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LETTER TO THE EDITOR

## On the quantum and semi-classical theories of a two-level atom interacting with a single-field mode

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**Abstract.** Formally exact solutions to the quantum and semi-classical models of a single atom interacting with a single-field mode in the dipole approximation are compared. It is shown that the quantum results tend to the semi-classical ones in the limit  $\bar{n} \rightarrow \infty$ , in disagreement with the results of Chang and Stehle.

In a recent publication, Chang and Stehle (1971) have performed a fully QED calculation on a system consisting of a single two-level atom interacting with a single monochromatic field mode in the dipole approximation and have compared their results with those obtained in the semi-classical approximation. They are led to the conclusion that whilst the QED and semi-classical theories agree at low intensities of the electromagnetic field, considerable differences occur at high intensities. (One particular property singled out for discussion was the Bloch–Siegert shift.) This could be an extremely important result, for it has long been assumed that the semi-classical and quantum theories should converge when the mean number of photons (in the quantum case) is very large—precisely the opposite situation to that found by Chang and Stehle.

The findings of Chang and Stehle have been challenged recently by several authors (Stenholm 1973a, b, Pegg 1973, Hannaford *et al* 1973, Cohen-Tannoudji *et al* 1973), who have all made fully quantum-mechanical calculations of the Bloch–Siegert shift (by different methods to those used by Chang and Stehle) and found results which differ from the latter's and which agree with the semi-classical results in the large photon number limit. However, the calculations of all these authors involve approximations at some stage, so that the problem cannot be considered completely resolved, and furthermore that rebuttals of the work of Chang and Stehle all involve calculations of the Bloch–Siegert shift only, and it is clearly desirable to investigate more generally the conditions under which the quantum and semi-classical theories could be expected to give essentially the same results.

We have previously published formally exact solutions to the problem of a single atom interacting with a single-field mode in the quantum case (Swain 1973a, b, to be referred to as I) and in the semi-classical case (Swain 1973c, to be referred to as II). In this letter we compare these exact solutions and show how the semi-classical theory results from the quantum theory when the number of photons involved in the quantum case is very large. The results are presented in a manner which makes the correspondence between the semi-classical and quantum theories most transparent.

We wish to solve the time-dependent Schrödinger equation

$$i \frac{d|\psi\rangle}{dt} = H|\psi\rangle \quad (1)$$

for the situations in which  $H$  describes the interaction between a single atom and a single mode in the dipole approximation for (a) the semi-classical case, and (b) the fully quantized case. For the semi-classical case we use the Schrödinger picture, so that

$$H_{sc} = E_\alpha |\alpha\rangle \langle \alpha| + E_\beta |\beta\rangle \langle \beta| + (V e^{-i\omega t} + V^* e^{i\omega t})(|\alpha\rangle \langle \beta| + |\beta\rangle \langle \alpha|) \quad (2)$$

whereas for the fully quantized case it is more convenient to use a partial interaction picture to eliminate the free-field contribution to the hamiltonian. That is, we take

$$|\psi_q\rangle = \exp[-i(a^\dagger a + \frac{1}{2})\omega t] |\phi_q\rangle \quad (3)$$

where  $|\phi_q\rangle$  satisfies an equation similar to (1) but with  $H$  now given by

$$H_q = E_\alpha |\alpha\rangle \langle \alpha| + E_\beta |\beta\rangle \langle \beta| + (gae^{-i\omega t} + g^* a e^{i\omega t})(|\alpha\rangle \langle \beta| + |\beta\rangle \langle \alpha|). \quad (4)$$

The hamiltonians (3) and (4) are now clearly related, and we would expect some correspondence between  $|\psi_{sc}\rangle$  and  $|\phi_q\rangle$ . (In equations (2)–(4),  $E_\alpha$  and  $E_\beta$  are the energy levels corresponding to the isolated atom's eigenstates  $|\alpha\rangle$  and  $|\beta\rangle$  respectively,  $V$  is a constant defining the amplitude of the monochromatic classical field whose frequency is  $\omega$ ,  $a$  and  $a^\dagger$  are the usual annihilation and creation operators for the quantized field, and  $g$  is a numerical coupling constant.)

We have shown elsewhere (I and II) that exact solutions of (1) with  $H$  given by (2) and (4) are, respectively, of the form

$$|\psi_{sc}(t)\rangle \equiv |q_{\gamma,j}(t)\rangle = \exp(-iq_{\gamma,j}t) \sum_{m=-\infty}^{\infty} [a_m(\gamma,j)|\alpha\rangle + b_m(\gamma,j)|\beta\rangle] e^{im\omega t} \quad (5)$$

and

$$|\phi_q(t)\rangle \equiv |d_{\gamma,k}(t)\rangle = \exp(-id_{\gamma,k}t) \sum_{n=0}^{\infty} [D_{\alpha,n}(\gamma,k)|\alpha\rangle + D_{\beta,n}(\gamma,k)|\beta\rangle] |n\rangle e^{in\omega t} \quad (6)$$

( $\gamma \equiv \alpha, \beta$ ;  $j$  and  $k$  are integers)

where the  $q$ ,  $a$  and  $b$  are constants defined explicitly in II, and the  $d$ , and  $D$  in I. (Actually in I we work in the Schrödinger picture and so find  $|\psi_q(t)\rangle$ ,  $|\phi_q(t)\rangle$  is obtained from it by application of (3)).

The wavefunctions (5) and (6) are of a similar form apart from the fact that the lower limits on the sums over  $n$  and  $m$  differ, and that the photon number eigenvector,  $n$ , appears in (6). The latter difference can be removed using a device due to Shirley (1965). He has shown that the time-dependent Schrödinger equation (1) with  $H$  given by (2) is completely equivalent to the time-independent Schrödinger equation

$$H_F |q(0)\rangle = q |q(0)\rangle \quad (7)$$

where  $H_F$  is the Floquet hamiltonian defined by equation (10) of Shirley's paper. However we find it more convenient to write out  $H_F$  as

$$H_F = E_\alpha |\alpha\rangle \langle \alpha| + E_\beta |\beta\rangle \langle \beta| + \sum_{m=-\infty}^{\infty} |m\rangle m \omega \langle m| + \sum_{m=-\infty}^{\infty} (V |m\rangle \langle m+1| + V^* |m+1\rangle \langle m|)(|\alpha\rangle \langle \beta| + |\beta\rangle \langle \alpha|) \quad (8)$$

where we have introduced, following Shirley, a set of states somewhat similar to the photon number eigenstates but capable of taking negative integer as well as positive integer values. These states merely denote Fourier components, but it is interesting

to observe how states analogous to the photon occupation states occur naturally even in the semi-classical theory. It is also worthwhile pointing out that the quantum hamiltonian may be written in the Schrödinger picture as

$$H = E_\alpha |\alpha\rangle \langle \alpha| + E_\beta |\beta\rangle \langle \beta| + \sum_{n=0}^{\infty} |n\rangle n\omega \langle n| + \sum_{n=0}^{\infty} (n+1)^{1/2} (g|n\rangle \langle n+1| + g^*|n+1\rangle \langle n|) (|\alpha\rangle \langle \beta| + |\beta\rangle \langle \alpha|). \quad (9)$$

The formal similarity of (8) and (9) is obvious.

A solution of (7) with (8) is

$$|q_{\gamma,j}(0)\rangle = \sum_{m=-\infty}^{\infty} [a_m(\gamma, j)|\alpha\rangle + b_m(\gamma, j)|\beta\rangle] |m\rangle \quad (10)$$

where the  $a_m$  and  $b_m$  are the same quantities which appear in (5). (We note that a solution of (7) with  $H_F$  given by (9) is exactly equation (6) with the  $\exp[i(-d+n\omega)t]$  factor omitted.) Hence if we introduce the Fourier component representation we should write (5) as

$$|q_{\gamma,j}(t)\rangle = \exp(-iq_{\gamma,j}t) \sum_{m=-\infty}^{\infty} [a_m(\gamma, j)|\alpha\rangle + b_m(\gamma, j)|\beta\rangle] |m\rangle \exp(im\omega t) \quad (11)$$

(6) and (11) differ in form only in the lower limits of the sums.

It is now appropriate to take the semi-classical limit of (6). Let  $N$  be a very large positive number, and set

$$n = N + \nu, \quad k = N + \kappa, \quad N \gg \nu, \kappa \quad (12)$$

in (6), which then becomes

$$|d_{\gamma, N+\kappa}(t)\rangle = \exp[-i(d_{\gamma, N+\kappa} - N\omega)t] \sum_{\nu=-N}^{\infty} [D_{\alpha, N+\nu}(\gamma, N+\kappa)|\alpha\rangle + D_{\beta, N+\nu}(\gamma, N+\kappa)|\beta\rangle] |N+\nu\rangle \exp(i\nu\omega t). \quad (13)$$

We now compare (13) with (11). In I and II we have shown that the properties of both types of system are determined by continued fractions  $\lambda$ ,  $\mu$ ,  $l$  and  $m$  which are defined differently in the quantum and semi-classical cases. From the definitions given in I and II one may easily show that

$$c_{N+\nu}^q(\gamma, N+\kappa) = c_{\nu}^{sc}(\gamma, \kappa) + O\left(\frac{1}{N}\right) \quad (14)$$

where  $c = \lambda, \mu, l$  or  $m$ , and  $\nu, \kappa \ll N$ . Having established this, it easily follows that

$$d_{\gamma, N+\kappa} - N\omega = q_{\gamma, \kappa} + O\left(\frac{1}{N}\right) \quad (15)$$

$$D_{\alpha, N+\nu}(\gamma, N+\kappa) = a_{\nu}(\gamma, \kappa) + O\left(\frac{1}{N}\right) \quad (16)$$

$$D_{\beta, N+\nu}(\gamma, N+\kappa) = b_{\nu}(\gamma, \kappa) + O\left(\frac{1}{N}\right). \quad (17)$$

For example,  $d_{\alpha, n}$  is defined by (21) of I. Hence  $d_{\alpha, N+\kappa} - N\omega$  satisfies

$$(d_{\alpha, N+\kappa} - N\omega) - E_{\alpha} - \kappa\omega - \frac{|g|^2 N [1 + (\nu/N)]}{m_{N+\nu-1}^q(\alpha, N+\kappa)} - \frac{|g|^2 N \{1 + [(\nu+1)/N]\}}{\mu_{N+\nu-1}^q(\alpha, N+\kappa)} = 0$$

whereas from II,  $q_{\alpha, \kappa}$  satisfies

$$q_{\alpha, \kappa} - E_{\alpha} - \kappa\omega - \frac{|V|^2}{m_{\kappa-1}^{sc}(\alpha, \kappa)} - \frac{|V|^2}{\mu_{\kappa+1}^{sc}(\alpha, \kappa)} = 0.$$

Using (14), (15) clearly follows if we make the correspondence

$$|g|^2 N \equiv |V|^2. \quad (18)$$

Equation (18) gives the connection between the quantum and classical field amplitudes, and  $N$  may clearly be interpreted as the mean number of photons present in the quantum situation. It is appropriate to point out here that in the quantum case one can deal with situations in which there may be a statistical distribution for the number of photons, whereas in the semi-classical case the field intensity is always precisely defined. The correspondence, (18) is therefore only valid if  $\delta N \ll N$ , where  $\delta N$  is the standard deviation of the photon distribution.

We have therefore shown that in the limit,  $N \rightarrow \infty$ , the quantum eigenvalue  $d$  tends to the corresponding semi-classical eigenvalue  $q$ , and the quantum eigenvector  $|d\rangle$  tends to the corresponding semi-classical eigenvector  $|q\rangle$ . It is apparent that if the eigenvectors and eigenvalues of two models are the same, then the properties of the two models must be identical.

We stress that the condition (12) must always be satisfied. If we are asking questions about the system which involve processes in which the number of photons present changes by a significant fraction of  $N$ , then (12) is not satisfied and our analysis is inappropriate. However, it is difficult to imagine such a situation arising in practice.

With the provisos already stated, we have therefore shown that the semi-classical theory results from the quantized field theory when the mean number of photons is allowed to approach infinity. The order of magnitude of the error involved is no greater than  $1/N$ . Our conclusions are in accordance with accepted practice and contrary to those of Chang and Stehle.

Finally we point out, as the other authors here quoted have done, that the semi-classical theory leads to predictions of the Bloch-Siegert shift which are in essential agreement with theory, in contrast with the theory of Chang and Stehle for two-level systems. In fact, it can be shown, using the semi-classical theory (II), that the Bloch-Siegert shift is given by the formula

$$\frac{\omega_0}{\omega} = \frac{\omega^2 - \frac{5}{2}|V|^2}{\omega^2 - \frac{3}{2}|V|^2}. \quad (20)$$

This remarkably simple formula is in good agreement with the experimental results of Morand and Theobald (1969) over the entire range of field strengths.

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