_1^\dagger\alpha_1 + \hbar\omega_2\alpha_2^\dagger\alpha_2 + \varepsilon_1(\alpha_1 + \alpha_1^\dagger) + \varepsilon_2(\alpha_2 + \alpha_2^\dagger) + \tfrac{1}{2}\hbar\omega_0\cos(\pi N)\sigma_z. \tag{9}$$

The form assumed by $H_{\rm B}$ enables the exact decoupling of the pseudo-spin variables from the bosonic ones simply regarding σ_z as a c-number, coincident with anyone between its two eigenvalues. Let us note, in addition, the nonlinear coupling between the two new field modes arising from the common interaction of the two old modes with the two-level system.

The knowledge of the constant of motion G, connected to a particular symmetry property of $H_{\rm SB}$, plays a central role in the possibility of obtaining the purely bosonic Hamiltonian $H_{\rm B}$. We are therefore led in a natural way to wonder whether an analogous decoupling of the two bosonic modes is feasible, with the help of a treatment based once more on symmetry arguments. The presence of the operator $\cos(\pi N)$ in $H_{\rm B}$ makes it very difficult to guess the structure of an eventual canonical transformation of the field operators which leaves $H_{\rm B}$ invariant, without introducing appropriate restrictive relations involving the characteristic parameters of the physical system appearing in $H_{\rm SB}$. If, however, we confine ourselves to the particular non-trivial case of Einstein bosons putting $\omega_1 = \omega_2 = \omega$, we may overcome the difficulty related to the cos-operator looking, from the beginning, for a symmetry transformation of H_B in the class of the canonical transformations which do not modify N. This last requirement is easily satisfied choosing the following one-parameter family of canonical transformations

$$\begin{cases} \tilde{\alpha}_1 = \alpha_1 \cos\vartheta + \alpha_2 \sin\vartheta \\ \tilde{\alpha}_2 = \alpha_1 \sin\vartheta - \alpha_2 \cos\vartheta \end{cases} \tag{10}$$

where ϑ has to be fixed, if possible, in such a way that

$$H_B(\tilde{\alpha}_1, \tilde{\alpha}_2, \tilde{\alpha}_1^\dagger, \tilde{\alpha}_2^\dagger) = H_B(\alpha_1, \alpha_2, \alpha_1^\dagger, \alpha_2^\dagger). \tag{11}$$

This condition is guaranteed by demanding that the linear terms in (9) be invariant under the transformation (10). We have

$$\varepsilon_1(\tilde{\alpha}_1 + \tilde{\alpha}_1^\dagger) + \varepsilon_2(\tilde{\alpha}_2 + \tilde{\alpha}_2^\dagger) = \tilde{\varepsilon}(\alpha_1 + \alpha_1^\dagger) + \tilde{\varepsilon}_2(\alpha_2 + \alpha_2^\dagger) \tag{12}$$

where

$$\begin{cases} \tilde{\varepsilon}_1 = \varepsilon_1 \cos\vartheta + \varepsilon_2 \sin\vartheta \\ \tilde{\varepsilon}_2 = \varepsilon_1 \sin\vartheta - \varepsilon_2 \cos\vartheta. \end{cases} \tag{13}$$

It is immediately verified that the conditions $\tilde{\varepsilon}_1 = \varepsilon_1$ and $\tilde{\varepsilon}_2 = \varepsilon_2$ may be simultaneously satisfied, in a non-trivial way, if

$$\cos\vartheta = \frac{\varepsilon_1^2 - \varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2} \qquad \sin\vartheta = \frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}. \tag{14}$$

Thus we arrive at the conclusion that the canonical transformation

$$\begin{cases} \tilde{\alpha}_1 = \dfrac{\varepsilon_1^2 - \varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2}\alpha_1 + \dfrac{2\varepsilon_1\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}\alpha_2 \\ \tilde{\alpha}_2 = \dfrac{2\varepsilon_1\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}\alpha_1 + \dfrac{\varepsilon_2^2 - \varepsilon_1^2}{\varepsilon_1^2 + \varepsilon_2^2}\alpha_2 \end{cases} \tag{15}$$

is a symmetry transformation for H_B provided that $\omega_1 = \omega_2 = \omega$. We are now in a position to follow the same idea as in the reduction of H_{SB} to H_B. Therefore we try to generate the canonical transformation expressed by (15) with the help of a suitable unitary operator. Noting that both $\tilde{\alpha}_1$ and $\tilde{\alpha}_2$ are linear combinations of α_1 and α_2, it appears reasonable to write such a unitary operator as $V = \exp(-i\eta K)$ where η is a real number while K is a Hermitian operator having the form

$$K = \Omega_1\alpha_1^\dagger\alpha_1 + \Omega_2\alpha_2^\dagger\alpha_2 + \lambda(\alpha_1^\dagger\alpha_2 + \alpha_1\alpha_2^\dagger) \tag{16}$$

with Ω_1, Ω_2 and λ adimensional real and positive coefficients to be determined. Instead of attempting a direct evaluation of $V^\dagger\alpha_1 V$ and $V^\dagger\alpha_2 V$ using the Baker–Hausdorff lemma, we introduce an auxiliary unitary operator defined as

$$S = \exp w(\alpha_1^\dagger\alpha_2 - \alpha_1\alpha_2^\dagger) \tag{17}$$

with w real parameter to be determined conveniently.

It is straightforward to derive $S^\dagger\alpha_1 S$ and $S^\dagger\alpha_2 S$ obtaining

$$\begin{cases} S^\dagger\alpha_1 S = \alpha_1\cos w + \alpha_2 \sin w \\ S^\dagger\alpha_2 S = -\alpha_1 \sin w + \alpha_2\cos w. \end{cases} \tag{18}$$

In passing, it is worthwhile underlining that the transformation (18) on the one hand cannot be obtained from (10) and on the other hand becomes a symmetry transformation of H_B if and only if w is a multiple of 2π. We may appreciate the advantage of introducing S evaluating $\tilde{K} = S^\dagger K S$. We easily get

$$\tilde{K} = \tilde{\Omega}_1\alpha_1^\dagger\alpha_1 + \tilde{\Omega}_2\alpha_2^\dagger\alpha_2 + \tilde{\lambda}(\alpha_1^\dagger\alpha_2 + \alpha_1\alpha_2^\dagger) \tag{19}$$

where

$$\begin{cases} \tilde{\Omega}_1 = \Omega_1\cos^2 w + \Omega_2 \sin^2 w - \lambda\sin 2w \\ \tilde{\Omega}_2 = \Omega_1 \sin^2 w + \Omega_2\cos^2 w + \lambda \sin 2w \\ \tilde{\lambda} = \frac{1}{2}(\Omega_1 - \Omega_2)\sin 2w + \lambda\cos 2w. \end{cases} \tag{20}$$

It is not difficult to convince oneself that the conditions:

$$\tilde{\Omega}_1 = 0 \qquad \tilde{\Omega}_2 = 1 \qquad \tilde{\lambda} = 0 \tag{21}$$

may be simultaneously satisfied provided that

$$\Omega_1 + \Omega_2 = 1 \qquad \Omega_1\Omega_2 = \lambda^2 \qquad \tan 2w = -\frac{2\lambda}{\Omega_1 - \Omega_2} \tag{22}$$

with $\Omega_1 \neq \Omega_2$. We still have two free parameters which may be conveniently fixed so that V generates the canonical transformation (10). To this end we now evaluate the expression of both $V^\dagger\alpha_1 V$ and $V^\dagger\alpha_2 V$:

$$\begin{aligned} V^\dagger\alpha_1 V &= S(S^\dagger e^{i\eta K} S)(S^\dagger\alpha_1 S)(S^\dagger e^{-i\eta K} S)S^\dagger \\ &= S e^{i\eta\alpha_2^\dagger\alpha_2}(\alpha_1\cos w + \alpha_2\sin w)e^{-i\eta\alpha_2^\dagger\alpha_2} S^\dagger \\ &= S(\alpha_1\cos w + \alpha_2 e^{-i\eta}\sin w)S^\dagger \\ &= (\cos^2 w + e^{-i\eta}\sin^2 w)\alpha_1 - \tfrac{1}{2}\sin 2w(1 - e^{-i\eta})\alpha_2. \end{aligned} \tag{23}$$

Proceeding in the same way yields:

$$V^\dagger\alpha_2 V = \tfrac{1}{2}\sin 2w(e^{-i\eta} - 1)\alpha_1 + (e^{-i\eta}\cos^2 w + \sin^2 w)\alpha_2. \tag{24}$$

From a comparison between (23) and (24) with (14) we easily derive that the operational equations $V^\dagger\alpha_1 V = \tilde{\alpha}_1$ and $V^\dagger\alpha_2 V = \tilde{\alpha}_2$ may be simultaneously satisfied provided that

$$\eta = \pi \qquad \cos 2w = \frac{\varepsilon_1^2 - \varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2} \qquad \sin 2w = \frac{-2\varepsilon_1\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2} \tag{25}$$

and that such conditions are compatible with those expressed by (21). This last prescription determines Ω_1, Ω_2 and λ in terms of ε_1 and ε_2

$$\Omega_1 = \frac{\varepsilon_2^2}{\varepsilon_1^2 + \varepsilon_2^2} \qquad \Omega_2 = \frac{\varepsilon_1^2}{\varepsilon_1^2 + \varepsilon_2^2} \qquad \lambda = \frac{\varepsilon_1\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}. \tag{26}$$

We have thus completed the construction of the unitary operator generating the symmetry transformation (14) of H_{B}. It has the form

$$V = \exp\left(\frac{\mathrm{i}\pi}{\varepsilon_1^2+\varepsilon_2^2}[\varepsilon_2^2\alpha_1^\dagger\alpha_1 + \varepsilon_1^2\alpha_2^\dagger\alpha_2 + \varepsilon_1\varepsilon_2(\alpha_1^\dagger\alpha_2 + \alpha_1\alpha_2^\dagger)]\right) \tag{27}$$

and of course is a constant of motion. This operator, although Hermitian, possesses a finite spectrum so that to carry our decoupling project further we must eventually look for a more appropriate Hermitian constant of motion implicitly embodied in V. It is useful for this scope to reconsider the canonical transformation (23) and (24) in order to show that it is possible to derive that

$$H_{\mathrm{B}}(\alpha_1, \alpha_2, \alpha_1^\dagger, \alpha_2^\dagger) = V^\dagger H_{\mathrm{B}} V \tag{28}$$

for any value of the real parameter η, provided only that conditions (26) are satisfied. This mathematically means that the operator

$$V(\eta) = \exp\left(\frac{\mathrm{i}\eta}{\varepsilon_1^2+\varepsilon_2^2}[\varepsilon_2^2\alpha_1^\dagger\alpha_1 + \varepsilon_1^2\alpha_2^\dagger\alpha_2 + \varepsilon_1\varepsilon_2(\alpha_1^\dagger\alpha_2 + \alpha_1\alpha_2^\dagger)]\right) \tag{29}$$

commutes with H_{B} for any η, and this property is a necessary and sufficient condition to assert that the Hermitian operator

$$K = \frac{\varepsilon_2^2}{\varepsilon_1^2+\varepsilon_2^2}\alpha_1^\dagger\alpha_1 + \frac{\varepsilon_1^2}{\varepsilon_1^2+\varepsilon_2^2}\alpha_2^\dagger\alpha_2 + \frac{\varepsilon_1\varepsilon_2}{\varepsilon_1^2+\varepsilon_2^2}(\alpha_1^\dagger\alpha_2 + \alpha_1\alpha_2^\dagger) \tag{30}$$

is a constant of motion for H_{B} as well as for H_{SB} if we consider that $T^\dagger K T = K$. Its eigenvalues are all non-negative integers because we know from (21) that it is unitarily equivalent to $\alpha_2^\dagger\alpha_2$. This amounts to saying that, if we transform H_{B} in accordance with (18) choosing $w = -\tan^{-1}(\varepsilon_2\varepsilon_1^{-1})$ so that $S^\dagger K S = \alpha_2^\dagger\alpha_2$, the operator $S^\dagger H_{\mathrm{B}} S = H$ has to commute with $\alpha_2^\dagger\alpha_2$. Therefore, noting that S commutes with $\cos(\pi N) = \cos(\pi\alpha_1^\dagger\alpha_1)\cos(\pi\alpha_2^\dagger\alpha_2)$ as well as with $\alpha_1^\dagger\alpha_1, \alpha_2^\dagger\alpha_2$, we may easily guess that

$$[S^\dagger[\varepsilon_1(\alpha_1 + \alpha_1^\dagger) + \varepsilon_2(\alpha_2 + \alpha_2^\dagger)]S, \alpha_2^\dagger\alpha_2] = 0. \tag{31}$$

In addition, the linearity of the canonical transformation accomplished by S enables us to come to the conclusion that H cannot present any linear dependence on the operators α_2 and $\alpha_2^\dagger$. We get an immediate confirmation of this fact from the following easily evaluated relation

$$S^\dagger[\varepsilon_1(\alpha_1 + \alpha_1^\dagger) + \varepsilon_2(\alpha_2 + \alpha_2^\dagger)]S = \varepsilon_{\mathrm{eff}}(\alpha_1 + \alpha_1^\dagger) \tag{32}$$

where

$$\varepsilon_{\mathrm{eff}} = \sqrt{\varepsilon_1^2 + \varepsilon_2^2}. \tag{33}$$

We may thus write down the explicit expression of $H = S^\dagger H_{\mathrm{B}} S$:

$$H = \hbar\omega(\alpha_1^\dagger\alpha_1 + \alpha_2^\dagger\alpha_2) + \varepsilon_{\mathrm{eff}}(\alpha_1 + \alpha_1^\dagger) + \frac{\hbar\omega_0}{2}\sigma_z\cos(\pi\alpha_1^\dagger\alpha_1)\cos(\pi\alpha_2^\dagger\alpha_2). \tag{34}$$

In this way we succeed in obtaining a transformed Hamiltonian where the two new bosonic modes can be decoupled and the diagonalization problem is exactly reduced, in each subspace where $\alpha_2^\dagger\alpha_2$ has a well defined value, to an effective single mode problem.

We wish to conclude by pointing out that the approach followed in this letter to obtain H from H_{SB} is extensible, without too many difficulties, to the case of M degenerate modes. For this model, in fact, besides the new constant of motion (30), we are able to construct, following iteratively the same procedure used in this letter, $M-1$ independent similar new constants of motion. More generally we believe that the systematic decoupling procedure outlined in this letter may be useful to investigate other Hamiltonian models as, for instance in quantum optics, some generalized Jaynes–Cummings models [7].

In conclusion, we have illustrated, in connection with a Hamiltonian model extensively present in the literature, a treatment by which new symmetry properties of the model can be effectively used to reduce a difficult diagonalization problem to a simple one.

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