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Exact analytical approach for spontaneous emission of atoms in the optical potential theory

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Abstract

Using a boundary condition proposed by Petrosky et al. [Physica A 173 (1991) 175], the optical potential (or model space) approach is generalized to study the decay problem. By making use of this method, the spontaneous emission of atoms in free space and cavities is dealt with in an exact analytical form without any approximation.

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1. Introduction

The problem of decay or dissipation of a quantum system interacting with an environment is a fundamental one appearing extensively in elementary particle physics, nuclear physics and atomic physics [1,2]. There are many methods to calculate the decay width and describe the dynamics of the quantum dissipation. Typical approaches are solving the time dependent Schrödinger equation, using scattering theory and building a master equation for the density matrix. However, all these approaches depend on certain approximations, such as the Wigner–Weisskopf approximation and the Markoff approximation [3]. Therefore, an exact analytical solution of this problem would help to develop the theory of decay. In this paper, we consider the optical potential theory [2,4] with applications to so-called cavity quantum electrodynamics [5].

The optical potential theory is a basic method to study elastic scattering problems and to calculate the width of the cross section peak. An optical potential can microscopically be derived in different ways, the most popular one being proposed by Feshbach using the projection operator technique [4]. In this theory, the Hamiltonian H, for the time independent Schrödinger equation $H\Psi = E\Psi$, is divided into two parts H_0 and V such that H_0 can be solved exactly. The whole Hilbert space is also divided into two arbitrary parts, the model space represented by the projection operator P and its supplementary space represented by another projection operator $Q = 1 - P$. Generally, this decomposition is selected according to different physical situations. For example, P

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is usually selected as the elastic channel or some bound states of H_0. Thus, one has a decomposition $\Psi = P\Psi + Q\Psi \equiv \Psi_P + \Psi_Q$, where Ψ_P and Ψ_Q obey

$$(H_{PP} - E)\psi_P + H_{PQ}\Psi_Q = 0 \tag{1}$$

and

$$(H_{QQ} - E)\Psi_Q + H_{QP}\Psi_P = 0 \tag{2}$$

for $H_{PP} = PHP$, $H_{QQ} = QHQ$, $H_{QP} = QHP$ and $H_{PQ} = PHQ$. If we focus on the model space, we have an effective Schrödinger equation

$$H_{\text{eff}}\Psi_P = E\Psi_P \tag{3}$$

for the non-Hermitian effective Hamiltonian

$$H_{\text{eff}} = H_{PP} + H_{PQ}\frac{1}{E - H_{QQ} + i\epsilon}H_{QP}, \tag{4}$$

with the so-called optical potential $V_{\text{opt}} = H_{\text{eff}} - p^2/2m$. Here ϵ is usually an infinitely small positive number representing the outgoing process. It should be noted that Eqs. (3) and (4) are exact and the effective Hamiltonian H_{eff} is energy dependent, therefore Eq. (3) should be solved self-consistently with respect to the energy. The physical meaning of Eq. (4) is clear: the first term represents the original interaction in the model space and the second term represents an interaction from outside the model space. In principle, the model space can be selected as a finite dimensional space, e.g., the space spanned by bound states. In this case, if the bound state energy is below the continuous spectrum, the calculation can be carried out easily for most cases. But when the bound state is embedded in the continuous spectrum, it is not known whether there is a solution.

Prigogine's group has proposed a new boundary condition called natural time ordering which is confirmed to be suitable to describe dissipative processes or decay problems [6,7]. Using the natural time ordering and an infinite order perturbation expansion, the boundary condition for the propagator is expressed in the form

$$f(z) = \int_{\Gamma} \frac{g(\omega_k)\,d\omega_k}{(\omega_k - \omega_i - z)}, \tag{5}$$

where ω_k and ω_i are the unperturbed state energy, z a complex number, $g(\omega_k)$ an arbitrary function and the inverse of the denominator is called the complex distribution. The integration denoted by Γ is first carried out by fixing z in the upper-half plane and then the limit $\text{Im } z \to -i\gamma$ is taken (for details see Refs. [6,7]).

By combining the boundary condition (5), exact solutions of the Schrödinger equation with the optical potential can be obtained for the spontaneous emission of two-level atoms both in free space and in a cavity. In this paper, the optical potential theory is generalized to calculate the decay by a self-consistent energy eigenequation with complex energy eigenvalues. As an application, the calculation of the spontaneous emission rates of atoms in free space as well as in a cavity [8] is exactly carried out. Notice that the spontaneous emission problem is still very important at present since it plays a critical role in laser cooling mechanisms and cavity quantum electrodynamics besides being extensively used in spectral theory [9,10]. As the Wigner–Weisskopf approximation is often used as a first order approximation in the calculation of the spontaneous emission of atoms, an exact soluble model is useful to check the efficiency of the Wigner–Weisskopf approximation and an exact calculation of the spontaneous emission is useful.

In fact, an exact complex spectral representation theory of the Hamiltonian as well as the Liouville–von Neumann operator may substantially reconcile some conflicts between the reversibility of the basic laws of physics and the irreversibility of most dynamic processes, such as dissipative structures, spontaneous emission of atoms, evolution process approaching equilibrium, quantum decoherence with wavefunction collapse and so on. The present approach, based on Fechbach's optical potential theory and the novel boundary condition of Prigogine's group, shows that the integral equation for the dissipation dynamics has consistent solutions for both the energy and the width of an arbitrary strength of interaction in explicit form when the dynamics of a system is formulated outside the Hilbert space of the system. Notice that the eigenstates obtained here do not belong to the usual Hilbert space of the system, but they lie in the so-called "rigged" Hilbert space introduced by Antoniou and Prigogine [11]. Therefore, the present study goes some way beyond traditional approaches in ordinary quantum mechanics, such as the Wigner–Weisskopf approximation and

the Born–Markov approximation. Actually, many interesting mesoscopic phenomena in cavity QED cannot be dealt with by these traditional methods and further generalizations of the method presented here may be applied to these problems successfully.

2. A simple illustration: the Friedrichs model

Although the Feshback theory [4] is extensively used to study scattering and bound states problems, its generalization can also be applied to the decay problem. Here, we first consider a simple model, the Friedrichs model [12], to show how the optical potential method is used to study the decay problem. Its Hamiltonian is

$$H = H_0 + V = e_1 |1\rangle\langle 1| + \int \omega(k) |k\rangle\langle k| \, dk + \int V_k (|k\rangle\langle 1| + |1\rangle\langle k|) \, dk, \quad (6)$$

where $|1\rangle$ is a discrete state with energy e_1 and $|k\rangle$ is a continuous state with energy ω_k of H where $e_1 > 0$ and $\omega_k \geq 0$. Obviously, the state $|1\rangle$ is embedded in the continuous spectrum. Let the projection operator be selected as

$$P = |1\rangle\langle 1|. \quad (7)$$

Then, as usual the effective Hamiltonian is

$$H_{\text{eff}} = \left(e_1 + \int \frac{V_k^2 \, dk}{E - \omega(k) + i\epsilon} \right) |1\rangle\langle 1|. \quad (8)$$

Since the model space is one dimensional, Eq. (3) becomes the transcendental equation

$$e_1 + \int \frac{V_k^2 \, dk}{E - \omega(k) + i\epsilon} = E. \quad (9)$$

which should be solved consistently for a complex energy E. However, the above equation has no solution. This can be shown as follows. Substituting $E = E_1 - i\gamma$ for real E_1 and γ into the above equation and separating its real and imaginary parts, we obtain two equations,

$$E_1 = e_1 + \int \frac{[E_1 - \omega(k)] V_k^2 \, dk}{[E_1 - \omega(k)]^2 + \gamma^2} \quad (10)$$

and

$$-\gamma = \gamma \int \frac{V_k^2 \, dk}{[E_1 - \omega(k)]^2 + \gamma^2}. \quad (11)$$

The only solution of Eq. (11) is $\gamma = 0$, but for $\gamma = 0$, Eq. (9) gives

$$\gamma = \pi \int V_k^2 \delta(E - \omega(k)) \, dk \neq 0, \quad (12)$$

except $V_k = 0$ at $E = \omega(k)$ occasionally. Therefore, we can conclude that Eq. (9) has no solution. This means that the subspace $|1\rangle$ must be excluded from the Hilbert space of the perturbed Hamiltonian H by the boundary condition implied in Eq. (9). In order to overcome the above contradiction, we invoke the natural time ordering approach for dissipative processes [6,7] with the substitution

$$\begin{aligned} \epsilon &\mapsto +\epsilon \quad \text{for } |1\rangle \to |k\rangle, \\ &\mapsto -\epsilon \quad \text{for } |k\rangle \to |1\rangle, \\ &\mapsto +\epsilon \quad \text{for } |k\rangle \to |k'\rangle, \end{aligned} \quad (13)$$

in Eq. (9). This implies the new boundary condition (5) for which the propagator in Eq. (9) is replaced by that in Eq. (5). According to Refs. [6,7], this results in a new equation,

$$e_1 - \int \frac{V_k^2 \, dk}{[\omega(k) - E]_{-i\gamma}^{+}} = E \quad (14)$$

and then the decay rate obeys

$$-\gamma = \gamma \int \frac{V_k^2 \, dk}{[E_1 - \omega(k)]^2 + \gamma^2} - \int_C \frac{V_k^2 \, dk}{\omega(k) - (E_1 - i\gamma)}, \quad (15)$$

where the contour C of the second integration is a small circle enclosing the singular point $E_1 - i\gamma$. Eqs. (10) and (15) have a solution, which means that the perturbed Hamiltonian has an eigenstate with a complex energy value $E_1 - i\gamma$ representing a decay state (for a detailed explanation see Refs. [6,7]).

3. Spontaneous emission of atoms in free space

For the spontaneous emission of an atom in free space, a two-level Hamiltonian in the rotating wave approximation [8] is

$$H = H_0 + V. \tag{16}$$

Here

$$H_0 = e_0|0\rangle\langle 0| + e_1|1\rangle\langle 1| + \int \omega(\lambda) a_\lambda^\dagger a_\lambda \, \mathrm{d}\lambda, \tag{17}$$

$$V = \int V(\lambda)\left(|1\rangle\langle 0| a_\lambda + |0\rangle\langle 1| a_\lambda^\dagger\right) \mathrm{d}\lambda, \tag{18}$$

where the natural unit $\hbar = 1$ is used; $|0\rangle$, $|1\rangle$, e_0 and e_1 are the atomic state vectors and the corresponding energies respectively; $\lambda = (\boldsymbol{k}, \sigma)$ represents the momentum and polarization of a photon and a_λ, $a_\lambda^\dagger$ and $\omega(\lambda)$ are the annihilation operator, creation operator and the frequency of the photon respectively. Denote the eigenstates of H_0 by $|a; \lambda_1\lambda_2\lambda_3\ldots\rangle$ where a denotes the atomic states, i.e., $a = 0, 1$, as follows.

The following subspaces are closed for the Hamiltonian (16),

$$\{|0, 0\rangle\}, \quad \{|1, 0\rangle, |0, \lambda\rangle\},$$
$$\{|1, \lambda\rangle, |0, \lambda, \lambda'\rangle\}, \ldots \tag{19}$$

We only consider a subspace $\{|1, 0\rangle, |0, \lambda\rangle\}$ and then select $|1, 0\rangle$ as a model space. Then we obtain two equations like Eqs. (15) and (10). If e_0 is set to zero and the energy shift is absorbed in e_1 as usual (i.e., $E_1 = e_1$), we only need to solve Eq. (15). Within the dipole approximation and after integration over the orientation of the momentum of the photon as well as summation of its polarization [8], Eq. (15) becomes

$$-\gamma = \gamma \frac{2}{3\pi c^3} \int \frac{\omega^3 \mu^2 \, \mathrm{d}\omega}{(E_1 - \omega)^2 + \gamma^2} - \frac{2}{3\pi c^3} \int_C \frac{\omega^3 \mu^2 \, \mathrm{d}\omega}{\omega - (E_1 - \mathrm{i}\gamma)}, \tag{20}$$

where μ is the matrix element of the atomic dipole moment. If μ is set to be constant as usually done the first term on the right hand side of Eq. (20) is divergent, as the dipole approximation is not valid at high frequencies. Actually, at high frequencies, the atomic wave functions are approximately given by $\varphi(r) \approx \exp(-\alpha r^2/2)$ and the interaction matrix is given by

$$V_k \propto \langle 0| z \exp(\pm \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})|1\rangle \approx \int \exp(-\alpha r^2 \pm \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \, \mathrm{d}^3 r \propto \exp(-k^2/4\alpha) \propto \exp(-\omega^2/\beta), \tag{21}$$

where α and β are positive constants representing the size of the atom. In order to make the calculation more simple, the following case is considered,

$$\mu^2 = \mu_0^2 \omega_0^3/\omega^3, \tag{22}$$

where μ_0 can be considered as an effective dipole moment. Then, we have

$$\gamma = \frac{2\mu_0^2\omega_0^3}{3\pi c^3}\left(2\pi - \gamma \int_{-E_1}^{\infty} \frac{\mathrm{d}\omega}{\omega^2 + \gamma^2}\right). \tag{23}$$

This gives an exact solution of the spontaneous emission of an atom in free space: If $E_1 \gg 0$ or $\gamma \ll 1$ we obtain

$$\gamma_1 = \frac{2\mu_0^2\omega_0^3}{3\pi c^3}(2\pi - \pi) = \frac{2\mu_0^2\omega_0^3}{3c^3}, \tag{24}$$

which is just the result of the Wigner–Weisskopf approximation. If $E_1 \to 0$ or $\gamma \gg 1$, we obtain

$$\gamma_2 = \frac{2\mu_0^2\omega_0^3}{3\pi c^3}(2\pi - \pi/2) = \frac{\omega_0^2\omega_0^3}{c^3}, \tag{25}$$

which means that Wigner–Weisskopf approximation is no longer valid. Therefore, we reach the conclusion that the width of spontaneous emission satisfies $\gamma_1 < \gamma < \gamma_2$.

In the model space the wave function is

$$|\Psi(t)\rangle \simeq \mathrm{e}^{-\mathrm{i}Et}|1, 0\rangle = \mathrm{e}^{-\mathrm{i}e_1 t - \gamma t}|1, 0\rangle \xrightarrow{t\to\infty} 0, \tag{26}$$

where the energy shift is absorbed into e_1 and the decay probability is γ. The exact solution can be found by

$$\varphi_\lambda = -\frac{V(\lambda)}{\left[\omega(\lambda) - e_1 + z\right]_{-\mathrm{i}\gamma}^{+}} \varphi_1, \tag{27}$$

where φ_1 may be chosen to be one or to be given by normalization. Then, the final spectral distribution is given by

$$|B(\omega(\lambda))|^2 = \frac{|V(\lambda)|^2}{[e_1 - \omega(\lambda)]^2 + \gamma^2} \tag{28}$$

or

$$A(\omega) = \int \frac{|V(\lambda)|^2}{[e_1 - \omega(\lambda)]^2 + \gamma^2} \rho(\omega)\, d\Omega = \frac{\gamma\pi^{-1}}{(e_1 - \omega)^2 + \gamma^2}. \tag{29}$$

where the energy shift is absorbed into e_1. Finally the wave function is given by (Eqs. (1)–(3) and boundary condition (5))

$$|\Psi\rangle \simeq |1, 0\rangle - \int d\lambda \frac{V(\lambda)}{[\omega(\lambda) - e_1 + z]^+_{-i\gamma}} |0, \lambda\rangle, \tag{30}$$

which has the same form as that derived by Petrosky et al. for the Friedrichs model using an infinite order perturbation series.

4. Spontaneous emission of atoms inside a cavity

The spontaneous emission for an atom in a cavity can be described by the following Hamiltonian [8],

$$H = H_a + H_c + H_w + W = H_0 + W, \tag{31}$$

where

$$H_0 = e_0 |0\rangle\langle 0| + e_1 |1\rangle\langle 1| + \omega a^+ a + \int \omega(\lambda) b_\lambda^+ b_\lambda \, d\lambda \tag{32}$$

and

$$W = \int \mu(\lambda)\left(a^+ b_\lambda + a b_\lambda^+\right) d\lambda + g(|1\rangle\langle 0| a + |0\rangle\langle 1| a^+). \tag{33}$$

Here as in Eqs. (17) and (18) $|0\rangle$, $|1\rangle$, e_0 and e_1 are the atomic state vectors and the energies respectively; ω, a^+ and a are the energy, annihilation and creation operators of a single mode photon field in the cavity respectively; λ represents the quantum number of the cavity wall system and b_λ, b_λ^+ and $\omega(\lambda)$ are the annihilation operator, creation operator and the energy of the wall-excitation. W contains both the interaction between the photon field and the wall and that between the atom and the photon field in the cavity. We only consider the following invariant space,

$$\{|1, 0, 0\rangle, |0, 1, 0\rangle, |0, 0, \omega_1\rangle\}, \tag{34}$$

where in the state $|\alpha, \beta, \gamma\rangle$ α represents the state of the atom, β is the number of the photons in the cavity and γ is the quantum number of the wall and the Hamiltonian in this subspace is

$$H = \begin{pmatrix} e_1 & g & 0 \\ g & \omega + e_0 & \mu(\lambda) \\ 0 & \mu(\lambda') & (\omega_\lambda + e_0)\delta(\lambda - \lambda') \end{pmatrix}. \tag{35}$$

If the projection operator (model space) is selected as

$$P = |1, 0, 0\rangle\langle 1, 0, 0| + |0, 1, 0\rangle\langle 0, 1, 0|, \tag{36}$$

then the effective Hamiltonian becomes

$$H_{\text{eff}} = \begin{pmatrix} e_1 & g \\ g & \omega \end{pmatrix} - \int d\lambda \begin{pmatrix} 0 \\ \mu(\lambda) \end{pmatrix} \times \frac{1}{[\omega(\lambda) - E]^+_{-i\gamma}} (0 \quad \mu(\lambda)) = \begin{pmatrix} e_1 & g \\ g & \omega + \int \mu^2(\lambda)\, d\lambda / [\omega(\lambda) - E]^+_{-i\gamma} \end{pmatrix} = \begin{pmatrix} e_1 & g \\ g & \omega + A + Bi \end{pmatrix}, \tag{37}$$

where e_0 is set to be zero and A and B are calculated as above. It is easy to obtain the eigenvalues

$$E_\pm = \tfrac{1}{2}\left\{e_1 + \omega + A + Bi \pm \sqrt{[e_1 - \omega - (A + Bi)]^2 + 4g^2}\right\}, \tag{38}$$

where A and B are functions of $E_\pm = E_{1\pm} - i\gamma_\pm$. This equation should be solved consistently for com-

plex energy. If the energy shift A is absorbed into e_1 and $\Delta = e_1 - \omega$, we have

$$E_{\pm} = \frac{1}{2}\left[e_1 + \omega + Bi \pm \sqrt{(\Delta - Bi)^2 + 4g^2} \right]$$
$$= \frac{1}{2}\left(e_1 + \omega + Bi \pm \sqrt{\Delta^2 - B^2 + 4g^2 - 2\Delta Bi} \right). \quad (39)$$

For a weak coupling of the cavity field to the atom, i.e., g is very small, we obtain

$$E_{\pm} \to \frac{1}{2}\left(e_1 + \omega + Bi \pm (e_1 - \omega - Bi) \right.$$
$$\left. \pm \frac{2g^2}{\Delta^2 + B^2}(\Delta - Bi) \right), \quad (40)$$

which means the atom will decay with the spontaneous emission rate

$$\gamma = \frac{g^2 B}{\Delta^2 + B^2} \quad (41)$$

and the cavity field will also decay with a width B. Similar results for the spontaneous emission rate of atoms in a cavity given in Refs. [5,8,9] are only approximate cases of the above result, which shows the enhancement and suppression of the spontaneous emission rates.

When the interaction between the atom and the field is strong, i.e., g is very large, we obtain

$$E_{\pm} = \frac{1}{2}\left[e_1 + \omega + Bi \pm g\left(2 + \frac{(\Delta - Bi)^2}{4g^2} \right) \right]$$
$$= \frac{1}{2}\left[e_1 + \omega \pm g\left(2 + \frac{\Delta^2 - B^2}{4g^2} \right) \right.$$
$$\left. + B\left(1 \mp \frac{\Delta}{2g} \right) i \right], \quad (42)$$

from which in the resonant case the decay width of the atom will be half that of a photon in the cavity (cavity damping).

It should be pointed out that there are other exactly solvable approaches for the problems of decay, dissipation and decoherence with wavefunction collapse [13]. For instance, in Refs. [14,15], the exact solution for the wavefunction of a particle, in constant or harmonic force fields, interacting with a bath of infinite harmonic oscillators was obtained to describe the dissipation process and the Brownian motion. In this sense, the physical meaning of the wavefunction for the dissipative system was clarified in comparison with the time dependent effective Hamiltonian treatment. In further works, we will analyze the relations between this approach and the present spectral representation of the Hamiltonian.

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References

[1] V. Weisskopf and E.Z. Wigner, Z. Phys. 63 (1930) 54; 65 (1930) 18.
[2] C.J. Joachain, Quantum collision theory (North-Holland, Amsterdam, 1975);
R.G. Newton, Scattering theory of waves and particles, 2nd Ed. (Springer, Berlin, 1982).
[3] W.H. Louisell, Quantum statistical properties of radiation (Wiley, New York, 1973).
[4] H. Feshbach, Ann. Phys. (NY) 5 (1958) 357; 19 (1962) 287.
[5] P.R. Berman, ed., Cavity quantum electrodynamics (Academic Press, New York, 1994).
[6] T. Petrosky, I. Prigogine and S. Tasaki, Physica A 173 (1991) 175.
[7] I. Prigogine, Phys. Rep. 219 (1992) 93.
[8] A.N. Oraevskii, Usp. Fiz. Nauk 164 (1994) 415.
[9] D.P. O'Brien, P. Meystre and H. Walther, Adv. At. Mol. Phys. 21 (1985) 1.
[10] E. Aromondo, W. Phillips and F. Strumia, eds., Laser manipulation of atoms and ions (North-Holland, Amsterdam, 1992).
[11] I. Antoniou and I. Prigogine, Physica A 192 (1993) 443.
[12] K. Friedrichs, Comm. Pure Appl. Math. 1 (1948) 361.
[13] C.P. Sun, Phys. Rev. A 43 (1994) 878.
[14] L.H. Yu and C.P. Sun, Phys. Rev. A 49 (1994) 592.
[15] C.P. Sun and L.H. Yu, Phys. Rev. A 51 (1995) 1845.