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ABSENCE OF ENERGY LEVEL CROSSING FOR THE GROUND STATE ENERGY OF THE RABI MODEL

MASAO HIROKAWA* AND FUMIO HIROSHIMA**

ABSTRACT. The Hamiltonian of the Rabi model is considered. It is shown in the light of quantum phase transition that the ground state energy of the Rabi Hamiltonian does not cross any other energies.

1. Introduction

Cavity quantum electrodynamics has supplied us with stronger interaction than the standard quantum electrodynamics (QED) does [8, 20]. Experimental physicists usually demonstrate the interaction by a two-level atom coupled with a one-mode light (i.e., single-mode laser) in a mirror cavity (i.e., a mirror resonator). The region that the strong interaction in cavity QED belongs to is called the strong coupling regime. At the dawn of the 21st century, the solid-state analogue of the strong interaction in a superconducting system was theoretically proposed in [15, 16], and it has been experimentally demonstrated in [3, 5, 23]. That is, the atom, the light, and the mirror resonator in cavity QED are respectively replaced by an artificial atom, a microwave, and a microwave resonator on a superconducting circuit. Here, the artificial atom is made by using a superconducting circuit based on some Josephson junctions. This replaced cavity QED is the so-called circuit QED. The circuit QED has been intensifying the coupling strength so that its region is beyond the strong coupling regime. This amazing region of the coupling strength between the artificial atom and the light is called the ultra-strong coupling regime in circuit QED [4, 6, 7, 17]. Then, experimental physicists have found some differences in physical phenomena between the two coupling regimes [6, 17]. As one of the striking differences, there is the following. In the strong coupling regime as well as in the weak coupling regime, the Jaynes-Cummings (JC) model is useful to explain the experimental results [8, 5]. The Hamiltonian of the JC model is obtained by applying the so-called rotating wave approximation (RWA) to the Rabi Hamiltonian. On the other hand, in the ultra-strong coupling regime, the JC model does not work, and thus, we need a help of the Rabi model [6, 17]. The current cutting-edge technology of circuit QED is beginning to show

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us the division between the two coupling regimes concretely. We are interested in how physics determines this division.

We will see a difference between the Rabi model and the JC model from a mathematical point of view in this paper. We pay particular attention to the energy level crossing for the ground state as well as for the excited states. It is well known that the energy level crossing for the ground state sometimes reveals a quantum phase transition [22]. It was shown [9, 10] that the models of the two-level atom coupled with the one-mode light such as the JC model turn out many energy level crossings as the coupling strength grows larger and larger, and then, the envelope made by some of the energy level crossings makes the ground state energy (see Fig.1 and Eq.(2.6)). That is, the ground state is constructed by a quantum phase transition. Such a type of quantum phase transition was pointed out by Preparata [19]. In other word, for the JC model the quantum phase transition in Rey's sense [21] takes place. Meanwhile, in 2010 Braak [1] had given a mathematically intriguing expressions of the eigenenergies of the Rabi model. Then, the following questions arise and are problems of interest to us in the case without the RWA: (i) are there any energy level crossings among them? If so, (ii) how do they take place? We can conjecture that the ground state energy of the Rabi model has no energy level crossing. In this paper we prove this fact with the functional-integral method [12, 11] as a corollary of the fact stating that the ground state energy of the Rabi model is simple (i.e., the ground state is unique). It reveals us that it is in the ultra-strong coupling regime of circuit QED that there is a big qualitative difference as well as quantitative one between the Rabi model and the JC model. This interests us in the problem whether a quantum phase transition lurks in the Rabi model.

2. Rabi Model

2.1. Definition. Let $\sigma_x, \sigma_y, \sigma_z$ be the 2×2 Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.1)$$

In this paper we adopt the natural unit: $\hbar = 1$. The renormalized Hamiltonian of the Rabi model is defined as a self-adjoint operator by

$$H_R = \Delta \sigma_z + \omega a^\dagger a + g \sigma_x (a + a^\dagger) \quad (2.2)$$

on the Hilbert space $\mathbb{C}^2 \otimes L^2(\mathbb{R})$. Here $\Delta > 0$ and $\omega > 0$ are respectively the atom transition frequency and the cavity resonance frequency, $g \in \mathbb{R}$ stands for a coupling constant, and a and a^\dagger denote the single mode bose annihilation and creation operators satisfying $[a, a^\dagger] = 1$ and $[a, a] = 0 = [a^\dagger, a^\dagger]$. It is given by

$$a = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{\omega}} \frac{d}{dx} + \sqrt{\omega} x \right), \quad a^\dagger = \frac{1}{\sqrt{2}} \left(-\frac{1}{\sqrt{\omega}} \frac{d}{dx} + \sqrt{\omega} x \right). \quad (2.3)$$

We are interested in studying spectral properties of eigenvalues of H_R , in particular crossing of the ground state energy.

The absence of crossing can be derived from the simplicity of the ground state energy of H_R . We will construct a path integral representation of e^{-tH_R} to show that the ground state energy is simple. This is a minor modification of recent

papers [12, 11], where the Feynman-Kac type formula with spin is established. In particular the spin-boson model is studied by path measure in [11] and we can apply it in this paper since the Rabi model can be regarded as the single mode photon version of the spin-boson model.

2.2. Two conjectures. Let us here consider the Rabi Hamiltonian H_R before the renormalization:

$$H_R = \Delta\sigma_z + \omega \left(a^\dagger a + \frac{1}{2} \right) + g\sigma_x (a + a^\dagger). \quad (2.4)$$

In this paper we follow the classification proposed in [2], and define the ultra-strong coupling regime by the region in which the dimensionless coupling strength $g/\omega > 0.1$. Applying the RWA to H_R , we have the JC Hamiltonian:

$$H_{JC} = \Delta\sigma_z + \omega \left(a^\dagger a + \frac{1}{2} \right) + g (\sigma_- a^\dagger + \sigma_+ a), \quad (2.5)$$

where $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$. We denote by E the ground state energy of H_{JC} . The JC model is a completely solvable model, and the eigenstate $\varphi_\nu = \varphi_\nu(g)$ of H_{JC} and its corresponding eigenvalue $E_\nu = E_\nu(g)$ are given for each $\nu \in \mathbb{Z}$ in the following procedure: Let

$$\varphi_g(x) = \left(\frac{\omega}{\pi} \right)^{1/4} e^{-\omega x^2/2}$$

be the normalized eigenvector associated with the lowest eigenvalue, 0, of the harmonic oscillator

$$\omega a^\dagger a = \frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega^2 x^2 - \omega \right).$$

Then Fock states are defined by

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(\prod_{i=1}^n a^\dagger \right) \varphi_g, \quad n = 0, 1, 2, \dots$$

for the single mode photon with $|0\rangle = \varphi_g$. Thus it follows that $L^2(\mathbb{R}) = \oplus_{n=0}^{\infty} \mathbb{C}|n\rangle$. We define the spin ground state $|-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and the spin excited state $|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ of $\Delta\sigma_z$. Then $\mathbb{C}^2 = \mathbb{C}|+\rangle \oplus \mathbb{C}|-\rangle$. Hence the total Hilbert space is represented as

$$\mathbb{C}^2 \otimes L^2(\mathbb{R}) = \oplus_{n=0}^{\infty} (\mathbb{C}|+\rangle \otimes |n\rangle \oplus \mathbb{C}|-\rangle \otimes |n\rangle).$$

We define states $|-, n\rangle$ and $|+, n\rangle$ by $|-, n\rangle = |-\rangle \otimes |n\rangle$ and $|+, n\rangle = |+\rangle \otimes |n\rangle$, respectively. Then,

$$\begin{cases} \varphi_0 = |-, 0\rangle, \\ \varphi_{+|\nu|} = \cos \theta_{|\nu|} |+, |\nu| - 1\rangle + \sin \theta_{|\nu|} |-, |\nu|\rangle, & \nu \neq 0, \\ \varphi_{-|\nu|} = -\sin \theta_{|\nu|} |+, |\nu| - 1\rangle + \cos \theta_{|\nu|} |-, |\nu|\rangle, & \nu \neq 0, \end{cases}$$

where $\theta_{|\nu|} = \theta_{|\nu|}(g) = \frac{1}{2} \tan^{-1} \left(\frac{2g\sqrt{|\nu|}}{2\Delta - \omega} \right)$ if $2\Delta \neq \omega$; $\theta_{|\nu|} = \pi/4$ if $2\Delta = \omega$, and

$$\begin{cases} E_0 = -\frac{(2\Delta - \omega)}{2}, \\ E_{\pm|\nu|} = \omega|\nu| \pm \sqrt{\frac{(2\Delta - \omega)^2}{4} + g^2|\nu|}, \quad \nu \neq 0. \end{cases}$$

Hence it follows that

$$H_{JC}\varphi_\nu = E_\nu\varphi_\nu.$$

According to [9, 10], the remarkable finding for E is the energy level crossings in the ultra-strong coupling regime: For each $n = 0, 1, 2, \dots$, there exists $g_{n+1} > 0$ such that E_{-n} and $E_{-(n+1)}$ cross each other at $g = g_{n+1}$, and

$$\begin{cases} E = E_{-n}, & \text{if } g < g_{n+1}, \\ E = E_{-n} = E_{-(n+1)}, & \text{if } g = g_{n+1}, \\ E = E_{-(n+1)}, & \text{if } g > g_{n+1}, \end{cases}$$

provided $2\Delta \geq \omega$. See Fig.1. In other words, as coupling constant g gets large, there exists $\nu_g \in \mathbb{Z}_-$ such that $E = E_{\nu_g}$, and moreover, ν_g is strictly decreasing and $\nu_g \rightarrow -\infty$ as $g \rightarrow \infty$. Namely, these energy level crossings take place and make the ground state energy E as the envelop of E_ν , $\nu = 0, -1, -2, \dots$ in Fig.1. We realize that the ground state energy E_{JC} is given by the envelope of the eigenenergies, E_{-n} , $n \in \mathbb{N}$, then. Thus, the asymptotic behavior of the ground state energy E_{JC} is

$$E_{JC} \sim -\frac{g^2}{4\omega} - \frac{(2\Delta - \omega)^2}{4g^2}\omega \quad \text{as } g \rightarrow \infty. \tag{2.6}$$

We also note that the ground-state entanglement [18] for the JC model. Namely, for instance, the ground state is a separable state for $g < g_1$, but it becomes an entangled state for $g \geq g_1$. The details on g_n and ν_g are in [9, 10].

In Fig.2 there is a numerical computation of the energy levels of H_R . It says that

- (C1) there is no energy level crossing between the ground state energy and the 1st excited state energy;
- (C2) we may say that there are just n energy level crossings between the $2n$ -th excited state energy and the $(2n + 1)$ -th excited state energy, $n = 1, 2, \dots$.

We give a comment on (C2). In [13, III.] it is shown by constructing eigenvectors concretely that there exist at least n energy level crossing.

In this paper, we will prove (C1).

3. Results and Proofs

Before going to show the Feynman-Kac formula of e^{-tH_R} , we prepare a probabilistic description of H_R .

Let $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ be elements of $SU(2)$. The rotation group in \mathbb{R}^3 has an adjoint representation on $SU(2)$. Let $n \in \mathbb{R}^3$ be a unit vector and $\theta \in [0, 2\pi)$. Thus we have $e^{(i/2)\theta n \cdot \sigma}$ satisfies that

$$e^{(i/2)\theta n \cdot \sigma} \sigma_\mu e^{-(i/2)\theta n \cdot \sigma} = (R\sigma)_\mu,$$

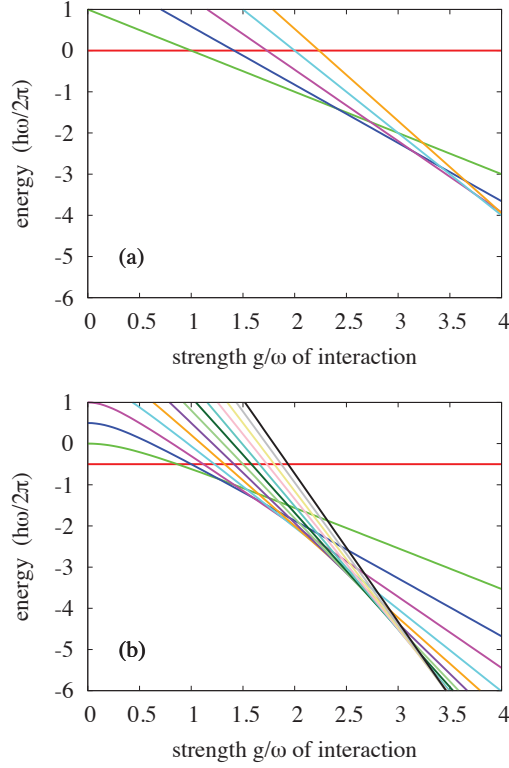


FIGURE 1. Energy level crossing among E_ν , $\nu = 0, -1, -2, \dots$, of the JC Hamiltonian. Each color indicates individual index ν of the energy E_ν . (a) $2\Delta = \omega$, (b) $2\Delta = 3\omega$.

where R denotes 3×3 matrix representing the rotation around n with angle θ . In particular for $n = (0, 1, 0)$ and $\theta = \pi/2$, we have

$$\begin{aligned} e^{(i/2)\theta n \cdot \sigma} \sigma_x e^{-(i/2)\theta n \cdot \sigma} &= \sigma_z, \\ e^{(i/2)\theta n \cdot \sigma} \sigma_z e^{-(i/2)\theta n \cdot \sigma} &= -\sigma_x. \end{aligned}$$

Set $U = e^{(i\pi/4)\sigma_y}$. Then

$$UH_RU^{-1} = \omega a^\dagger a + g\sigma_z(a + a^\dagger) - \Delta\sigma_x. \tag{3.1}$$

Since φ_g is strictly positive, we can define the unitary operator $U_g : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}, \varphi_g^2 dx)$ by $U_g f = \varphi_g^{-1} f$. We set the probability measure $\varphi_g^2 dx$ on \mathbb{R} by $d\mu$. Thus UH_RU^{-1} is transformed to the operator:

$$U_g UH_RU^{-1} U_g^{-1} = \frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega x \frac{d}{dx} \right) + g\sigma_z \sqrt{2\omega} x - \Delta\sigma_x \tag{3.2}$$

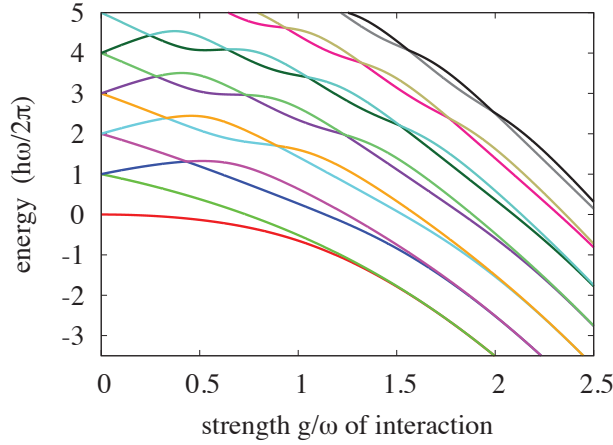


FIGURE 2. Energy level of H_R for $2\Delta = \omega$. Each color indicates the n th level of the energy for $n = 1, 2, \dots$ from the bottom, where the 0th level energy means the ground state energy.

in $\mathbb{C}^2 \otimes L^2(\mathbb{R}, d\mu)$. Let us introduce $\mathbb{Z}_2 = \{-1, +1\}$ to redefine the Hamiltonian (3.2) on a set of scalar functions. We identify $\mathbb{C}^2 \otimes L^2(\mathbb{R}, d\mu)$ with

$$\mathcal{H} = L^2(\mathbb{R} \times \mathbb{Z}_2, d\mu) = \left\{ f = f(x, \sigma) \left| \sum_{\sigma \in \mathbb{Z}_2} \int |f(x, \sigma)|^2 d\mu(x) < \infty \right. \right\} \quad (3.3)$$

by $\mathbb{C}^2 \otimes L^2(\mathbb{R}, d\mu) \ni \begin{bmatrix} f_+(x) \\ f_-(x) \end{bmatrix} \mapsto f(x, \sigma) \in \mathcal{H}$. Thus under this identification (3.2) is transformed to the operator H :

$$Hf(x, \sigma) = \left\{ \frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega x \frac{d}{dx} \right) + g\sqrt{2\omega\sigma x} \right\} f(x, \sigma) - \Delta f(x, -\sigma), \quad \sigma \in \mathbb{Z}_2 \quad (3.4)$$

in \mathcal{H} . Thus we have the lemma below:

Lemma 3.1. *The operator H_R in $\mathbb{C}^2 \otimes L^2(\mathbb{R})$ is unitarily equivalent to H in \mathcal{H} .*

In what follows we deal with H instead of H_R . Let

$$h = \frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega x \frac{d}{dx} \right)$$

and $(X_t)_{t \geq 0}$ be the Ornstein-Uhlenbeck process on a probability space $(\mathcal{X}, \mathcal{B}, P^x)$. We have $P^x(X_0 = x) = 1$

$$\int d\mu(x) \mathbb{E}_{P^x} [X_t] = 0, \quad \int d\mu(x) \mathbb{E}_{P^x} [X_t X_s] = \frac{e^{-|t-s|\omega}}{2\omega}.$$

Here $\mathbb{E}_Q[\dots]$ denotes the expectation with respect to a probability measure Q . The generator of X_t is given by $-h$ and

$$(f, e^{-th}g)_{\mathcal{H}} = \int d\mu(x) \mathbb{E}_{P^x} \left[\overline{f(X_0)} g(X_t) \right].$$

The distribution $\rho_t(x, y)$ of X_t under P^x is given by

$$\rho_t(x, y) = \varphi_g(x)^{-1} K_t(x, y) \varphi_g(y), \tag{3.5}$$

where $K_t(x, y)$ denotes the Mehler kernel:

$$K_t(x, y) = \frac{1}{\sqrt{\pi(1 - e^{-2t})}} \exp\left(\frac{4xye^{-t} - (x^2 + y^2)(1 + e^{-2t})}{2(1 - e^{-2t})}\right).$$

See e.g., [14, 3.10.4] for the detail of Ornstein-Uhrenbeck processes and harmonic oscillators. In order to show the spin part by a path measure we introduce a Poisson process. Let $(N_t)_{t \geq 0}$ be a Poisson process on some probability space $(\mathcal{X}', \mathcal{B}', \nu)$ with unit intensity, i.e.,

$$\mathbb{E}_\nu [\mathbb{1}_{N_t=n}] = \frac{t^n}{n!} e^{-t}, \quad n \geq 0.$$

We define $\sigma_t = (-1)^{N_t} \sigma$, $\sigma \in \mathbb{Z}_2$, for $t \geq 0$. Let $\sum_{\sigma \in \mathbb{Z}_2} \int d\mu(x) \mathbb{E}_{P^x} \mathbb{E}_\nu [\dots] = \mathbb{E} [\dots]$.

Theorem 3.2. [Feynman-Kac formula] *The following equalities hold:*

$$(\Delta > 0) \quad (f, e^{-tH} g)_{\mathcal{H}} = e^t \mathbb{E} \left[\overline{f(X_0, \sigma_0)} g(X_t, \sigma_t) e^{-g\sqrt{2\omega} \int_0^t \sigma_s X_s ds} \Delta^{N_t} \right], \tag{3.6}$$

$$(\Delta = 0) \quad (f, e^{-tH} g)_{\mathcal{H}} = e^t \mathbb{E} \left[\mathbb{1}_{N_t=0} \overline{f(X_0, \sigma)} g(X_t, \sigma) e^{-g\sigma\sqrt{2\omega} \int_0^t X_s ds} \right]. \tag{3.7}$$

Proof. Let $\Delta > 0$. By a minor modification of [12, Theorem 5.10] we can see that

$$(f, e^{-tH} g)_{\mathcal{H}} = e^t \mathbb{E} \left[\overline{f(X_0, \sigma_0)} g(X_t, \sigma_t) e^{-g\sqrt{2\omega} \int_0^t \sigma_s X_s ds} e^{\int_0^t \log \Delta dN_s} \right]. \tag{3.8}$$

Here $\int_0^t f(N_s) dN_t = \sum_{r, N_{r+} \neq N_{r-}} f(N_r)$. Since $e^{\int_0^t \log \Delta dN_s} = e^{\log \Delta^{N_t}} = \Delta^{N_t}$,

(3.6) follows. In the case of $\Delta = 0$ only the set $N_t = 0$ contributes to the path integral. Then

$$(f, e^{-tH} g)_{\mathcal{H}} = e^t \mathbb{E} \left[\overline{f(X_0, \sigma_0)} g(X_t, \sigma_t) e^{-g\sqrt{2\omega} \int_0^t \sigma_s X_s ds} \mathbb{1}_{N_t=0} \right]. \tag{3.9}$$

Then (3.7) follows. □

Corollary 3.3. [Uniqueness] *Let $E_0 = \inf \sigma(H)$. Then we have*

$$\dimker(H - E_0) = 1,$$

i.e., the ground state of H_R is unique.

Proof. Let $f, g \geq 0$ but not identically zero. Then for sufficiently small $\epsilon > 0$, we see that both $\Omega_f = \{(x, \sigma) \in \mathbb{R} \times \mathbb{Z}_2 | f(x, \sigma) > \epsilon\}$ and $\Omega_g = \{(x, \sigma) \in \mathbb{R} \times \mathbb{Z}_2 | g(x, \sigma) > \epsilon\}$ have positive measures. We have by (3.6),

$$(f, e^{-tH} g) \geq \epsilon e^t \mathbb{E} \left[\mathbb{1}_{\Omega_f}(X_0, \sigma_0) \mathbb{1}_{\Omega_g}(X_t, \sigma_t) e^{-g\sqrt{2\omega} \int_0^t \sigma_s X_s ds} \Delta^{N_t} \right].$$

Since Ω_f is a subset of $\mathbb{R} \times \mathbb{Z}_2$, we have $\Omega_f = \bigcup_{\sigma \in \mathbb{Z}_2} (\Omega_f^\sigma, \sigma)$. Thus either Ω_f^+ or Ω_f^- ($\subset \mathbb{R}$) have at least a positive measure. Suppose that Ω_f^+ has a positive measure. Similarly we see that $\Omega_g = \bigcup_{\sigma \in \mathbb{Z}_2} (\Omega_g^\sigma, \sigma)$ and suppose that Ω_g^+ is a

positive measure. Let Ω be the set of paths starting from the inside of $(\Omega_f^+, +)$ and arriving at the inside of $(\Omega_g^+, +)$. We see that

$$\mathbb{E}[\mathbb{1}_\Omega] = \mathbb{E}\left[\mathbb{1}_{\Omega_f^+}(X_0)\mathbb{1}_{\Omega_g^+}(X_t)\mathbb{1}_{N_t=\text{even}}\right].$$

By using the distribution ρ_t of X_t we have

$$\mathbb{E}[\mathbb{1}_\Omega] = \sum_{n=0}^{\infty} \frac{t^{2n}}{(2n)!} e^{-t} \int_{\Omega_f^+} dx \int_{\Omega_g^+} dy \varphi_g(x) K_t(x, y) \varphi_g(y) > 0.$$

Hence we conclude that Ω has a positive measure and

$$(f, e^{-tH}g) \geq \epsilon e^t \mathbb{E}\left[\mathbb{1}_\Omega e^{-g\sqrt{2\omega} \int_0^t \sigma_s X_s ds} \Delta^{N_t}\right] > 0.$$

Thus e^{-tH} is a positivity improving operator. Thus $\dimker(H - E_0) = 1$ follows from the Perron-Frobenius theorem. \square

Corollary 3.4. [No crossing] *The ground state energy of H_R has no crossing for all the values of g and Δ .*

Let us define the self-adjoint operator K by

$$K = \frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega x \frac{d}{dx} \right) - |g|\sqrt{2\omega}|x| - \Delta\sigma_x. \tag{3.10}$$

It is trivial to see that $H - K \geq 0$ as self-adjoint operator, and we can see that

$$\epsilon - \Delta \leq \inf \sigma(H), \tag{3.11}$$

where $\epsilon = \inf \sigma\left(\frac{1}{2} \left(-\frac{d^2}{dx^2} + \omega x \frac{d}{dx} \right) - |g|\sqrt{2\omega}|x|\right)$. We state more strong statement. By using the Feynman-Kac formula we have the inequality below.

Corollary 3.5. *We have the inequality: $|(f, e^{-tH}g)| \leq (|f|, e^{-tK}|g|)$.*

Proof. By the Feynman-Kac formula we have

$$|(f, e^{-tH}g)_{\mathscr{H}}| \leq e^t \mathbb{E}\left[|f(X_0, \sigma_0)g(X_t, \sigma_t)| e^{|g|\sqrt{2\omega} \int_0^t X_s ds} \Delta^{N_t}\right]. \tag{3.12}$$

Then the corollary follows. \square

4. Concluding Remarks

In this paper we have proved the first conjecture (C1) that the numerical computation predicts, while the JC model has many energy level crossings for the ground state energy in the ultra-strong coupling regime of circuit QED though it has no energy level crossing in the weak and strong coupling regimes. It shows that it is in the ultra-strong coupling regime that there is a big qualitative difference as well as quantitative one between the JC model and the Rabi model.

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