The rotating wave approximation (RWA) of quantum optics: serious defect

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Abstract

The rotating wave approximation (RWA) is an integral part of the foundations of quantum optics and it is also used extensively in atomic and condensed-matter physics. Here we prove that the model has a serious defect, viz. the spectrum has no lower bound, for all models of physical interest. As a result, the reservoir is not passive (since energy can be extracted from it without limit) and hence the second law of thermodynamics is not satisfied. An alternative to the RWA is discussed.

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The rotating wave approximation (RWA) is an integral part of the foundations of quantum optics and is discussed in both the old and the more modern textbooks and review articles [1–6]. It concerns the interaction of a reservoir, consisting of an infinite number of oscillators, with either a two-level atom or a cavity mode or a charged harmonic oscillator. Here, we will concentrate on the latter case as this will provide us with a clear-cut method for making it clear that the model has a serious defect.

The RWA Hamiltonian, for an oscillator of frequency ω_0 interacting with a reservoir, has the form

$$H_{RWA} = \hbar\omega_0 a^\dagger a + \sum_j \hbar\omega_j b_j^\dagger b_j + \sum_j (\lambda_j a^\dagger b_j + \lambda_j^* a b_j^\dagger), \tag{1}$$

where a and b_j are operators satisfying the commutation relations

$$[a, a^\dagger] = 1, [b_j, b_j^\dagger] = 1 \quad \text{for all } j. \tag{2}$$

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Our purpose here is to show that the energy of this system has no lower bound and hence we are dealing with an unphysical system. In order to obtain an upper bound for the ground-state energy, we choose a variational wave-function $\psi = |\alpha > \prod_j |\beta_j >$ which is a direct product of coherent states [2,7] associated with the non-interacting oscillators. Explicitly,

$$\psi = \exp(\alpha a^+ - \tfrac{1}{2}|\alpha|^2)\prod_j \exp(\beta_j b_j^+ - \tfrac{1}{2}|\beta_j|^2)\psi_0, \tag{3}$$

where ψ_0 is the vacuum state, defined by

$$a\psi_0 = 0, \qquad b_j\psi_0 = 0, \quad \text{for all } j \text{ and } \langle\psi_0,\psi_0\rangle = 1. \tag{4}$$

Note that ψ is a simultaneous eigenfunction of a and the b_j, with corresponding eigenvalues α and β_j,

$$a\psi = \alpha\psi, \qquad b_j\psi = \beta_j\psi \quad \text{for all } j. \tag{5}$$

It follows that the expectation value of the RWA Hamiltonian is

$$\langle\psi, H_{RWA}\psi\rangle = \hbar\omega_0|\alpha|^2 + \sum_j (\hbar\omega_j|\beta_j|^2 + \lambda_j\alpha^*\beta_j + \lambda_j^*\alpha\beta_j^*). \tag{6}$$

For a given value of α, we minimize this quantity if we choose

$$\beta_j = -\frac{\lambda_j^*}{\hbar\omega_j}\alpha. \tag{7}$$

Then

$$\langle\psi, H_{RWA}\psi\rangle = \left(\hbar\omega_0 - \sum_j \frac{|\lambda_j|^2}{\hbar\omega_j}\right)|\alpha|^2. \tag{8}$$

Therefore, if the coupling satisfies the condition

$$\sum_j \frac{|\lambda_j|^2}{\hbar\omega_j} > \hbar\omega_0, \tag{9}$$

then, by choosing $|\alpha|$ large enough, the expectation of the RWA Hamiltonian can be made as large and negative as we please. Since the expectation of any self-adjoint operator is within the spectrum of the operator, this implies that the spectrum of the RWA Hamiltonian would have no lower bound. However, the common lore in the quantum optics community is that this is only of concern for physical systems with low-frequency oscillators (ω_0) and strong coupling (λ_j), in contrast to the situation in quantum optics where the frequencies are high ($\sim 10^{15}$ Hz). We will now prove that this is a fallacy.

To investigate the condition (9) in detail, we must consider the physical system from which the RWA Hamiltonian was obtained by discarding certain terms. For this purpose, we consider the independent-oscillator (IO) model [8], which is sufficiently general to describe any system with linear passive dissipation.

In particular, it describes non-relativistic quantum electrodynamics (NRQED). For the IO model

$$\lambda_j = -\frac{\hbar}{2}\left(\frac{m_j\omega_j^3}{m\omega_0}\right)^{1/2}, \tag{10}$$

where m is the oscillator mass while m_j and ω_j and are the mass and frequency of the jth reservoir oscillator. Then, it can be shown that the condition given by (9) can be written as

$$\frac{1}{4\pi}\int_{-\infty}^{\infty} d\omega \, \mathrm{Re}\{\tilde{\mu}(\omega + iO^+)\} > m\omega_0^2, \tag{11}$$

where $\tilde{\mu}(\omega)$ is the Fourier transform of the memory term appearing in the generalized quantum Langevin equation associated with the IO model [8]. For the Ohmic case [8], where the reservoir spectrum is chosen to give rise to a Markovian equation of motion for the oscillator [1–6],

$$\mathrm{Re}\{\tilde{\mu}(\omega + iO^+)\} = \zeta, \tag{12}$$

where ζ is the frequency-independent friction constant. For the more physical case, of a radiation reservoir [8]

$$\mathrm{Re}\{\tilde{\mu}(\omega + iO^+)\} = m\tau_e \frac{\omega^2}{1 + \omega^2\tau_e^2}, \tag{13}$$

where $\tau_e = 2e^2/3mc^3$. In either case the integral on the left-hand side of (11) is divergent, so (9) is satisfied with a vengeance. In other words, even when dealing with high ω_0 values, corresponding to the situation in quantum optics, problems arise in both models. These are perhaps the models of most interest but it can be shown that similar conclusions hold for other models often found in the literature. Thus, for all models of physical interest, the left-hand side of (8) is actually divergent so that the spectrum has no lower bond. This implies that, no matter what state the system is in, energy can always be extracted from it by having it go into a lower-energy state. Hence, (the Kelvin–Planck formulation [9]) of the second law of thermodynamics is violated. We conclude that the RWA model has a serious defect.

We wish to emphasize that this defect is not confined to the RWA Hamiltonian. In particular, the defect occurs for a pair of coupled oscillators (where each sum in (1) has only a single term), for which a normal mode with negative frequency arises if the coupling constant is sufficiently large. As is well known, to avoid this problem one must choose a positive-definite Hamiltonian. This automatically ensures that the energy spectrum is bounded from below.

What is the nature of the difficulties arising from the use of H_{RWA}? The RWA is constructed to reproduce the first-order perturbation expression for the transition amplitude. However, nothing else is given correctly (see below), including electromagnetic energy shifts (Lamb shifts), mass renormalization and the power spectrum of the reservoir.

Is it possible to repair the RWA to obtain a positive-definite Hamiltonian so that the energy spectrum has a lower bound? Yes, but the problem is that there is an infinity of possibilities, i.e. the repair is not unique. For example, two possibilities that might come immediately to mind are

$$H_1 = \hbar\omega_0 a^\dagger a + \sum_j \hbar\omega_j \left(b_j + \frac{\lambda_j^*}{\hbar\omega_j} a \right)^\dagger \left(b_j + \frac{\lambda_j^*}{\hbar\omega_j} a \right)$$

$$= H_{RWA} + \sum_j \frac{|\lambda_j|^2}{\hbar\omega_j} a^\dagger a , \tag{14}$$

and

$$H_2 = \hbar\omega_0 \left\{ a + \sum_j \frac{\lambda_j}{\hbar\omega_0} b_j \right\}^+ \left\{ a + \sum_j \frac{\lambda_j}{\hbar\omega_0} b_j \right\} + \sum_j \hbar\omega_j b_j^+ b_j$$

$$= H_{RWA} + \frac{1}{\hbar\omega_0} \left(\sum_j \lambda_j b_j \right)^+ \left(\sum_j \lambda_j b_j \right) . \tag{15}$$

Since each term in both H_1 and H_2 is positive definite, it follows that the lower bound on the expectation of both Hamiltonians is zero. However, in order to resolve the problem of non-uniqueness, we are forced to the conclusion that we need to return to the original physical Hamiltonian of which H_{RWA} is a truncated form. This is in fact the IO model discussed above.

In particular, the H of NRQED (which, as already mentioned, is a particular case of the IO model) contains $a^+ b_j^+$ and ab_j terms, plus self-interaction terms, in addition to the RWA terms [8]. Thus, it might be thought that it would be even harder to solve than the RWA model, which in fact is generally solved only under restrictive assumptions. However, when expressed in terms of coordinate and momentum operators (instead of creation and annihilation operators), it turns out that the unitarily transformed H of NRQED has a remarkably simple form (see eq. (4.1) of Ref. [8] and the discussion about unitary transformation in Section V of this reference) which enabled an exact solution to be obtained [8]. Based on this solution, we have recently carried out a detailed analysis of the consequences vis-à-vis the corresponding results obtained from the RWA model. In particular, we obtained the master equation for a charged oscillator interacting with the electromagnetic field and found that its form differs from that generally obtained using the RWA, in that there is no electromagnetic (Lamb) shift for the oscillator and that an explicit expression is given for the decay rate [10]. Furthermore, it can be verified that the spectrum of the reservoir is the Planck spectrum [11], in contrast to that given by the RWA model [1–6]. The IO model has also been used to prove that, in contrast to existing expositions in the literature (which are mainly based on use of the RWA model), there is in fact no quantum regression theorem [12].

We conclude that use of the RWA should be confined only to the calculation of transition amplitudes for first-order absorption and emission, where the non-RWA

terms do not contribute. For the calculation of other physical quantities, such as energy shifts and power spectrum, the use of the RWA leads to results at variance with these obtained (more easily in fact) from an exact more physical model [3].

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