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Applying the variational principle to a spin-boson Hamiltonian

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Ground states of a spin-boson Hamiltonian, describing *one* two-level system (a spin) coupled to *infinitely* many harmonic oscillators (bosons), are studied. This spin-boson Hamiltonian is a prototype for the description of *a "small" system (e.g., a molecule) coupled to its environment.* The respective ground-state vector(s) are approximated by a linear combination of two *coherent*-state vectors corresponding to the two levels of the spin. Interest concentrates mainly on phase-transition phenomena (generation of superselection rules) in case the parameters of the Hamiltonian (level splitting of the spin, frequencies of the field modes, and coupling constants) exhibit an infrared singularity. The resulting phase diagrams are shown to satisfy reasonably well the rigorous bounds derived by Spohn, and in particular distinguish between the superohmic, ohmic, and subohmic regime in the sense of Leggett. Nevertheless, the approximation method used is simple enough so that everything can be explicitly calculated. Former results by Pfeifer as well as results by Emery and Luther, Zwerger and Harris and Silbey are extended and discussed.

I. GROUND STATES OF SYSTEMS WITH INFINITELY MANY DEGREES OF FREEDOM

When the variational principle is applied to some Hamiltonian H this is based on the assumption, that a ground-state vector ξ exists satisfying

$$H\xi = E_0\xi, \tag{1a}$$

$$\frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle} \geqslant E_0, \tag{1b}$$

where ψ is an arbitrary nonzero vector in the underlying Hilbert space. For systems with *finitely* many degrees of freedom this assumption is known or may at least expected to hold true in many cases.

For systems with *infinitely* many degrees of freedom (such as the radiation or a phonon field, or a molecule coupled to such fields) there is no similar guarantee at all, even if the respective Hamiltonian is known to be lower bounded. This is no pathology. It reflects the fact that the "observables" of infinite systems can be represented on "different" Hilbert spaces in a physically *non*equivalent manner, corresponding to different values of classical, possibly macroscopic observables.[1-7] As a consequence, the ground state looked for may "live" in a different representation. Since all infinite-dimensional Hilbert spaces with countable basis can be identified by a unitary mapping, it is not the Hilbert spaces which are "different," but much more the way the relevant observables (operators) act, i.e., the *representation*.

To illustrate this phenomenon, denote by E_0 the infinimum (i.e., the largest lower bound)

$$E_0 := \inf_{\psi\neq 0} \frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle}, \tag{2}$$

and consider some sequence of normalized vectors ξ_n, $n = 1,2,3,\ldots$, such that $\langle\xi_n|H\xi_n\rangle$ converges to E_0. Suppose, furthermore, that the expectation values $\langle\xi_n|T\xi_n\rangle$ converge to some expectation value $\phi(T)$ for arbitrary observables T of the system. Then one cannot expect that there is some vector ξ in the *original* Hilbert space implementing this expectation value by

$$\phi(T) = \langle\xi|T\xi\rangle. \tag{3}$$

Nevertheless, it can always be shown by use of the Gel'fand–Naimark–Segal representation (see Ref. 8, Sec. III; Ref. 7, Sec. II) that there exists a vector fulfilling condition (3) in some "different" Hilbert space belonging to a new representation of the system's observables.

Hence the essential new element arising in the discussion of infinite systems is the variety of physically inequivalent representations. State vectors of different representations are separated by a superselection rule.[1-7] Trying to approximate some ground state with the variational principle may result in a state ϕ (equal to the expectation value functional) which lives in a different representation, physically inequivalent to the original representation one started with. Furthermore, ground states separated by a superselection rule may occur.

II. THE SPIN-BOSON HAMILTONIAN

The following spin-boson Hamiltonian[7,9-21]

$$H^\epsilon = \hbar\epsilon\sigma_1 \otimes \mathbf{1} \tag{4a}$$

$$+ \mathbf{1} \otimes \sum_{n=1}^{\infty} \hbar\omega(n) a_n^* a_n \tag{4b}$$

$$+ \hbar\sigma_3 \otimes \sum_{n=1}^{\infty} \lambda(n)(a_n + a_n^*) \tag{4c}$$

will be used to illustrate the general statements in Sec. I. It refers to *one* two-level system (a "spin," described by 2×2 matrices, in particular, the Pauli matrices $\sigma_j, j = 1,2,3$) coupled to *infinitely* many bosons described by boson operators a_n, $n = 1,2,3,\ldots$, fulfilling the canonical commutation relations

$$[a_n, a_{n'}] = 0, \quad [a_n, a_{n'}^*] = \delta_{nn'}. \tag{5}$$

The term (4a) refers to the isolated two-level system with level splitting $2\hbar\epsilon$, the term (4b) to the isolated boson field, whereas (4c) is a kind of dipole-type coupling. The frequencies $\omega(n)$, $n = 1,2,3,...$, are strictly positive and the coupling constants $\lambda(n)$ real numbers, supposed to fulfill

$$\sum_{n=1}^{\infty} \frac{|\lambda(n)|^2}{\omega(n)} < \infty, \quad \sum_{n=1}^{\infty} |\lambda(n)|^2 < \infty, \tag{6}$$

the first of which guarantees that the Hamiltonian (4) is lower bounded [see, e.g., Ref. 7, Eq. (I.57)]. Main interest will be concentrated on the situation where the infrared divergence or infrared singularity (in short, IR singularity)

$$\sum_{n=1}^{\infty} \frac{|\lambda(n)|^2}{\omega(n)^2} = \infty \tag{7}$$

arises. Its strength is measured[9] by the coefficient ζ in the relation

$$\sum_{n=1}^{\infty} |\lambda(n)|^2 \exp[-\omega(n)|t|] \propto |t|^{-\zeta} \quad (\text{for large } |t|). \tag{8}$$

Here, "$\propto$" means "proportional to." For ζ strictly larger than 2, no IR divergence arises. In the terminology of Leggett *et al.*[10] this situation is called "superohmic." For $1 < \zeta \leqslant 2$ the IR divergence (7) holds true. It is called subohmic if $1 < \zeta < 2$, and ohmic for $\zeta = 2$.

The spin-boson Hamiltonian describes the coupling of a two-level system to a "bath" of infinitely many harmonic oscillators. It is used in many different circumstances (superconducting quantum interference devices,[10] coupling of a molecule to the radiation field,[11,22] or a phonon field, etc.). Here, it is considered as a *prototype for the coupling of a "small" system to its environment.*

III. APPLYING THE VARIATIONAL PRINCIPLE TO THE SPIN-BOSON HAMILTONIAN

The variational principle is used here to determine an *approximate* ground state of the spin-boson Hamiltonian (4). The ansatz taken is a linear combination of two *coherent-state vectors,*

$$\Omega := a\begin{bmatrix} W(\alpha)\Psi_F \\ 0 \end{bmatrix} + b\begin{bmatrix} 0 \\ W(\beta)\Psi_F \end{bmatrix}, \tag{9a}$$

$$a,b\in\mathbb{C}, \quad |a|^2 + |b|^2 = 1, \tag{9b}$$

where

$$W(\xi) := \exp\left[\sum_{n=1}^{\infty} \xi(n)a_n^* - \xi(n)^* a_n\right], \tag{10a}$$

$$\xi := [\xi(1),\xi(2),\xi(3),...], \quad \xi(n)\in\mathbb{C}, \tag{10b}$$

defines *unitary operators* satisfying the *Weyl canonical commutation relations.*[4,6,7] Here, ξ (and α,β above) are (appropriate) sequences of complex numbers and Ψ_F is the *Fock vector*, i.e., the ground-state vector of the Hamiltonian (4b) of the free field fulfilling

$$\langle \Psi_F | W(\xi)\Psi_F \rangle = \exp\left[-\frac{1}{2}\sum_{n=1}^{\infty} |\xi(n)|^2\right]. \tag{11}$$

Note that the expectation value with respect to a state vector $[W(\xi)\Psi_F]$ is properly defined even if ξ is *not* square summable [the unitary operator $W(\xi)$ itself is then only formally defined].

Later on the slightly more restricted class of states implemented by vectors

$$\Omega := a\begin{bmatrix} W(-\alpha)\Psi_F \\ 0 \end{bmatrix} + b\begin{bmatrix} 0 \\ W(\alpha)\Psi_F \end{bmatrix}, \tag{12a}$$

$$|a|^2 + |b|^2 = 1 \tag{12b}$$

will be investigated. It has been studied by Emery and Luther,[12] Zwerger (Ref. 13: Appendix), Silbey and Harris [cf. Ref. 15: Eqs. (95)–(99), and Refs. 23, 24] precisely in the same context of the spin-boson model.

The optimal coefficients a, b and sequences α, β are determined by the variational principle. The respective calculations are tedious but straightforward and will be published elsewhere. Interest is concentrated here on situations of *broken inversion symmetry*,[9,11,13,6,7,25,26] i.e., the case where the ground state is *not* unique. This situation arises if and only if the lowest-energy expectation value can be reached with a state vector Ω fulfilling

$$\langle \Omega | (\sigma_3 \otimes \mathbf{1})\Omega \rangle = |a|^2 - |b|^2 \neq 0. \tag{13}$$

The respective ground-state vectors are then given by (12) and its "mirror image"[9,11,6,27]

$$b\begin{bmatrix} W(-\beta)\Psi_F \\ 0 \end{bmatrix} + a\begin{bmatrix} 0 \\ W(-\alpha)\Psi_F \end{bmatrix}. \tag{14}$$

Checking if the inversion symmetry is broken can be done by calculation of the *infimum of energy expectation values* $\langle \Omega | H^\epsilon \Omega \rangle$, under the restriction that the variable

$$u := \langle \Omega | (\sigma_3 \otimes \mathbf{1})\Omega \rangle = |a|^2 - |b|^2 \tag{15}$$

takes a fixed (but arbitrary) prescribed value within the interval $[-1,+1]$. The infimum of these energy expectation values [with Ω being of the form (12)] is denoted by $E^\epsilon(u)$. *Hence the inversion symmetry is broken if and only if there exists some nonzero* $u_0\in[-1,+1]$ *such that*

$$E^\epsilon(u_0) \leqslant E^\epsilon(0). \tag{16}$$

In the sequel the functions

$$F(s) := \sum_{n=1}^{\infty} \left[\frac{\lambda(n)}{\omega(n)+s}\right]^2, \quad s\geqslant 0, \tag{17a}$$

$$L(s) := \sum_{n=1}^{\infty} \frac{\lambda(n)^2}{\omega(n)} \left[\frac{s}{\omega(n)+s}\right]^2, \quad s\geqslant 0, \tag{17b}$$

will be used (and assumed to be continuous). Furthermore, the auxiliary positive variable σ is defined to be either equal to zero or a solution of the equation

$$\frac{1}{2}\ln\left[\frac{2|\epsilon|}{(1-u^2)^{1/2}}\right] = \frac{1}{2}\ln(\sigma) + F(\sigma). \tag{18}$$

A first bunch of results is summarized as follows.

● The energy $E^\epsilon(u)$ is given by

$$E^\epsilon(u) := \min_\sigma\left\{(1-u^2)\left[L(\sigma) - \frac{1}{2}\sigma\right]\right\} - \sum_{n=1}^{\infty} \frac{|\lambda(n)|^2}{\omega(n)}, \quad u\in[-1,1], \tag{19}$$

where the minimum is taken over all solutions σ of Eq. (18) and $\sigma = 0$.

● The complex scalars a and b can be chosen as

$$a = +\sqrt{\tfrac{1}{2}(1+u)}, \tag{20a}$$

$$b = -\sqrt{\tfrac{1}{2}(1-u)}. \tag{20b}$$

Both could be multiplied with (the same) arbitrary complex scalar of modulus 1.

● The sequences α and β are real and given by

$$\alpha(j) = -\frac{\lambda(j)}{\omega(j)}\left[1-\frac{2\sigma|b|^2}{\omega(j)+\sigma}\right], \quad j=1,2,..., \tag{21a}$$

$$\beta(j) = \frac{\lambda(j)}{\omega(j)}\left[1-\frac{2\sigma|a|^2}{\omega(j)+\sigma}\right], \quad j=1,2,..., \tag{21b}$$

with σ being that one solution of Eq. (18) or zero, respectively, which minimizes $[L(\sigma)-(1/2)\sigma]$ in Eq. (19). The formulas (19)–(21) are also true (but not very interesting) in the "trivial" case $u=\pm 1$.[11,7]

For spin-boson Hamiltonians with IR singularity it is very convenient to introduce the *coupling strength* ρ, replacing the coupling constants $\lambda(n)$ in the Hamiltonian (4) by

$$\sqrt{\rho/2}\,\lambda(n), \quad n=1,2,3,... . \tag{22}$$

This parameter ρ just allows us to scale simultaneously all coupling constants. It is normalized by appropriate normalization of the coupling constants such that

$$\left\{\sum_{n=1}^{\infty}|\lambda(n)|^2\exp[-\omega(n)|t|]\right\}|t|^{\zeta}=1 \tag{23}$$

(for large $|t|$),

where the constant ζ, $1<\zeta\leqslant 2$, describes the strength of the IR singularity [see Eq. (8)]. Equations (18) and (19) will then be written as

$$\ln\left[\frac{2|\epsilon|}{(1-u^2)^{1/2}}\right]=\ln(\sigma)+\rho F(\sigma), \tag{24a}$$

$$E^{\epsilon}(u)=\min_{\sigma}\left\{(1-u^2)\left[\frac{\rho}{2}L(\sigma)-\frac{1}{2}\sigma\right]\right\} -\frac{\rho}{2}\sum_{n=1}^{\infty}\frac{|\lambda(n)|^2}{\omega(n)}, \quad u\in[-1,1], \tag{24b}$$

with F and L being based on normalized (23) coupling constants.

IV. THE PHASE DIAGRAM OF THE SPIN-BOSON MODEL

Evaluating the function (17a) for the *subohmic* $(1<\zeta<2)$ and *ohmic* $(\zeta=2)$ situation with *normalized coupling constants* gives

$$F_{\text{subohmic}}(\sigma)\cong\Gamma(2-\zeta)\sigma^{\zeta-2}+\text{const}, \tag{25a}$$

$$F_{\text{ohmic}}(\sigma)\cong-\ln\sigma+\text{const} \tag{25b}$$

for small σ, with $\Gamma(\cdot)$ being the gamma function.

The above estimates (25) for the function F can be used to give some preliminary results concerning the phase diagram of the spin-boson model. If the term

$$\ln(\sigma)+\rho F(\sigma) \tag{26}$$

in Eq. (24a) converges to some *finite* value or to $+\infty$ (but *not* to $-\infty$) for $\sigma\to 0$, one has symmetry breaking for ϵ small enough: Since F is positive, the function (26) takes a global minimum, say $g\in\mathbb{R}$, and for all pairs of values $(|\epsilon|,u)$ such that

$$\ln\left[\frac{2|\epsilon|}{(1-u^2)^{1/2}}\right]<g, \tag{27}$$

Eq. (24a) has no proper solution, i.e., the "solution" $\sigma=0$ must be used for the evaluation of the energy expectation values (24b). If this is the case for $(|\epsilon|,0)$, it will be still the case for $(|\epsilon|,u)$ with $0<u<\nu$ and ν appropriately chosen. Hence for these values of u the minimal-energy function (24b) takes the constant value

$$-\frac{\rho}{2}\sum_{n=1}^{\infty}\frac{|\lambda(n)|^2}{\omega(n)}. \tag{28}$$

Therefore the minimal-energy function $E^{\epsilon}=E^{\epsilon}(u)$ has at least two global minima and the inversion symmetry is broken.

In the *subohmic* situation, Eq. (25a) implies that this scenario is fulfilled for arbitrarily chosen coupling constant $\rho>0$; *hence the inversion symmetry is broken if only the level splitting ϵ is small enough.* This behavior is characteristic for the subohmic regime.[9,10,7,18,28]

In the *ohmic* situation, Eq. (25b) implies that the above scenario is fulfilled precisely for coupling constant $\rho\geqslant 1$; *hence the inversion symmetry is broken if only the coupling strength ρ exceeds 1 and if the level splitting ϵ is small enough.* This behavior is characteristic for the ohmic regime.[9,10,7,18,28] It will be seen below that approximation of ground states by coherent states (which is investigated here) may even lead to a broken symmetry for coupling strength $\rho<1$, which does *not* conform to the rigorous bounds developed by Spohn!

Besides, the presently studied approximation distinguishes between the ohmic and the subohmic regime, which is not the case in the (Hartree) approximation used by Pfeifer.[11]

In the following, a representative ohmic example [cf. Ref. 11 and Ref. 7: (I.32)] will be studied with frequencies and coupling constants chosen as

$$\omega(\mathbf{k}):=|\mathbf{k}|, \quad \mathbf{k}\in\mathbb{R}^3, \tag{29a}$$

$$\lambda(\mathbf{k}):=\frac{1}{\sqrt{4\pi|\mathbf{k}|}}, \quad \mathbf{k}\in\mathbb{R}^3, \quad |\mathbf{k}|\leqslant\Lambda, \tag{29b}$$

$$\lambda(\mathbf{k}):=0, \quad \mathbf{k}\in\mathbb{R}^3, \quad |\mathbf{k}|>\Lambda. \tag{29c}$$

The wave vector $\mathbf{k}$ is chosen here as a *continuous* parameter. The corresponding continuous-mode spin-boson Hamiltonian is thought of being approximated by a discrete-mode Hamiltonian (4), which might be a little bit critical from a mathematical point of view (cf. Ref. 29: Appendix A.2). These (probably minor) difficulties will not be discussed further here. The functions F and L corresponding to the parameters (29) are given by

$$F(s)=-\ln s+\ln(s+\Lambda)-\Lambda/(s+\Lambda) \tag{30}$$

and

$$L(s)=s\Lambda/(s+\Lambda). \tag{31}$$

Equation (30) or a direct calculation show that the parameters (29) fulfill the normalization condition (23). The ultraviolet-cutoff constant Λ can be identified with

$$\Lambda = \int_0^\infty F(\sigma)d\sigma = \int_{\mathbf{R}^3} \frac{\lambda(\mathbf{k})^2}{\omega(\mathbf{k})} d\,\mathbf{k}. \tag{32}$$

The minimal-energy function (24b) turns then out to be

$$E^\epsilon(u) = \min_\sigma \left[(1-u^2)\frac{\sigma}{2}\left(\frac{\rho\Lambda}{\sigma+\Lambda} - 1\right)\right] - \frac{\rho}{2}\sum_{n=1}^\infty \frac{|\lambda(n)|^2}{\omega(n)} \tag{33a}$$

$$= \min_\sigma \left\{ \frac{2|\epsilon|^2}{\sigma} \exp[-2\rho F(\sigma)]\left(\frac{\rho\Lambda}{\sigma+\Lambda} - 1\right)\right\} - \frac{\rho}{2}\sum_{n=1}^\infty \frac{|\lambda(n)|^2}{\omega(n)}, \tag{33b}$$

where the last equation is a consequence of (24a). If the minimum in Eq. (33) is taken for $\sigma \neq 0$, one must have

$$\rho\Lambda/(\sigma+\Lambda) - 1 \leqslant 0, \tag{34}$$

which implies that

$$\sigma \geqslant \Lambda(\rho - 1), \tag{35}$$

being a restriction only for $\rho > 1$, since σ is always positive. On the other hand, the unique minimum of the function

$$\ln(\sigma) + \rho F(\sigma) = (1-\rho)\ln(\sigma) + \rho\ln(\sigma+\Lambda) - \frac{\rho\Lambda}{\sigma+\Lambda} \tag{36}$$

is taken at

$$\sigma = \Lambda(\sqrt{\rho} - 1), \quad \rho \geqslant 1, \tag{37}$$

which is to say that the solution of Eq. (24a) is uniquely determined under the constraint (35) or zero if no solution is available fulfilling (35); see Fig. 1. For $\rho < 1$ the latter is never the case. For $\rho \geqslant 1$ the "solution" $\sigma = 0$ gives rise to a broken symmetry, the situation being similar to that one described in the second paragraph of this section. Hence for $\rho \geqslant 1$ and

$$\ln(2|\epsilon|) < \ln[\Lambda(\rho-1)] + \rho\left\{\ln\left[\frac{\Lambda(\rho-1)+\Lambda}{\Lambda(\rho-1)}\right] - \frac{\Lambda}{\Lambda(\rho-1)+\Lambda}\right\} \tag{38a}$$

$$= (1-\rho)\ln[\Lambda(\rho-1)] + \rho\ln(\Lambda\rho) - 1 \tag{38b}$$

$$= \ln[\Lambda(\rho-1)] + \rho\left\{\ln\left[\frac{\rho}{(\rho-1)}\right] - \frac{1}{\rho}\right\} \tag{38c}$$

the inversion symmetry is broken [use (35) and (24a)]. For $\rho = 1$, Eq. (38a) specializes to

$$\ln(2|\epsilon|) < \ln(\Lambda) - 1, \tag{39a}$$

$$|\epsilon| < \Lambda/2e \cong 0.18\Lambda. \tag{39b}$$

Since

$$\lim_{\sigma\to\infty} \rho\left\{\ln\left[\frac{\rho}{(\rho-1)}\right] - \frac{1}{\rho}\right\} = 0, \tag{40a}$$

$$\ln(\Lambda\rho) \geqslant (1-\rho)\ln[\Lambda(\rho-1)] + \rho\ln(\Lambda\rho) - 1, \tag{40b}$$

the latter holding for arbitrary $\rho \geqslant 1$, it follows that the region of broken symmetry described by Eq. (38) is bounded by its "asymptote"

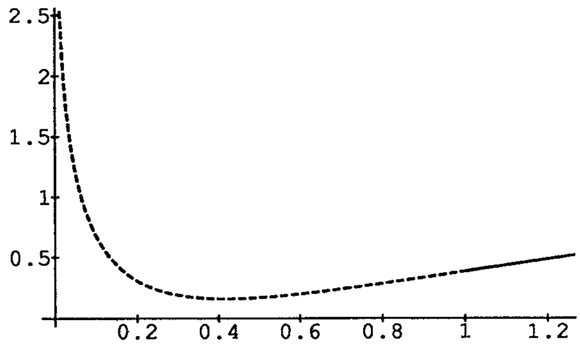

FIG. 1. Plot of the function $[\sigma \to \ln(\sigma) + \rho F(\sigma)]$ of Eq. (36) with parameters $\Lambda = 1$ and $\rho = 2$: It is relevant only if $[\rho L(\sigma) - \sigma]$ is negative [outlined curve; see Eq. (35)]. Otherwise (dashed curve) the "solution" of (24a) is given by $\sigma = 0$.

$$\rho \to \tfrac{1}{2}\Lambda\rho. \tag{41}$$

See Fig. 2. For large coupling strength the difference between this asymptote and the phase-transition line is given by $(1/4)\Lambda$, which is small with respect to the height of the phase-transition line. The correct asymptote, derived by Spohn[9] and recovered below, does *not* contain the factor 1/2.

The inversion symmetry of the spin-boson model studied is broken (with respect to the approximation used) if and only if there exists a nonzero $u_0 \in [-1, 1]$ such that the minimal-energy function (33) takes equally low (or lower) values at u_0 as it takes at $u = 0$. This was the case for the "solutions" with $\sigma = 0$. In the following the "proper" solutions ($\sigma \neq 0$) will be looked at. Rewriting Eq. (33b) leads to

$$E^\epsilon(u) = \min_\sigma \left[\frac{2|\epsilon|^2}{\sigma}\left(\frac{\sigma}{\sigma+\Lambda}\right)^{2\rho} \times \exp\left(+\frac{2\rho\Lambda}{\sigma+\Lambda}\right)\left(\frac{\rho\Lambda}{\sigma+\Lambda} - 1\right)\right] - \frac{\rho}{2}\sum_{n=1}^\infty \frac{|\lambda(n)|^2}{\omega(n)}. \tag{42}$$

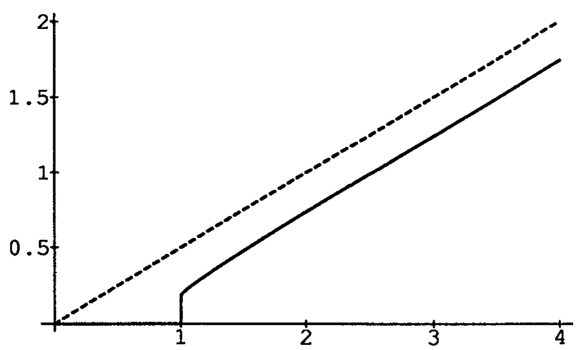

FIG. 2. Phase-transition diagram of the ohmic spin-boson model with parameters (29), determined by the $\sigma = 0$ "solutions" of Eq. (24a). The modulus $|\epsilon|$ of the level splitting ϵ is plotted vs the coupling strength ρ. The phase-transition line is proportional to Λ which has been set to $\Lambda = 1$ here. The inversion symmetry is broken for pairs $(|\epsilon|,\rho)$ lying below the (full) phase-transition line. The dashed line refers to the "asymptote" (41). *This phase diagram results also if the class of states (12) studied by Harris and Silbey* (Ref. 15) *is used.* The complete calculation admits a richer set of parameters with broken symmetry.

If $(|\epsilon|,0)$ gives rise to a proper solution of Eq. (24a) and fulfills (35), then the same is true for any pair of values $(|\epsilon|,u)$ with $u\in[-1, 1]$ and *σ increases with increasing u* [use (35) and (37)].

Equation (42) can be shown (by use of the transformation $\tau := \Lambda/\sigma + \Lambda$) to imply that *the inversion symmetry can only be broken for $\rho > 1/2$* (the rigorous bound by Spohn stating that phase transitions for suitably chosen nonzero level splitting ϵ may arise only for $\rho > 1$!). More precisely, *the inversion symmetry can be shown to be broken if and only if the level splitting ϵ fulfills*

$$\ln(2\epsilon) < \ln[\Lambda(2\rho-1)] + \rho\left\{\ln\left[\frac{\Lambda(2\rho-1)+\Lambda}{\Lambda(2\rho-1)}\right] - \frac{\Lambda}{\Lambda(2\rho-1)+\Lambda}\right\} \tag{43a}$$

$$= (1-\rho)\ln[\Lambda(2\rho-1)] + \rho\ln(2\Lambda\rho) - \tfrac{1}{2} \tag{43b}$$

$$= \ln[\Lambda(2\rho-1)] + \rho\left\{\ln\left[\frac{2\rho}{(2\rho-1)}\right] - \frac{1}{2\rho}\right\}. \tag{43c}$$

The phase-transition line [characterized by Eq. (43a) where "$<$" is replaced by "$=$"] is proportional to Λ. Just as in (40) and (41) it follows that the region of broken symmetry described by Eq. (43) is bounded by its asymptote

$$\rho \to \Lambda\rho. \tag{44}$$

See Figs. 3 and 4. For large coupling strength the difference between the asymptote and the phase-transition line is given by $3\Lambda/8$, which is small with respect to the height of the phase-transition line. This asymptote does *not* contain the factor 1/2 as in Eq. (41) and coincides with the correct one derived by Spohn.[9] It also coincides precisely with the phase-transition line of Pfeifer.[11]

For $\rho \to 1/2$ one finds that $\ln(2|\epsilon|)$ has to be infinitely small in order to get a broken symmetry, i.e., $|\epsilon| \to 0$. For $\rho = 1$ one arrives at $\sigma = \Lambda$ and the criterion (43) specializes to

$$\ln(2|\epsilon|) < \ln(2\Lambda) - \tfrac{1}{2}, \tag{45a}$$

$$|\epsilon| < \Lambda e^{-1/2} \cong 0.61\Lambda. \tag{45b}$$

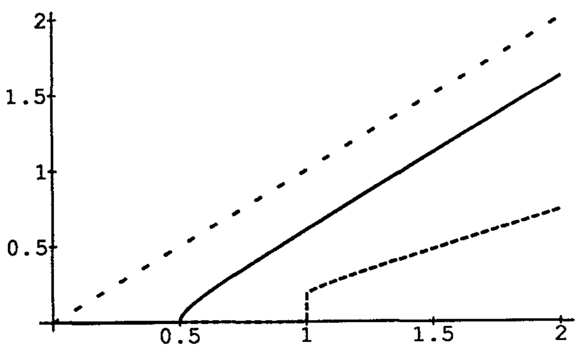

FIG. 3. Phase diagram of the ohmic spin-boson model characterized by the parameters (29). This phase diagram results if the class of coherent states (9) is used to approximate the ground states of the model. The modulus $|\epsilon|$ of the level splitting ϵ is plotted vs the coupling strength ρ. The inversion symmetry is broken for pairs $(|\epsilon|,\rho)$ lying below the (full) phase-transition line. The line $(\rho,\epsilon=0)$ belongs to the region of broken symmetry. The (lower) dashed line corresponds to Fig. 2. The (upper) dashed line refers to the "asymptote" (44). The phase-transition lines are proportional to Λ which has been set to $\Lambda = 1$.

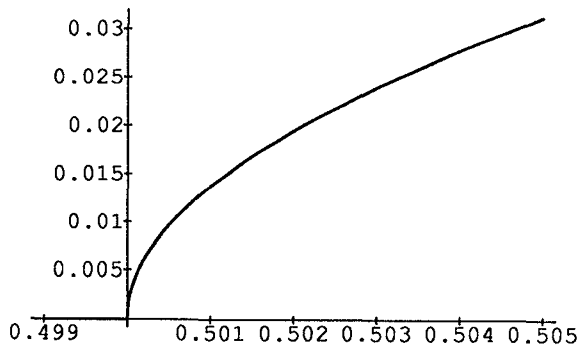

FIG. 4. Detail from Fig. 3: For $|\epsilon| > 0$ the inversion symmetry can only be broken (in the present approximation) if the coupling strength fulfills $\rho > 1/2$.

In summary, if one starts with the (ohmic) parameters (29) of the spin-boson Hamiltonian and approximates the ground states by coherent states (9) one arrives at the phase diagram in Fig. 3, determined by Eq. (43). The (lower) dashed line is the phase-transition line of Fig. 2, which arises if coherent states (12) instead of (9) are used to approximate the ground states (see Sec. VI). The "asymptote" of Fig. 3 has been derived rigorously by Spohn,[9,26] i.e., without restricting oneself to coherent states. It is the phase-transition line proposed by Pfeifer.[11]

It might be notable that the inversion symmetry remains unbroken in the *superohmic* case (i.e., if there is *no* IR singularity) if the level splitting ϵ is small enough. This follows from Eqs. (18) and (19) since $F(\sigma)$ and $L(\sigma)/\sigma^2$ converge to some finite value for $\sigma \to 0$.

V. GROUND STATES OF THE SPIN-BOSON MODEL REVISITED

The minimal-energy ground-state vectors of the form of (9) can be expressed as

$$\begin{pmatrix} aW\left[-\dfrac{\lambda}{\omega}\left(1-\dfrac{2\sigma|b|^2}{\omega+\sigma}\right)\right]\Psi_F \\ bW\left[+\dfrac{\lambda}{\omega}\left(1-\dfrac{2\sigma|a|^2}{\omega+\sigma}\right)\right]\Psi_F \end{pmatrix}, \quad a,b\in\mathbb{C}, \tag{46a}$$

$$a = +\sqrt{\tfrac{1}{2}(1+u)}, \tag{46b}$$

$$b = -\sqrt{\tfrac{1}{2}(1-u)}. \tag{46c}$$

The structure of *superselection sectors* containing such state vectors will be investigated in the present section.

For state vectors η and ϕ lying in different superselection sectors the "transition probabilities" $|\langle\eta|T\phi\rangle|^2$ vanish for arbitrary observables (operators) T of the system under consideration. In the case of the spin-boson system all observables are built up from spin operators (Pauli matrices) and boson operators (5). In spectroscopy, a choice for the operator T could, for example, be the electric dipole moment operator (or the respective 2×2 matrix if the molecule studied is considered as a two-level system). Note that transition probabilities with respect to *all* observables vanish if the respective states are separated by a *super*selection rule. A candidate for a molecular superselection rule is chirality.[11,7,27,30]

For coherent states the structure of superselection sectors is easily derived. Proofs of the following observations can be given just as in (Ref. 7, Sec. II.6).

Observation 1: Coherent-state vectors $W(\chi)\Psi_F$ and $W(\xi)\Psi_F$ are separated by a superselection rule if and only if

$$\sum_{n=1}^{\infty} |\chi(n)-\xi(n)|^2 = \infty. \tag{47}$$

Observation 2: The two vectors

$$W\left[-\frac{\lambda}{\omega}\left(1-\frac{2\sigma|b|^2}{\omega+\sigma}\right)\right]\Psi_F, \tag{48a}$$

$$W\left[+\frac{\lambda}{\omega}\left(1-\frac{2\sigma|a|^2}{\omega+\sigma}\right)\right]\Psi_F \tag{48b}$$

are *not* separated by a superselection rule if $\sigma\neq 0$. Hence the state vector (46) implements a *pure state* [note that the coupling strength ρ has been omitted in Eqs. (48)].

Proof: Apply observation 1.

For $\sigma=0$ the state vectors (48) are separated by a superselection rule if the IR singularity holds. Hence for $\sigma=0$, Eq. (46) does not refer to a *pure* state. The pure ground-state vectors are given in this case by the state vectors

$$\begin{bmatrix} W(-\lambda/\omega)\Psi_F \\ 0 \end{bmatrix}, \tag{49a}$$

$$\begin{bmatrix} 0 \\ W(+\lambda/\omega)\Psi_F \end{bmatrix}. \tag{49b}$$

These vectors coincide with the rigorously derivable ground-state vectors in the "trivial" case[11] with level splitting $\epsilon=0$.

Observation 3: The state vector (46) and its "mirror image" (14)

$$\begin{pmatrix} bW\left[-\frac{\lambda}{\omega}\left(1-\frac{2\sigma|a|^2}{\omega+\sigma}\right)\right]\Psi_F \\ aW\left[+\frac{\lambda}{\omega}\left(1-\frac{2\sigma|b|^2}{\omega+\sigma}\right)\right]\Psi_F \end{pmatrix}, \tag{50}$$

are separated by a superselection rule if the IR singularity holds and if $|a|^2\neq|b|^2$. In the case $|a|^2=|b|^2$ (corresponding to $u=0$) the two states implemented by the state vectors (46) and (50) coincide.

Proof: Apply observation 1.

Observation 4: Consider two state vectors of the type of (46) with corresponding a,b,σ and $\tilde{a},\tilde{b},\tilde{\sigma}$, respectively. Let σ and $\tilde{\sigma}$ be nonzero. These state vectors are separated by a superselection rule if and only if $|a|\neq|\tilde{a}|$, i.e., if and only if

$$|a|^2-|b|^2=:u\neq\tilde{u}:=|\tilde{a}|^2-|\tilde{b}|^2. \tag{51}$$

Note that the minimal-energy states obtained by minimizing the function E^{ϵ} with respect to u always have *nonzero* σ if $\epsilon\neq 0$.

Proof: Apply observation 1.

Observation 5 (without proof): Consider the spin-boson model with special parameters (29). *Then symmetry-broken pure "ground states" of the type of (46) corresponding to different modulus of the level splitting* ϵ (holding constant the other parameters of the model) *are separated by a superselection rule.* Note that the level splitting changes only the spin part of the Hamiltonian: A change of the coupling strength ρ, on the other hand, would be much more drastic.

In summary, ground-state vectors of the type of (9) have a strong tendency to be separated by a superselection rule. A change of the level splitting ϵ or the coupling strength ρ will almost inevitably change the ground-state's sector.

VI. DISCUSSING THE VARIATIONAL ANSATZ OF HARRIS AND SILBEY

Approximation of ground states by state vectors of the type of (12) leads to a similar variational problem as before. Since the spin-boson Hamiltonian (4) has the same expectation values with respect to the vector states

$$\begin{bmatrix} W(-\alpha)\Psi_F \\ 0 \end{bmatrix}, \tag{52a}$$

$$\begin{bmatrix} 0 \\ W(\alpha)\Psi_F \end{bmatrix}, \tag{52b}$$

it follows by explicit consideration of the 2×2 eigenvalue problem that the inversion symmetry can only be broken if the corresponding outer-diagonal terms vanish. *In the case of a broken symmetry*, one recovers the ground states (49) of the spin-boson model with level splitting $\epsilon=0$. *Hence the expectation value of* $(\sigma_3\otimes\mathbf{1})$ *with respect to pure minimal-energy states is either* 0 *or* ± 1. In the latter case the respective energy is given as

$$-\frac{\rho}{2}\sum_{n=1}^{\infty}\frac{|\lambda(n)|^2}{\omega(n)} \tag{53}$$

with the coupling strength ρ now being explicitly mentioned.

An explicit calculation leads to the minimal energy

$$E^{\epsilon}(u)=\min_{\sigma}\left[\frac{\rho}{2}L(\tilde{\sigma})-\frac{1}{2}\tilde{\sigma}\right]-\frac{\rho}{2}\sum_{n=1}^{\infty}\frac{|\lambda(n)|^2}{\omega(n)} \tag{54}$$

with the minimum taken over solutions $\tilde{\sigma}$ of

$$\ln[2|\epsilon|(1-u^2)^{1/2}]=\ln(\tilde{\sigma})+\rho F(\tilde{\sigma}) \tag{55}$$

and $\tilde{\sigma}=0$. The functions F and L are defined as before. Note that on the left-hand side of Eq. (55), $2|\epsilon|$ is indeed multiplied and not divided by $(1-u^2)^{1/2}$ as before! Similarly, there is no term $(1-u^2)$ missing on the right-hand side of (54).

The remarks made at the beginning of this section imply that in case of a broken symmetry the minimum of (54) is taken at $\tilde{\sigma}=0$ for all $u\in[-1,1]$, i.e., either (55) has no proper solution or the corresponding

$$\frac{\rho}{2}L(\tilde{\sigma})-\frac{1}{2}\tilde{\sigma} \tag{56}$$

is positive. This implies, in particular, that

$$\tilde{\sigma}<\rho\left[\sum_{j=1}^{\infty}\frac{\lambda(j)^2}{\omega(j)}\right] \tag{57}$$

must hold for all $u\in[-1,1]$.

With the particular choice (29) for frequencies and coupling constants of the spin-boson model, positivity of Eq. (56) can be sharpened to read [cf. (35)]

$$\sigma < \Lambda(\rho - 1) \cong \left[\int_{\mathbf{R}^3} \frac{\lambda(\mathbf{k})^2}{\omega(\mathbf{k})} d\mathbf{k} \right] (\rho - 1), \tag{58}$$

which *leads to the phase diagram of Fig. 2* determined by Eq. (38). Hence the line of phase transition starts at $\rho = 1$, which has been conjectured to be the correct result.[9] On the other hand, it is not very satisfying that the line of phase transition makes a "jump" at $\rho = 1$ and exhibits a wrong asymptotic behavior (41).

The explicit calculation shows that the test function α in (12) is of the form

$$\alpha = \frac{\sqrt{\rho/2}\lambda}{\omega + \tilde{\sigma}}, \tag{59}$$

and therefore the minimal-energy states (12) for some given value of $u := (|a|^2 - |b|^2)$ are of the form

$$\begin{pmatrix} aW\left[-\dfrac{\sqrt{\rho/2}\lambda}{(\omega + \tilde{\sigma})} \right] \Psi_F \\ bW\left[+\dfrac{\sqrt{\rho/2}\lambda}{(\omega + \tilde{\sigma})} \right] \Psi_F \end{pmatrix}, \tag{60a}$$

$$a = +\sqrt{\tfrac{1}{2}(1+u)}, \tag{60b}$$

$$b = -\sqrt{\tfrac{1}{2}(1-u)}. \tag{60c}$$

Therefore the case $\tilde{\sigma} \neq 0$ gives rise to vectors in the Fock sector only (use observation 1 in the last section). This fits nicely together with the statement above that a broken symmetry can arise only if $\tilde{\sigma} = 0$. Hence *for fixed coupling strength ρ only three different representations (separated by a superselection rule) arise if an IR singularity holds*: the representations *containing* the vectors

$$\begin{pmatrix} W(-\sqrt{\rho/2}\,\lambda/\omega)\Psi_F \\ 0 \end{pmatrix}, \tag{61a}$$

$$\begin{pmatrix} 0 \\ W(+\sqrt{\rho/2}\,\lambda/\omega)\Psi_F \end{pmatrix}, \tag{61b}$$

$$\sqrt{1/2} \begin{pmatrix} \Psi_F \\ \Psi_F \end{pmatrix}, \tag{61c}$$

respectively. The first two [(61a) and (61b)] refer to broken, and the last one (61c) to unbroken inversion symmetry (depending on the level splitting ϵ). A change in the level splitting ϵ does only change the sector if the phase-transition line is crossed. A change of the coupling strength ρ, on the other hand, will change the sector considered, if the inversion symmetry is broken.

It might be notable that the minimum in Eq. (54) is *never* taken at $\tilde{\sigma} = 0$ for systems without IR singularity (apart from situations where $u = \pm 1$ or $\epsilon = 0$), i.e., in the superohmic situation. Hence *no* breaking of the inversion symmetry will take place for superohmic parameters of the spin-boson Hamiltonian if the "Harris–Silbey" coherent states (12) are used to approximate its ground states. This is a satisfying result. A similar result does *not* hold if the more general ansatz (9) for the ground states is used (cf. the final paragraph of Sec. IV).

VII. CONCLUDING REMARKS

In comparison with the *Hartree method of Pfeifer*,[11] approximation by states of the type of (9) and (12) has several advantages.

- The phase diagrams clearly distinguish between the superohmic, ohmic, and subohmic regime (all these regimes gave identical results in Ref. 11).
- The characteristic behavior in the ohmic regime is reproduced, i.e., in order to get a broken inversion symmetry one needs a certain coupling strength for the coupling between spin and field.[9]
- The characteristic behavior of the subohmic regime is reproduced, i.e., there is symmetry breaking for low coupling strengths if the level splitting of the spin is only small enough (but nonzero).[9]

Giving reasonable results, the "ground states" (46) and (60) discussed are still very simple: All questions concerning separation by superselection rules and the structure of sectors can be explicitly solved.

The *variational ansatz (12) used by Harris and Silbey* may be preferred to the more general approach (9) due to its simplicity: Once the functions F and L are calculated, the phase diagram can almost immediately be drawn. Though the possible expectation values of $(\sigma_3 \otimes \mathbf{1})$, i.e., the values of the "order parameter" are restricted to 0 and ± 1 (the latter referring to broken inversion symmetry), the results should *not* be considered as pathological: Rigorous estimates (see Ref. 9, theorem 3) show that the expectation value of $(\sigma_3 \otimes \mathbf{1})$ "jumps" by at least $1/\sqrt{\rho}$ at the phase-transition line. The "jump" from 0 to ± 1 in the Harris–Silbey approach may be too large sometimes, but reflects the actual situation. Note that with the more general ansatz (9) there need not be a jump at all at the phase-transition line! On the other hand, the wrong asymptotic behavior (41) of the Harris–Silbey ansatz (12) is somewhat disturbing. Besides, the comparison of the two approaches with vector states (9) and (12) illustrates that results concerning ground states, and the respective phase diagrams may but need not improve when the "basis set" of the variational calculation is extended.

The state vectors (9) and (12) are *not* of product form, contrary to the state vectors

$$\begin{pmatrix} a \\ b \end{pmatrix} \otimes [W(\xi)\Psi_F], \tag{62a}$$

$$|a|^2 + |b|^2 = 1 \tag{62b}$$

used by Pfeifer.[11] Nevertheless, the (pure) *broken-symmetry* ground states with respect to the ansatz of Harris and Silbey (12) *turn out* to be product states (61a) and (61b). This changes when the more general form (9) is used. There the ground states (46) are *never of product form* (apart from the case with trivial level splitting), since they always correspond to some $\sigma \neq 0$ (though $\sigma = 0$ may be the "solution" of (18) and (24a) for $u \in [-\nu, +\nu]$, with $\nu < 1$). The same is true for the correct ground states.[28] Hence there would be some interest in replacing the original factorization (spin $\otimes$ field) by another one creating a "quasiparticle" with respect to which the ground states factorize. To a certain extent, this happens in the broken-symmetry case: The two ground states (46) and (50) are separated by a superselection rule and the "observable algebra" of the quasiparticle is a two-dimensional commutative one. The two projections P_L and P_R generating this two-dimensional commutative algebra admit the ground states (46) and (50), respectively, as eigenstates with eigenvalue 1. These "left- and right-handed" ground states (and their respective sectors consisting of *all* eigenstates of P_L and P_R, respectively, with eigenvalue 1) are *not* mixed up by the spin-boson dynamics. They are candidates for chiral molecular ground states,[11,30,31] the "naked" molecule being replaced by a "quasimolecule" which partially encorporates the influence of the environment.

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