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Numerical analysis of Dicke's model for one atom

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Abstract. Using the Green function technique, we calculate the transition probability amplitude for one atom interacting with a one-mode electromagnetic field, without assuming the rotating-wave approximation (RWA). The effects of the RWA are studied in the time and frequency domains. In the time domain, the periodicity of the typical RWA results is broken; in the frequency domain, the Bloch–Siegert shift is obtained.

1. Introduction

The problem of one atom interacting with an electromagnetic field was solved a long time ago (Jaynes and Cummings 1963, Allen and Eberly 1975) using the rotating-wave approximation (RWA). This approximation leads directly to a periodic solution for the probability amplitude of emission of a photon. There is a periodic transfer of energy from the atom to the field, and vice versa.

In the present work, the effects of the counter-rotating terms in the Hamiltonian (Ramírez and Orszag 1982) are considered, with the following results:

(i) The periodic behaviour, typical of the RWA, is destroyed.

(ii) A frequency shift is obtained. This shift is the well known Bloch–Siegert shift.

Analytical expressions for the Bloch–Siegert shift have been obtained by several authors (Shirley 1965, Swain 1973a, 1974, Hannaford *et al* 1973, Stenholm 1973, Ahamad and Bullough 1974, Cohen-Tannoudji *et al* 1973).

Swain (1973b) calculated the eigensolutions of Dicke's Hamiltonian, arriving at continued-fraction expressions for the eigenstates and eigenvalues. From there, he was able to obtain the time behaviour of the system. Walls (1972), using the resolvant technique, found the second-order perturbation approximation for the emission probability and the shift. Here, eigenvalue and eigenfunction calculations are avoided. Instead, the direct application of the Green function technique allow us to determine, in a compact and straightforward calculation, the time behaviour and Bloch–Siegert shift of Dicke's model, to any order, and compare these results with the RWA results.

At the end, a short comparison of this work with that of Shirley (1965) and Swain (1973a) is given.

2. The method

Consider the Hamiltonian of an atom interacting via an electromagnetic field:

$$H = \omega a^+ + \omega_0 S_z + K(a + a^+)(S^+ + S^-) = H_0 + K(a + a^+)(S^+ + S^-). \tag{1}$$

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This Hamiltonian operates on a Hilbert space $\{|\sigma\rangle \otimes |n\rangle\}$, where $|\sigma\rangle = |\pm\frac{1}{2}\rangle$ represents the atomic state vector. The atomic Hamiltonian is $\omega_0 S_z$, obeying the equation

$$\omega_0 S_z |\pm\tfrac{1}{2}\rangle = \pm\tfrac{1}{2}\omega_0 |\pm\tfrac{1}{2}\rangle. \tag{2}$$

The state $|n\rangle = [(a^+)^n/(n!)^{1/2}]|0\rangle$ represents the state of n photons. Let $|\sigma, n\rangle = |\sigma\rangle \otimes |n\rangle$ be the eigenstates of H_0, and $|\nu\rangle$ the eigenstates of H, with eigenvalue Ω_ν. Then we can expand $|\nu\rangle$ as a linear superposition of $|\sigma, n\rangle$.

The time evolution operator can be written as

$$\exp(-itH) = \sum_\nu \exp(-i\Omega_\nu t)|\nu\rangle\langle\nu|. \tag{3}$$

Let $|i\rangle$ and $|f\rangle$ be two eigenstates of the system. The probability amplitude of the transition $|i\rangle \to |f\rangle$ is given by

$$a_{fi}(t) = \langle f|\exp(-itH)|i\rangle = \sum \exp(-i\Omega_\nu t)\langle f|\nu\rangle\langle\nu|i\rangle, \tag{4}$$

and its Fourier transform is

$$a_{fi}(\Omega) = \int_{-\infty}^{0} dt\, a_{fi}(t) \exp[it(\Omega - \Omega_\nu - i\eta)] + \int_0^\infty dt\, a_{fi}(t) \exp[it(\Omega - \Omega_\nu + i\eta)], \tag{5}$$

where η is a small parameter to ensure the convergence of $a_{fi}(\Omega)$. The limit $\eta \to 0^+$ will be taken later on.

Defining the Green function as

$$G(\Omega) = \frac{1}{\Omega - H} = \sum_\nu \frac{|\nu\rangle\langle\nu|}{\Omega - \Omega_\nu}, \tag{6}$$

we can write

$$a_{fi}(\Omega) = i^{-1}[G_{fi}(\Omega - i\eta) - G_{fi}(\Omega + i\eta)], \tag{7}$$

where $G_{fi} = \langle f|G|i\rangle$.

We can now write the probability amplitude $a_{fi}(t)$ in terms of the Green function (Zubarev 1960):

$$\begin{aligned} a_{fi}(t) &= \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\Omega \exp(-it\Omega)[G_{fi}(\Omega - i\eta) - G_{fi}(\Omega + i\eta)] \\ &= \frac{1}{2\pi i}\oint d\Omega \exp(-it\Omega) G_{fi}(\Omega), \end{aligned} \tag{8}$$

where the closed integral is taken in the positive sense and enclosing the real axis, as shown in figure 1. Obviously, this integral is zero everywhere except at the poles of $G(\Omega)$. These poles correspond to the eigenstates of H (equation (6)).

We can write $a_{fi}(t)$ in terms of the residues of G_{fi} as

$$a_{fi}(t) = \sum_\nu \exp(-it\Omega_\nu)\, \mathrm{res}[G_{fi}(\Omega)]_{\Omega_\nu}. \tag{9}$$

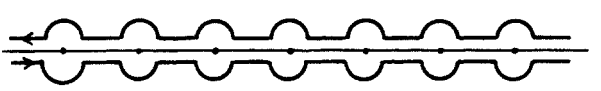

Figure 1. Path taken for the integral appearing in equation (8). The dots correspond to the poles of $G(\omega_0)$.

3. Calculation of the Green function

Consider the identity (Roessler *et al* 1980)

$$(\Omega - H)G(\Omega) = 1. \tag{10}$$

Taking the matrix elements of equation (10), between the states $\langle \sigma n|$ and $|\sigma' n'\rangle$, inserting $\Sigma_\tau |\tau m\rangle\langle \tau m| = 1$ and using the matrix elements of our Hamiltonian,

$$H_{\sigma n,\tau m} = \delta_{\sigma\tau}\,\delta_{nm}(\omega n + \sigma\omega_0) + K\,\delta_{\sigma,-\tau}(\sqrt{m}\,\delta_{n,m-1} + \sqrt{m+1}\,\delta_{n,m+1}), \tag{11}$$

we can write equation (10) in the form

$$(\Omega - \omega\cdot n - \sigma\omega_0)G_{\sigma n,\sigma' n'}(\Omega) - K[\sqrt{n+1}\,G_{(-\sigma,n+1),(\sigma',n')}(\Omega) + \sqrt{n}\,G_{(-\sigma,n-1),(\sigma',n')}(\Omega)] = \delta_{\sigma\sigma'},\,\delta_{nn'}. \tag{12}$$

Define

$$Q_m^\sigma = \Omega - m\omega - \sigma\omega_0 \tag{13}$$

and

$$X_m^\sigma = K\sqrt{m+1}\,G_{(-\sigma m+1)(\sigma' n')}/G_{(\sigma m)(\sigma' n')}. \tag{14}$$

With the definitions (13) and (14), equation (12) can be now written as

$$Q_n^\sigma - X_n^\sigma - K^2 n/X_{n-1}^{-\sigma} = \delta_{\sigma\sigma'}\,\delta_{nn'}/G_{\sigma n,\sigma n}. \tag{15}$$

Taking $(\sigma' n') = (\sigma n)$, we have

$$G_{(\sigma n)(\sigma n)}(\Omega) = 1/(Q_n^\sigma - X_n^\sigma - K^2 n/X_{n-1}^{-\sigma}). \tag{16}$$

From equation (15) we readily obtain

$$X_m^\sigma = Q_m^\sigma - K^2 m/X_{m-1}^{-\sigma} \qquad (m < n) \tag{17}$$

or

$$X_m^\sigma = K^2(m+1)/(Q_{m+1}^{-\sigma} - X_{m+1}^{-\sigma}) \qquad (m > n). \tag{18}$$

Iterating equations (17) and (18), we obtain equations (19) and (20) respectively:

$$\frac{K^2 n}{X_{n-1}^{-\sigma}} = \cfrac{K^2 n}{Q_{n-1}^{-\sigma} - \cfrac{K^2(n-1)}{Q_{n-2}^{\sigma} - \cfrac{K^2(n-2)}{Q_{n-3}^{-\sigma} - \cfrac{K^2(n-3)}{Q_{n-4}^{\sigma} - \cdots}}}} \tag{19}$$

$$X_n^\sigma = \cfrac{K^2(n+1)}{Q_{n+1}^{-\sigma} - \cfrac{K^2(n+2)}{Q_{n+2}^{\sigma} - \cfrac{K^2(n+3)}{Q_{n+3}^{-\sigma} - \cfrac{K^2(n+4)}{Q_{n+4}^{\sigma} - \cdots}}}}. \tag{20}$$

Introducing equations (19) and (20) into (16), we get an explicit expression for $G_{\sigma n,\sigma n}$.

Making use of equation (14), once $G_{\sigma n,\sigma n}$ is known, we can calculate $G_{(-\sigma n+1)(\sigma n)}$, $G_{(\sigma n+2)(\sigma n)}$, ... For example

$$G_{(-\sigma n+1)(\sigma n)} = (X_n^\sigma/K\sqrt{n+1})G_{(\sigma n)(\sigma n)}. \tag{21}$$

Since X_n^σ and $G_{(\sigma n)(\sigma n)}$ are known, equation (21) allow us to calculate $G_{(-\sigma n+1)(\sigma n)}$.

4. Approximate results in the $(K\sqrt{n}/\omega_0) \to 0$ limit

We will study the transition $|i\rangle = |\frac{1}{2}, n\rangle \to |f\rangle = |-\frac{1}{2}, n+1\rangle$.

In the case $K = 0$, the poles of G correspond to

$$\Omega_{l\pm} = \omega(n + 2l + \tfrac{1}{2}) \pm \Delta, \qquad l = 0, \pm 1, \pm 2 \ldots, \tag{22}$$

where $\Delta = (\omega_0 - \omega)/2$.

If the interaction is turned on ($K \neq 0$), the poles will still come in pairs, but will be shifted with respect to the undisturbed value (equation (22)).

With the use of equations (16), (19), (20) and (21), we can estimate the location of the poles up to K^2. The lth pole is located approximately at

$$\Omega_{l\pm} \approx \frac{-2\omega K^2 \pm R_{n+2l}\theta^2}{\theta^2 + 2K^2(n+2l+1)} + \omega(n + 2l + \tfrac{1}{2}), \tag{23}$$

where

$$\theta = 2\omega + \Delta,$$

$$R_n = \left[K^2(n+1) + \left(\Delta + \frac{K^2(n+1)}{\theta}\right)^2 + \frac{4\omega^2 K^4}{\theta^4} + \frac{2K^2\Delta^2(n+1)}{\theta^2} + \frac{K^4}{\theta^2}[2(n+1)^2 - 1]\right]^{1/2}. \tag{24}$$

The residues for $l = 0$ and $l = 1$ are given approximately by

$$R_s(\Omega_{0\pm}) \approx \frac{\pm K\sqrt{n+1}}{2R_n}, \qquad R_s(\Omega_{1\pm}) \approx \frac{K^3\sqrt{n+1}(n+2)}{2(2\omega+\Delta)^2(2\omega-\Delta)}\left(1 \pm \frac{\Delta}{R_{n+2}}\right). \tag{25}$$

A simple quantum mechanical argument shows that in general

$$R_s(\Omega_{l\pm}) \sim (K\sqrt{n+1}/\omega_0)^{4l-1}. \tag{26}$$

5. Numerical results

Equation (9) can be rewritten in the form

$$a_{fi}(t) = -\sum_{l=[n/2]}^{\infty} \exp(-i\Omega_l t)(C_l \cos \varepsilon_l t + iS_l \sin \varepsilon_l t), \tag{27}$$

where $[n/2]$ is the integer part of $n/2$, $f = (-, n+1)$, $i = (+, n)$ and

$$\begin{aligned} &\varepsilon_l = \tfrac{1}{2}(\Omega_{l+} - \Omega_{l-}), \qquad &&\Omega_l = \tfrac{1}{2}(\Omega_{l+} + \Omega_l), \\ &S_l = R_s(\Omega_{l+}) - R_s(\Omega_{l-}), \qquad &&C_l = -R_s(\Omega_{l+}) - R_s(\Omega_{l-}). \end{aligned} \tag{28}$$

The most important contribution to the summation given in equation (27) is the term $-iS_0 \sin(\varepsilon_0 t)$; basically, up to a correction of the order of $K^2(n+1)/\omega_0^2$, $|S_0|^2$ represents the maximum value of the transition probability $P(t)$.

If we now take the limit $n \to \infty$, $K\sqrt{n+1} \to 0$, then

$$S_l \approx S_{-l} \qquad C_l \approx -C_{-l} \qquad \Omega_l \approx (n + \tfrac{1}{2} + 2l)\omega \qquad \varepsilon_l \approx \varepsilon_0 \tag{29}$$

and $a_{fi}(t)$ can be written approximately as

$$a_{fi}(t) \approx -i\left(S_0 \sin \varepsilon_0 t + 2\sum_{l=1}^{\infty} (S_l \cos 2l\omega t \sin \varepsilon_0 t - C_l \sin 2l\omega t \cos \varepsilon_0 t)\right). \tag{30}$$

We have computed $P(t) = |a_{fi}(t)|^2$, $\varepsilon_0(\omega/\omega_0)$ and $S_0(\omega/\omega_0)$ for $K^2(n+1)/\omega_0^2 = 0.01$ and 0.1.

In figure 2(*a*) we show ε_0 as a function of ω/ω_0 for $K^2(n+1)/\omega_0^2 = 0.01$, and in figure 2(*b*) we plot S_0 as a function of ω/ω_0 for the same coupling constant. These graphs are practically unchanged when n varies from zero to ∞, keeping $K^2(n+1)/\omega_0^2$ fixed. When the curves are compared with the results using the RWA, the deviation from the RWA is of the order of $K^2(n+1)/\omega_0^2 \sim 0.01$.

Figure 3 shows ε_0 and S_0 versus ω/ω_0 for $K^2(n+1)/\omega_0^2 = 0.1$. The dependence on n is again small (n taking the values 0 and ∞ for fixed $K\sqrt{n}/\omega_0$), but now the deviation from the RWA is appreciable, of the order of $K^2(n+1)/\omega_0^2 \sim 0.1$. Notice also that the

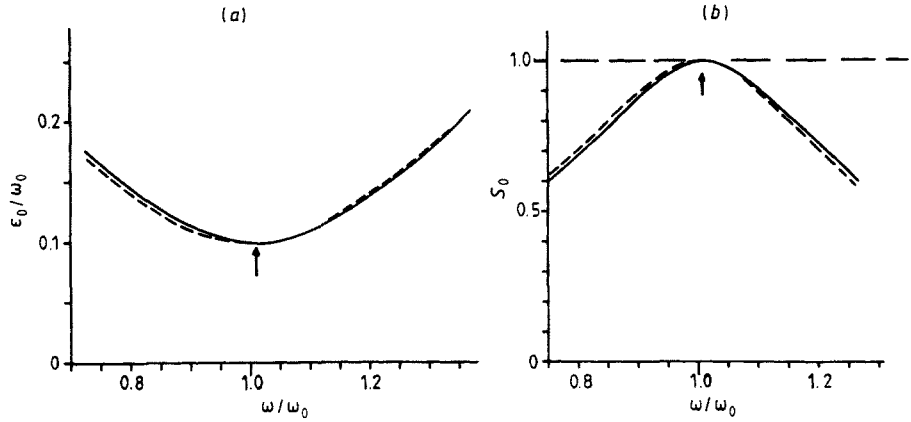

Figure 2. (*a*) ε_0/ω_0 and (*b*) S_0 versus ω/ω_0 for $K^2(n+1)/\omega_0^2 = 0.01$. The broken curves correspond to the RWA. The full curves are the exact curves for both $n = 0$ and $n = 10^4$ (their difference is of the order of 10^{-4}).

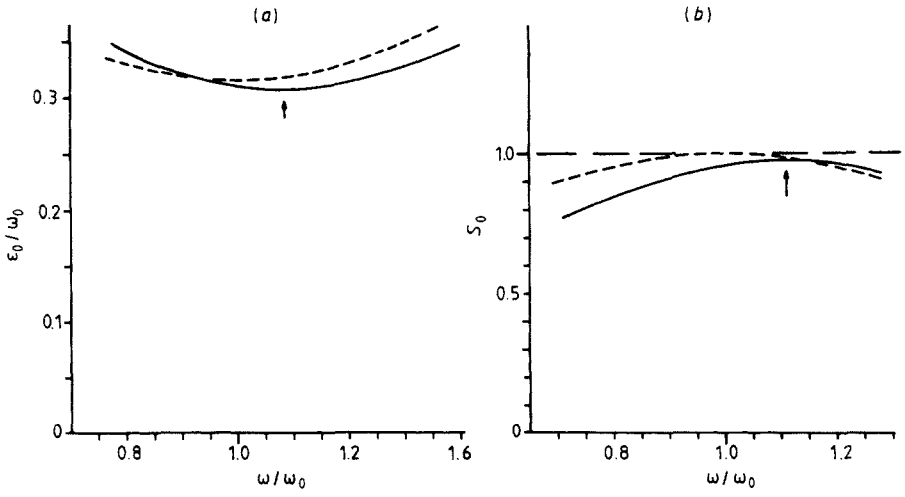

Figure 3. (*a*) ε_0/ω_0 and (*b*) S_0 versus ω/ω_0 for $K^2(n+1)/\omega_0^2 = 0.1$. The full curves are the exact curves, and the broken curves correspond to the RWA. Notice that the maximum S_0 is at $\omega/\omega_0 = 1.11$, while the minimum ε_0/ω_0 is at $\omega/\omega_0 = 1.084$ (see the arrows).

Table 1. Values of the amplitude and frequency for the first two harmonics, for various values of n, detuning and coupling constant.

n	$K^2(n+1)$	ω	Ω_0	ε_0	S_0	C_0	Ω_1	ε_1	S_1	C_1
0	0.01	0.8	0.3944	0.1452	0.6841	4.11×10^{-4}	1.9984	0.207	1.0×10^{-4}	-4.1×10^{-4}
10^4	0.01	0.8	0	0.14518	0.6843	0	1.6	0.1452	1.148×10^{-4}	-1.946×10^{-4}
0	0.1	0.8	0.3388	0.3412	0.8431	0.0222	1.9159	0.5342	−0.0129	−0.0218
10^4	0.1	0.8	0	0.3422	0.8553	0	1.6	0.3423	-1.428×10^{-3}	-7.648×10^{-3}
0	0.1	1.11	0.5055	0.3086	0.9740	0.0080	2.7200	0.5133	−0.0042	−0.00803
10^4	0.1	1.107	0	0.3091	0.9759	0	2.214	0.3091	−0.0015	−0.00351
0	0.1	1	0.4471	0.3113	0.9559	0.1075	2.4390	0.5192	-5.473×10^{-3}	−0.1070
10^6	0.1	1	0.5	0.3119	0.9596	0	2.5	0.3139	-1.397×10^{-3}	-4.437×10^{-3}

maximum of S_0 is shifted with respect to ω_0. This maximum is located at $\omega/\omega_0 = 1.11$ for $n = 0$ and at $\omega/\omega_0 = 1.107$ for $n = \infty$. This is the Bloch–Siegert shift.

Shirley's (1965) semiclassical calculation of the shift gives $\omega/\omega_0 \approx 1.1025$, and Swain's (1973a) result gives $\omega/\omega_0 = 1.1137$ for $n \to \infty$.

Notice also that the maximum value of S_0 does not coincide with the minimum of the frequency of the first harmonic. This minimum corresponds to $\omega/\omega_0 = 1.084$.

Some numerical values of the amplitudes and frequencies of the various harmonics have been tabulated (table 1). For this table the value $\omega_0 = 1$ was taken.

In figure 4(*a*) we have plotted $P(t) = |a_{fi}(t)|^2$ against $\omega_0 t$ for $K^2(n+1)/\omega_0^2 = 0.1$ and $\omega/\omega_0 = 0.8$. There is a noticeable difference between the RWA and the two exact curves for $n = 0$ and $n = \infty$. The small difference between these last two curves shows that there is only a weak dependence on n, for $K^2(n+1)/\omega_0^2$ fixed.

In figure 4(*b*) we again show $P(t)$ against $\omega_0 t$ for $K^2(n+1)/\omega_0^2 = 0.1$, but with the value of ω/ω_0 that gives the maximum S_0. In this case it corresponds to $\omega/\omega_0 = 1.1$ for $n = 10^4$ and $\omega/\omega_0 = 1.11$ for $n = 0$. These curves are compared with the one using the RWA for $\omega/\omega_0 = 1$.

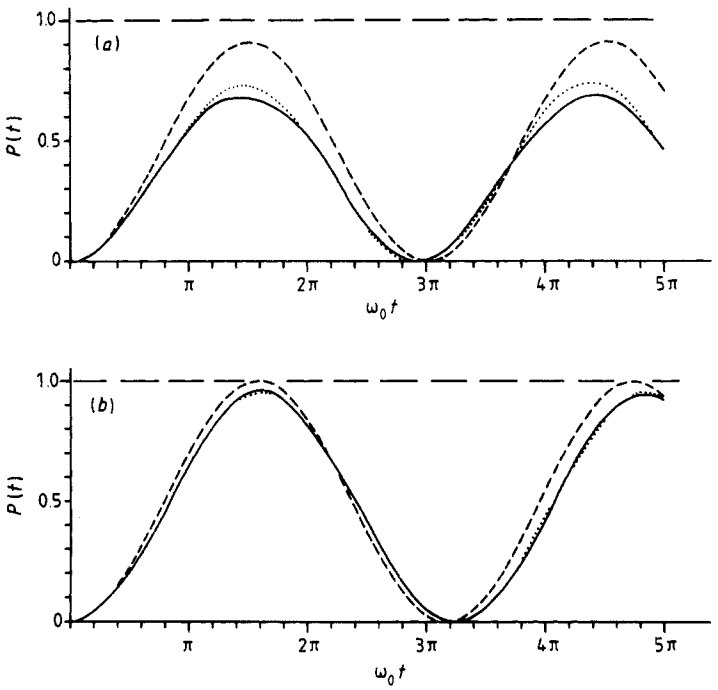

Figure 4. (*a*) $P(t)$ versus $\omega_0 t$ for $K^2(n+1)/\omega_0^2 = 0.1$ and a detuning $\omega/\omega_0 = 0.8$. The broken curve corresponds to the RWA, the dotted curve is the exact curve for $n = \infty$, and the full curve is the exact curve for $n = 0$. (*b*) $P(t)$ versus $\omega_0 t$ for $K^2(n+1)/\omega_0^2 = 0.1$ and $\omega/\omega_0 = \{\text{maximum } S_0\}$. The broken curve corresponds to the RWA and $\omega/\omega_0 = 1$, the full curve to the exact curve for $n = 0$ and $\omega/\omega_0 = 1.11$, and the dotted curve to the exact curve for $n = 10^4$ and $\omega/\omega_0 = 1.1$.

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