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An Expression of the Ground State Energy of the Spin-Boson Model

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Abstract

An expression of the ground state energy E_{SB} of the spin-boson Hamiltonian H_{SB} is considered. The expression in the cases of both massive and massless bosons is given by a nonperturbative method.

The spin-boson model, which describes a two-level system coupled to a quantized Bose field, has been investigated as a simplified model for atomic systems interacting with a quantized radiation or phonon field ([LCDFGW, Am, Ar1, D, FaNV, Gér, HüSp1, HüSp2, Sp1, ArHi1, JP3] and references therein). Several properties of the ground states of the model are of interest. Especially, we are interested in expressions of the ground state energy of the model, because for each Hamiltonian we can actually observe its energies only at every state, neither the Hamiltonian nor the state according to the standard quantum theory. For the spin-boson Hamiltonian H_{SB}, recently attention has been paid to the ground states as the eigenvectors of H_{SB} with eigenvalue equal to the infimum of its spectrum to develop nonperturbative method ([Sp3, (ii) on p.5], [ArHi1, ArHi2]) and analyze spectral properties and the process of radiative decay ([HüSp1, HüSp2]). Talking of the ground states of this type model, we here note that in [T1, T2, T3, T4] Tomonaga argued the ground state of the model which has relation to the spin-boson model in order to get rid of physical difficulties caused by applying the perturbation theory to the model. Moreover, recently Bach, Fröhlich and Sigal argued the ground state, spectrum and resonance for a model of nonrelativistic quantum electrodynamics ([BaFrSig1, BaFrSig2, BaFrSig3, BaFrSig4]). Especially they established the method of renormalization group to investigate resonances in quantum electrodynamics, which is of great value for many who deal with problems on the resonances in the case of massless bosons. For the generalized spin-boson model, Arai and the author showed that, under certain conditions, there exists a ground state of the generalized model in [ArHi2] by a nonperturbative method, and we gave a formula for the asymptotic behavior of the ground state energy of the generalized model in the strong coupling region ([ArHi2, Proposition 1.4]). In this paper we focus our attention on the expression of the ground state energy of the (standard) spin-boson Hamiltonian H_{SB} in the cases of both massive and massless bosons. Especially, it is important that we clarify the expression in the case of massless bosons, because we cannot apply the regular perturbation theory to H_{SB} in the case. Thus we try nonperturbative approach to our problem in this paper.

For physical reality, we consider the situation where bosons move in the 3-dimensional Euclidean space $\mathbf{R}^3$. We take a Hilbert space of bosons to be

$$\mathcal{F}_b = \mathcal{F}\left(L^2\left(\mathbf{R}^3\right)\right) = \bigoplus_{n=0}^{\infty}\left[\otimes_s^n L^2\left(\mathbf{R}^3\right)\right], \tag{1}$$

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the symmetric Fock space over $L^2(\mathbf{R}^3)$ ($\otimes_s^n \mathcal{K}$ denotes the n-fold symmetric tensor product of a Hilbert space $\mathcal{K}$, $\otimes_s^0 \mathcal{K} \equiv \mathbf{C}$). Let Ω_0 be the Fock vacuum in $\mathcal{F}_b$.

In this paper, we set both of $\hbar$ and c one, i.e., $\hbar = c = 1$, where $\hbar$ is the Planck constant divided by 2π, and c the velocity of the light. A function ω_r is given by

$$\omega_r(k) := \sqrt{|k|^2 + m^2}, \qquad m \geq 0,\ k \in \mathbf{R}^3,$$

which is the energy of the relativistic bosons with mass m and momentum k.

We denote by $d\Gamma(\omega_r)$ the second quantization of the multiplication operator ω_r on $L^2(\mathbf{R}^3)$ and set

$$H_b = d\Gamma(\omega_r) = \int_{\mathbf{R}^3} dk\, \omega_r(k) a^+(k) a(k),$$

where $a(k)$ and $a^+(k)$ are the operator-valued distribution kernels of the smeared annihilation and creation operators respectively:

$$a(f) = \int_{\mathbf{R}^3} dk\, a(k) f(k), \tag{2}$$

$$a^+(f) = \int_{\mathbf{R}^3} dk\, a^+(k) f(k) \tag{3}$$

for every $f \in L^2(\mathbf{R}^3)$ on $\mathcal{F}_b$.

Remark 1. In [ArHi1, ArHi2], we used the definition,

$$a(f) = \int_{\mathbf{R}^3} dk\, a(k) f(k)^*, \qquad f \in L^2(\mathbf{R}^3),$$

as the annihilation operator $a(f)$ according to the custom for mathematics, where $f(k)^*$ denotes the complex conjugate of $f(k)$ $(k \in \mathbf{R}^3)$, but we here employ (2) as the definition of $a(f)$ according to the way of physics.

The Segal field operator $\phi_s(f)$ $(f \in L^2(\mathbf{R}^3))$ is given by

$$\phi_s(f) := \frac{1}{\sqrt{2}} \left(a^+(f) + a(f) \right). \tag{4}$$

Let λ be a real-valued continuous function on $\mathbf{R}^3$ satisfying the following conditions:

(A) $\quad \lambda(k) = \lambda(-k)$ $(k \in \mathbf{R}^3)$, and $\lambda, \lambda/\omega_r \in L^2(\mathbf{R}^3)$.

Remark 2. Since $\lambda, \lambda/\omega_r \in L^2(\mathbf{R}^3)$, we have $\lambda/\sqrt{\omega_r} \in L^2(\mathbf{R}^3)$.

The Hamiltonian of the spin-boson model is defined by

$$H_{SB} := \frac{\mu}{2} \sigma_3 \otimes I + I \otimes H_b + \sqrt{2} \alpha \sigma_1 \otimes \phi_s(\lambda)$$

acting in the Hilbert space

$$\mathcal{F} := \mathbf{C}^2 \otimes \mathcal{F}_b = \mathcal{F}_b \oplus \mathcal{F}_b, \tag{5}$$

where σ_1, σ_3 are the standard Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In (5), we identified $\mathbf{C}^2 \otimes \mathcal{F}_b$ with $\mathcal{F}_b \oplus \mathcal{F}_b$. So, H_{SB} has the following representation on $\mathcal{F}_b \oplus \mathcal{F}_b$ and we employ it in this paper:

$$H_{SB} = \begin{pmatrix} H_b + \frac{\mu}{2} & \sqrt{2}\alpha\phi_s(\lambda) \\ \sqrt{2}\alpha\phi_s(\lambda) & H_b - \frac{\mu}{2} \end{pmatrix}.$$

For a linear operator T on a Hilbert space, we denote its domain by $D(T)$. It is well-known that H_{SB} is self-adjoint with $D(H_{SB}) = D(I \otimes H_b)$ and

$$-\frac{|\mu|}{2} - \alpha^2 \left\| \frac{\lambda}{\sqrt{\omega_r}} \right\|_{L^2}^2 \leq H_{SB},$$

where $\| \cdot \|_{L^2}$ denotes the norm of $L^2(\mathbf{R}^3)$.

For a self-adjoint operator T bounded from below, we denote by $E(T)$ the infimum of the spectrum $\sigma(T)$ of T:

$$E(T) = \inf \sigma(T).$$

In this paper, an eigenvector of T with eigenvalue $E(T)$ is called a *ground state* of T (if it exists). We say that T has a (resp. unique) ground state if $\dim\ker(T - E(T)) \geq 1$ (resp. $\dim\ker(T - E(T)) = 1$). We call $E(T)$ the *ground state energy* of T if T is a Hamiltonian.

For H_{SB} we set

$$E_{SB}(\mu, \alpha) := E(H_{SB}).$$

By the variational principle ([Ar1, Theorem 2.4] and [D, p.161]), we have

$$E_{SB}(\mu, \alpha) \leq -\frac{|\mu|}{2} e^{-2\alpha^2 \|\lambda/\omega_r\|_{L^2}^2} - \alpha^2 \left\| \frac{\lambda}{\sqrt{\omega_r}} \right\|_{L^2}^2. \tag{6}$$

Under certain assumptions, we know that H_{SB} has a ground state ([HüSp1, ArHi1, Sp3] and see Remark 4(1) in this paper).

DEFINITION 1. We say *a vector* $\Psi \in \mathcal{F} \equiv \mathcal{F}_b \oplus \mathcal{F}_b$ *overlaps with a ground state* $\Omega_{SB}(\mu, \alpha)$ if and only if there exists the ground state $\Omega_{SB}(\mu, \alpha)$ of H_{SB} such that

$$\langle \Psi \, , \, \Omega_{SB}(\mu, \alpha) \rangle_{\mathcal{F}} \neq 0,$$

where $\langle \quad , \quad \rangle_{\mathcal{F}}$ is the standard inner product of $\mathcal{F} \equiv \mathcal{F}_b \oplus \mathcal{F}_b$.

From now on, according to the custom for the physicists, all the inner products of the Hilbert spaces appearing in this paper have the linearity on the right hand side.

If a ground state $\Omega_{SB}(\mu, \alpha)$ of H_{SB} exists, for $\Omega_{SB}(\mu, \alpha)$ we set

$$\Omega_{SB}(\mu, \alpha) = \begin{pmatrix} \Omega_1 \\ \Omega_2 \end{pmatrix} \in \mathcal{F} \equiv \mathcal{F}_b \oplus \mathcal{F}_b.$$

It is well known that, if $f \in L^2(\mathbf{R}^3)$, we can define a self-adjoint operator $P(f)$ by

$$P(f) := i\left\{a^+(f) - a(f)\right\},$$

thus, if $\lambda/\omega_r \in L^2(\mathbf{R}^3)$, we have two unitary operators $U_\pm$ defined by

$$U_\pm := \exp\left[\pm i\alpha P(\lambda/\omega_r)\right]. \tag{7}$$

We define two unit vectors $\Omega_\pm \in \mathcal{F} \equiv \mathcal{F}_b \oplus \mathcal{F}_b$ by

$$\Omega_\pm := \frac{1}{2}\begin{pmatrix} U_+\Omega_0 \mp U_-\Omega_0 \\ U_+\Omega_0 \pm U_-\Omega_0 \end{pmatrix}.$$

We have the following proposition on an upper bound of the ground state energy:

PROPOSITION 2. *Assume (A). Then,*

$$\begin{aligned}
&E_{SB}(\mu,\alpha) \\
\leq\; & -\alpha^2 \int_{\mathbf{R}^3} dk \frac{\lambda(k)^2}{\omega_r(k)} \\
& - \lim_{\beta\to\infty} \frac{1}{\beta} \ln\Bigg\{ 1 + \beta\frac{|\mu|}{2} \exp\left[-2\alpha^2 \int_{\mathbf{R}^3} dk \frac{\lambda(k)^2}{\omega_r(k)^2}\right] \\
& \qquad + \sum_{\ell=1}^{\infty} \left(\frac{\mu}{2}\right)^{2\ell} \int_0^{\beta} d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{2\ell-1}} d\beta_{2\ell} \\
& \qquad\qquad \exp\left[-2\alpha^2 \int_{\mathbf{R}^3} dk \frac{\lambda(k)^2}{\omega_r(k)^2}\left(2G_{\beta_1,\cdots,\beta_{2\ell}}(k) + 2\ell\right)\right] \\
& \qquad + \sum_{\ell=1}^{\infty} \left(\frac{|\mu|}{2}\right)^{2\ell+1} \int_0^{\beta} d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{2\ell}} d\beta_{2\ell+1} \\
& \qquad\qquad \exp\Bigg[-2\alpha^2 \int_{\mathbf{R}^3} dk \frac{\lambda(k)^2}{\omega_r(k)^2}\Big(2G_{\beta_1,\cdots,\beta_{2\ell}}(k) \\
& \qquad\qquad\qquad + 2F_{\beta_1,\cdots,\beta_{2\ell+1}}(k) + (2\ell+1)\Big)\Bigg]\Bigg\},
\end{aligned}$$

where

$$\begin{aligned}
G_{\beta_1,\cdots,\beta_{2\ell}}(k) &= -\sum_{p=1}^{\ell} e^{-(\beta_{2p-1}-\beta_{2p})\omega_r(k)} \\
&\quad + \sum_{p,q=1;p<q}^{\ell} \left(e^{-\beta_{2p-1}\omega_r(k)} - e^{-\beta_{2p}\omega_r(k)}\right)\left(e^{\beta_{2q-1}\omega_r(k)} - e^{\beta_{2q}\omega_r(k)}\right) \\
&\leq 0,
\end{aligned} \tag{8}$$

$$F_{\beta_1,\cdots,\beta_{2\ell+1}}(k) = e^{\beta_{2\ell+1}\omega_r(k)} \sum_{p=1}^{\ell} \left(e^{-\beta_{2p-1}\omega_r(k)} - e^{-\beta_{2p}\omega_r(k)}\right) \leq 0. \tag{9}$$

Remark 3. The upper bound (6) of $E_{SB}(\mu,\alpha)$ by the variational principle ([Ar1, Theorem 2.4], [D, p.161]) is given by estimating $G_{\beta_1,\cdots,\beta_{2\ell}}(k)$ and $F_{\beta_1,\cdots,\beta_{2\ell+1}}(k)$ at 0 from above in our Proposition, which is the most rough estimation in ours.

The statement of our main theorem is made as follows:

THEOREM 3. *Assume (A).*
(i) *Suppose that a ground state $\Omega_{SB}(\mu,\alpha)$ of H_{SB} exists.*

(i)$_+$ *If Ω_+ overlaps with the ground state $\Omega_{SB}(\mu,\alpha)$, then $E_{SB}(\mu,\alpha)$ is given by*

$$
\begin{aligned}
&E_{SB}(\mu,\alpha)\\
= &-\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)}\\
&-\lim_{\beta\to\infty}\frac{1}{\beta}\ln\Bigg\{1+\beta\frac{\mu}{2}\exp\left[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\right]\\
&\qquad +\sum_{\ell=1}^{\infty}\left(\frac{\mu}{2}\right)^{2\ell}\int_0^\beta d\beta_1\int_0^{\beta_1} d\beta_2\cdots\int_0^{\beta_{2\ell-1}} d\beta_{2\ell}\\
&\qquad\quad \exp\left[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\left(2G_{\beta_1,\cdots,\beta_{2\ell}}(k)+2\ell\right)\right]\\
&\qquad +\sum_{\ell=1}^{\infty}\left(\frac{\mu}{2}\right)^{2\ell+1}\int_0^\beta d\beta_1\int_0^{\beta_1} d\beta_2\cdots\int_0^{\beta_{2\ell}} d\beta_{2\ell+1}\\
&\qquad\quad \exp\Bigg[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\Big(2G_{\beta_1,\cdots,\beta_{2\ell}}(k)\\
&\qquad\qquad\qquad +2F_{\beta_1,\cdots,\beta_{2\ell+1}}(k)+(2\ell+1)\Big)\Bigg]\Bigg\},
\end{aligned}
$$

where $G_{\beta_1,\cdots,\beta_{2\ell}}$ and $F_{\beta_1,\cdots,\beta_{2\ell+1}}$ are given in (8) and (9) respectively.

(i)$_-$ *If Ω_- overlaps with the ground state $\Omega_{SB}(\mu,\alpha)$, then $E_{SB}(\mu,\alpha)$ is given by*

$$
\begin{aligned}
&E_{SB}(\mu,\alpha)\\
= &-\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)}\\
&-\lim_{\beta\to\infty}\frac{1}{\beta}\ln\Bigg\{1-\beta\frac{\mu}{2}\exp\left[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\right]\\
&\qquad +\sum_{\ell=1}^{\infty}\left(\frac{\mu}{2}\right)^{2\ell}\int_0^\beta d\beta_1\int_0^{\beta_1} d\beta_2\cdots\int_0^{\beta_{2\ell-1}} d\beta_{2\ell}\\
&\qquad\quad \exp\left[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\left(2G_{\beta_1,\cdots,\beta_{2\ell}}(k)+2\ell\right)\right]\\
&\qquad -\sum_{\ell=1}^{\infty}\left(\frac{\mu}{2}\right)^{2\ell+1}\int_0^\beta d\beta_1\int_0^{\beta_1} d\beta_2\cdots\int_0^{\beta_{2\ell}} d\beta_{2\ell+1}\\
&\qquad\quad \exp\Bigg[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\Big(2G_{\beta_1,\cdots,\beta_{2\ell}}(k)\\
&\qquad\qquad\qquad +2F_{\beta_1,\cdots,\beta_{2\ell+1}}(k)+(2\ell+1)\Big)\Bigg]\Bigg\},
\end{aligned}
$$

where $G_{\beta_1,\cdots,\beta_{2\ell}}$ and $F_{\beta_1,\cdots,\beta_{2\ell+1}}$ are given in (8) and (9) respectively.

(ii) *(for massive bosons) Let $m > 0$. Then there exists a ground state $\Omega_{SB}(\mu,\alpha)$ of H_{SB}. Moreover, if*

$$\frac{1}{2}|\mu|\left(1 - e^{-2\alpha^2\|\lambda/\omega_r\|^2_{L^2}}\right) < m,$$

then either Ω_+ or Ω_- overlaps with the ground state $\Omega_{SB}(\mu,\alpha)$ at least.
(iii) *(for massive or massless bosons) Let $m \geq 0$, and $|\alpha|\|\lambda/\omega_r\|^2_{L^2} < 1$. Then there exists a ground state $\Omega_{SB}(\mu,\alpha)$ of H_{SB}. Moreover, if $\lambda/\omega_r^2 \in L^2(\mathbf{R}^3)$ with*

$$|\mu\alpha|\left\|\frac{\lambda}{\omega_r^2}\right\|_{L^2} < \frac{1}{2},$$

then either Ω_+ or Ω_- overlaps with the ground state $\Omega_{SB}(\mu,\alpha)$ at least.

Remark 4. (1) Spohn showed a necessary and sufficient condition for existence of a ground state of H_{SB} (condition (A) implies the condition) whose statement appears in [Sp3, Comment (ii) after Theorem 1], and its proof in his unpublished note (1991) was clarified in [Sp4].

(2) In the case of massive bosons, by applying regular perturbation theory (e.g. [RSi3, Theorem XII.8 and Theorem XII.9]), we can easily obtain an expression of the ground state energy of the spin-boson model as the perturbation series. For instance, Davies had the expression in the case of massive bosons by regarding $I \otimes H_b + \sqrt{2}\alpha\sigma_1 \otimes \phi_s(\lambda)$ and $\frac{\mu}{2}\sigma_3 \otimes I$ as the free part and perturbation term respectively ([D, Theorem 10]): Let $\mu < 0$ and $\alpha > 0$. By inserting $|\mu|/2$, $\alpha^2\|\lambda/\sqrt{\omega_r}\|^2_{L^2}$, and $\|\lambda/\sqrt{\omega_r}\|^{-1}_{L^2}\lambda$ into ε, Λ, and f in [D, Theorem 10], we know that F_1, F, N, and the Hamiltonian $\mathbf{H}$ in [D, Theorem 10] is given by $\omega_r > 0$, H_b, $\alpha^2\|\lambda/\omega_r\|^2_{L^2}$, and

$$H'_{SB} := -\frac{\mu}{2}\sigma_1 \otimes I + I \otimes H_b + \sqrt{2}\alpha\sigma_3 \otimes \phi_s(\lambda)$$

respectively. We note here that H_{SB} and H'_{SB} are unitary equivalent (see Lemma 2(i) in this paper). So, by [D, Theorem 10], for sufficiently small $|\mu|$,

$$E_{SB}(\mu,\alpha) = -\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)} - \frac{|\mu|}{2}\exp\left[-2\alpha^2\int_{\mathbf{R}^3} dk\frac{\lambda(k)^2}{\omega_r(k)^2}\right] + 0\left(\mu^2\right).$$

For arbitrary fixed $m > 0$ and $\mu \neq 0$ (resp. $\alpha \neq 0$), sufficiently small $|\alpha|$ (resp. $|\mu|$) satisfies the inequality in (ii). Thus Theorem 3(i)$_\pm$ with (ii) may be regarded as a result which improves the one obtained by regular perturbation theory. Note that (10) is a nonperturbative estimate in α, since the left hand side of (10) is non-polynomial in α.

(3) To author's best knowledge, Theorem 3(i)$_\pm$ with (iii) is the first which establishes a concrete expression of the ground state energy of the spin-boson model H_{SB} in the case of *massless bosons.*

COROLLARY. *Assume (A). Fix* $\alpha \in \mathbf{R}$.
(i) *Suppose that, for* $\mu, \mu' > 0$, $\Omega_{SB}(\mu,\alpha)$ *and* $\Omega_{SB}(\mu',\alpha)$ *exist, and* Ω_+ *overlaps with both of them. Then*

$$E_{SB}(\mu',\alpha) \leq E_{SB}(\mu,\alpha) \text{ if } \mu < \mu'.$$

(ii) *Suppose that, for* $\mu, \mu' < 0$, $\Omega_{SB}(\mu,\alpha)$ *and* $\Omega_{SB}(\mu',\alpha)$ *exist, and* Ω_- *overlaps with both of them. Then*

$$E_{SB}(\mu',\alpha) \geq E_{SB}(\mu,\alpha) \text{ if } \mu < \mu'.$$

The basic idea to prove our main theorem is as follows: If there exist a ground state $\Omega_{SB}(\mu,\alpha)$ of H_{SB} and a vector $\Psi \in \mathcal{F} \equiv \mathcal{F}_b \oplus \mathcal{F}_b$ such that Ψ overlaps with $\Omega_{SB}(\mu,\alpha)$, then by Bloch's formula ([Blo, (12)] and see Lemma 2.4 in this paper), we have

$$E_{SB}(\mu,\alpha) = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln\langle\Psi\,,\,e^{-\beta H_{SB}}\Psi\rangle_{\mathcal{F}}.$$

So, our problem is reduced to that of how to find such Ψ that we now try to calculate $\langle\Psi\,,\,e^{-\beta H_{SB}}\Psi\rangle_{\mathcal{F}}$ in the concrete. In the following section, we shall use several unitary transformations and the Du Hammel formula so that we can apply the Feynman-Kac-Nelson formula for the free field, and we shall find that either Ω_+ or Ω_- is one of the answers for the problem above. Here, it is important that we employ the Feynman-Kac-Nelson formula for the *free field* because we can calculate actually and concretely the ground state energy of the spin-boson model.

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