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A comparison of quantum and semi-classical theories of the interaction between a two-level atom and the radiation field

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Abstract. The interaction of a two-level atom with a single mode of the radiation field is considered both in a fully quantized and a semi-classical theory. With only the dipole and rotating-wave approximations the Liouville equations are solved to give the exact behaviour of the diagonal elements of the density operator and of their semi-classical analogue. The results suggest experimentally verifiable differences between the two theories.

1. Introduction

We shall discuss here a two-level atom interacting with the electromagnetic field in a lossless cavity, particularly with a view to comparing the quantum and semi-classical results. Numerous authors, for example Crisp and Jaynes (1969), Scully and Sargent (1972), Swain (1972a, b; 1973a, b), have discussed the semi-classical theory in general and this problem in particular. Jaynes and Cummings (1963), in one of the early papers on the theory, have discussed the model we shall consider from a somewhat different point of view, and arrive at results that are consistent with ours.

Consider a single atom at rest in a lossless cavity one of whose modes has a frequency near one of the transition frequencies of the atom; we suppose that all other modes of the cavity have somehow been suppressed, so that it suffices to consider the interaction of that one mode with the pair of atomic states of interest. For completeness, and in order to clarify the notation, we shall briefly outline a derivation of the equations of motion; Fleck (1966), Louisell (1964, p 212 ff), and others give somewhat more detailed accounts.

If only one cavity mode, $\boldsymbol{u}(\boldsymbol{r})$ is excited, we may write the electric field as†

$$\boldsymbol{E}(\boldsymbol{r}, t) = (\tfrac{1}{2}\hbar\omega)^{1/2}\boldsymbol{u}(\boldsymbol{r})(a\,\mathrm{e}^{-\mathrm{i}\omega t} + a^{\dagger}\,\mathrm{e}^{\mathrm{i}\omega t})$$

where ω is the frequency of the cavity mode, and a is the usual normalized amplitude; in the interaction picture it is a constant. In the semi-classical theory a is a c number, while in the quantum theory it is, of course, an annihilation operator.

If the cavity is sufficiently well tuned to an atomic transition, only two of the atomic levels, $|1\rangle$ and $|2\rangle$, contribute. We will take

$$E_1 = 0, \qquad E_2 = \hbar\omega_0,$$

† We use Heaviside–Lorentz (ie, rationalized Gaussian) units, and have defined the normalized amplitudes to be 90° out of phase with the customary ones.

and shall denote the atomic transition operator by

$$b\,\mathrm{e}^{-\mathrm{i}\omega_0 t} = |1\rangle\langle 2|;$$

in the interaction picture b is also a constant.

The atom interacts with the field via a dipole moment. If the atom is at rest at the origin the interaction energy is

$$H' = -\boldsymbol{p}\,.\,\boldsymbol{E}(0,t) = \hbar g(b\,\mathrm{e}^{-\mathrm{i}\omega_0 t} + b^{\dagger}\,\mathrm{e}^{\mathrm{i}\omega_0 t})(a\,\mathrm{e}^{-\mathrm{i}\omega_0 t} + a^{\dagger}\,\mathrm{e}^{\mathrm{i}\omega_0 t}), \tag{1}$$

where $g = -e(\omega/2\hbar)^{1/2}\boldsymbol{u}(0)\,.\,\langle 2|\boldsymbol{r}|1\rangle$. Keeping only resonant terms†, we have

$$H_{\mathrm{I}} = \hbar g(a^{\dagger}b\,\mathrm{e}^{-\mathrm{i}\nu t} + ab^{\dagger}\,\mathrm{e}^{\mathrm{i}\nu t}), \tag{2}$$

where the frequency mismatch between cavity and atom is

$$\nu = \omega_0 - \omega.$$

In the interaction picture the density operator evolves according to

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H_{\mathrm{I}}, \rho(t)]. \tag{3}$$

Let us write

$$\rho(t) = \sum_{i,j=1}^{2} |i\rangle\rho_{ij}(t)\langle j|,$$

where the quantities

$$\rho_{ij}(t) = \langle i|\rho(t)|j\rangle \tag{4}$$

are density operators for the radiation field. The Liouville equation (3) can then be written as four coupled equations for the $\rho_{ij}(t)$. If we suppose that the atom is initially in a stationary state or mixture then $\rho_{12}(0) = 0$, and we can describe the behaviour of the diagonal terms by two coupled equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{11}(t) = g^2\int_0^t \mathrm{d}t'\,\{\exp[\mathrm{i}\nu(t-t')](a^{\dagger}\rho_{22}(t')a - \rho_{11}(t')a^{\dagger}a) + \exp[-\mathrm{i}\nu(t-t')](a^{\dagger}\rho_{22}(t')a - a^{\dagger}a\rho_{11}(t'))\}, \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{22}(t) = -g^2\int_0^t \mathrm{d}t'\,\{\exp[\mathrm{i}\nu(t-t')](aa^{\dagger}\rho_{22}(t') - a\rho_{11}(t')a^{\dagger}) + \exp[-\mathrm{i}\nu(t-t')](\rho_{22}(t')aa^{\dagger} - a\rho_{11}(t')a^{\dagger})\}. \tag{6}$$

Except for the approximations that went into equation (2), and the restriction that

$$\rho_{12}(0) = 0$$

these equations are exact.

† The non-resonant terms may be included as a perturbation, as in Jaynes and Cummings (1963), or in a formally exact treatment, as in Swain (1973a). However, it does not seem worthwhile to do so without including also the effects of other atomic levels—whose frequency mismatch is less than that of the anti-resonant terms.

2. The quantum-mechanical problem

Let us denote the joint probability of finding the atom in state j (=1, 2) and the field in a state with n photons by $p_j(n, t)$:

$$p_j(n, t) = \langle n|\rho_{jj}(t)|n\rangle. \tag{7}$$

From equations (5) and (6) we see that

$$\frac{\mathrm{d}}{\mathrm{d}t}p_1(n, t) = 2ng^2\int_0^t \mathrm{d}t' \cos \nu(t-t')(p_2(n-1, t')-p_1(n, t')), \tag{8}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}p_2(n-1, t) = -\frac{\mathrm{d}}{\mathrm{d}t}p_1(n, t). \tag{9}$$

These equations can readily be solved using Laplace transforms. The results can be written compactly in terms of a generating function as

$$\begin{aligned} G_1(y, t) &= \sum_{n=0}^{\infty} p_1(n, t)\,\mathrm{e}^{-ny} \\ &= \sum_{n=0}^{\infty} \frac{\mathrm{e}^{-ny}}{4g^2n+\nu^2}\{p_1(n, 0)[2g^2n+\nu^2+2g^2n\cos t(\nu^2+4g^2n)^{1/2}] \\ &\quad + p_2(n-1, 0)2g^2n[1-\cos t(\nu^2+4g^2n)^{1/2}]\}, \end{aligned} \tag{10}$$

$$\begin{aligned} G_2(y, t) &= \sum_{n=0}^{\infty} p_2(n, t)\,\mathrm{e}^{-ny} \\ &= \sum_{n=1}^{\infty} \frac{\mathrm{e}^{-(n-1)y}}{4g^2n+\nu^2}\{p_2(n-1, 0)[2g^2n-\nu^2+2g^2n\cos t(\nu^2+4g^2n)^{1/2}] \\ &\quad + p_1(n, 0)2g^2n[1-\cos t(\nu^2+4g^2n)^{1/2}]\}. \end{aligned} \tag{11}$$

The probabilities $p_1(n, t)$ and $p_2(n, t)$ can be read off directly from these expressions. For the atom, the probabilities for finding it in its ground and excited states are given by $G_1(0, t)$ and $G_2(0, t)$, respectively. For the field, the statistical properties at time t can be determined from $G_1(y, t)+G_2(y, t)$.

3. The semi-classical problem

For the semi-classical problem the field amplitudes a and $a^\dagger$ become c numbers; in order to emphasize the distinction between the two models we shall denote them by α and α^*. The quantities $\rho_{ij}(t)$ of equation (4) are, of course, also no longer operators, but distribution functions for α; we shall denote them by $\mathscr{P}_{ij}(\alpha, t)$. Corresponding, in a sense, to the photon-number distributions $p_j(n, t)$ of equation (7), we have here intensity distributions

$$\mathscr{p}_j(|\alpha|^2, t) = \tfrac{1}{2}\int_0^{2\pi} \mathscr{P}_{jj}(\alpha\,\mathrm{e}^{\mathrm{i}\phi}, t)\,\mathrm{d}\phi.$$

(Of course, since α is still normalized as the quantum-mechanical amplitude, the intensity of the field is not $|\alpha|^2$ but $\frac{1}{2}\hbar\omega|\boldsymbol{u}(\boldsymbol{r})|^2|\alpha|^2$.)

Since all quantities are c numbers, equations (5) and (6) immediately give

$$\frac{\mathrm{d}}{\mathrm{d}t}\wp_1(x,t) = 2xg^2\int_0^t \mathrm{d}t' \cos\nu(t-t')(\wp_2(x,t')-\wp_1(x,t')) \tag{12}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\wp_2(x,t) = -\frac{\mathrm{d}}{\mathrm{d}t}\wp_1(x,t). \tag{13}$$

The solutions may be obtained in exactly the same way as before.

In order to preserve the analogy to equations (10) and (11) we express the solutions in terms of generating functions

$$\begin{aligned} F_1(s,t) &= \int_0^\infty \mathrm{d}x\,\wp_1(x,t)\,\mathrm{e}^{-sx} \\ &= \int_0^\infty \mathrm{d}x\frac{\mathrm{e}^{-sx}}{4g^2+\nu^2}\{\wp_1(x,0)[2g^2x+\nu^2+2g^2x\cos t(\nu^2+4g^2x)^{1/2}] \\ &\quad +\wp_2(x,0)2g^2x[1-\cos t(\nu^2+4g^2x)^{1/2}]\}, \end{aligned} \tag{14}$$

$$\begin{aligned} F_2(s,t) &= \int_0^\infty \mathrm{d}x\,\wp_2(x,t)\,\mathrm{e}^{-sx} \\ &= \int_0^\infty \mathrm{d}x\frac{\mathrm{e}^{-sx}}{4g^2x+\nu^2}\{\wp_2(x,0)[2g^2x+\nu^2+2g^2x\cos t(\nu^2+4g^2x)^{1/2}] \\ &\quad +\wp_1(x,0)2g^2x[1-\cos t(\nu^2+4g^2x)^{1/2}]\}. \end{aligned} \tag{15}$$

The functions F_j do not strictly correspond to the G_j of the quantum-mechanical problem. Glauber's P representation (Glauber 1963) permits one to define an intensity distribution corresponding to $\wp_j(\alpha, t)$ for the quantum-mechanical problem. It then becomes clear that the quantum analogue of F is not

$$G_j(y,t) = \mathrm{tr}[\rho_{jj}(t)\exp(-ya^\dagger a)],$$

but

$$F'_j(s,t) = \mathrm{tr}\left(\rho_{jj}(t)\sum_{k=0}^{\infty}\frac{(-s)^k}{k!}(a^\dagger)^k a^k\right).$$

It can be shown (Louisell 1964, p 119), that

$$G(y,t) = F'(1-\mathrm{e}^{-y},t),$$

so that the two functions approach each other in the classical limit, ie for large $\langle x\rangle$ or $\langle n\rangle$, or for small s or y. We would thus expect both the quantum and semi-classical systems to behave in similar ways in the classical limit. That, however, need not be true, as we shall see for the second example below.

It is clear from a comparison of equations (8) and (12) that for large values of n the solution for the quantum-mechanical $p_j(n, t)$ approaches the semi-classical $\wp_j(x, t)$ to $O(1/n)$. This result agrees precisely with the result of Swain (1973b), who has solved the problem of equation (1), ie without the rotating-wave approximation. The difference in behaviour between the two theories arises from the differing physical interpretations of the functions $\wp$ and p, and not from their mathematical differences.

4. Initially chaotic field

A chaotic state of the radiation field may be obtained, for example, by a thermal excitation of the cavity mode. For such a field having a mean energy $\hbar\omega\bar{n}$, and for the atom initially in its ground state,

$$p_1(n, 0) = (\bar{n}+1)^{-1}(1+1/\bar{n})^{-n}$$

$$p_2(n, 0) = 0.$$

The corresponding intensity distributions are (Glauber 1963)

$$\not{p}_1(x, 0) = \bar{n}^{-1}\,\mathrm{e}^{-x/\bar{n}}$$

$$\not{p}_2(x, 0) = 0.$$

With this initial state, the probability for finding the atom in the ground state at time t is, from equation (10),

$$G_1(0, t) = (\bar{n}+1)^{-1}\sum_{n=0}^{\infty}\frac{(1+1/\bar{n})^{-n}}{4g^2n+v^2}[2g^2n+v^2+2g^2n\cos t(4g^2n+v^2)^{1/2}] \tag{16}$$

for the quantum theory; or, from equation (14),

$$F_1(0, t) = (\bar{n})^{-1}\int_0^{\infty}\mathrm{d}x\frac{\mathrm{e}^{-x/\bar{n}}}{4g^2x+v^2}[2g^2x+v^2+2g^2x\cos t(4g^2x+v^2)^{1/2}] \tag{17}$$

for the semi-classical theory. Clearly the two theories do not differ very wildly: the series of equation (16) converges fairly slowly for even moderate values of $\bar{n}$, so that the sum may be well approximated by an integral, and the terms in the sum approach the form of the integrand of equation (56) for large $\bar{n}$.

The behaviour of $G_1(0, t)$ is shown in figure 1 for some selected values of the parameters. I do not show $F_1(0, t)$, since its behaviour is not enlighteningly different.

5. Initially coherent field

This is essentially a classical field with a well defined intensity; we shall suppose that the field is initially in a stationary state, so that only the intensity and not the phase are well defined. Lasers and masers produce fairly good approximations to such fields. If we take the atom to be initially in the ground state again, then

$$\not{p}_1(x) = \delta(x-x_0)$$

$$\not{p}_2(x) = 0,$$

where x_0 is the normalized intensity of the field. The corresponding photon number distributions are (Glauber 1963)

$$p_1(n) = (x_0^n/n!)\,\mathrm{e}^{-x_0}$$

$$p_2(n) = 0.$$

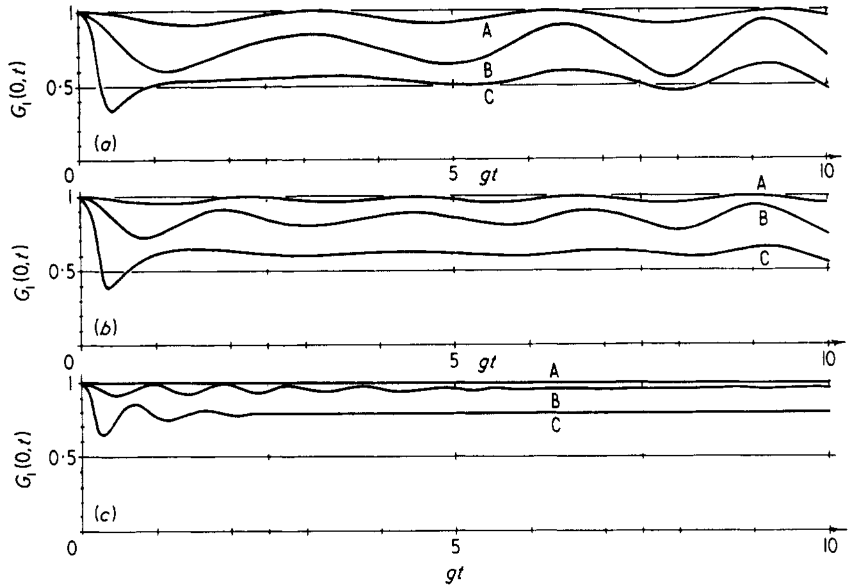

Figure 1. Behaviour, in quantum theory, of $G_1(0, t)$, the probability of finding an atom in the ground state at time t, plotted as a function of the dimensionless parameter gt. The radiation field is initially in a chaotic (eg, thermally excited) state of various strengths; values of the mean numbers of initial photons, $\bar{n}$, are 0·1 (curves A), 1·0 (curves B) and 10 (curves C). The three graphs are for: (*a*) cavity and atom perfectly matched, $\nu = 0$; (*b*) cavity and atom slightly mismatched, $\nu = 2g$; (*c*) cavity and atom quite mismatched, $\nu = 6g$. See equation (16).

If the atom is initially in the ground state, the probability of finding it there at t is, again from equation (10),

$$G_1(0, t) = \mathrm{e}^{-x_0} \sum_{n=0}^{\infty} \frac{x_0^n/n!}{4g^2n+\nu^2}[2g^2n+\nu^2+2g^2n \cos t(4g^2n+\nu^2)^{1/2}], \qquad (18)$$

for the quantum theory; or, from equation (14),

$$F_1(0, t) = (4g^2x_0+\nu^2)^{-1}[2g^2x_0+\nu^2+2g^2x_0 \cos t(4g^2x_0+\nu^2)^{1/2}], \qquad (19)$$

for the semi-classical theory.

The differences between the two theories are considerably greater than in the previous case, and these differences do not disappear in the classical limit. That is, while it is true that the Poisson distribution becomes very sharply peaked about $n = x_0$, that peak is only *relatively* narrow, having a width of about $x_0^{1/2}$. Thus even for large x_0 the semi-classical theory predicts regular oscillations of the probability of finding the atom in its ground state, while the quantum theory predicts fluctuations in that probability that are superpositions of many terms with incommensurable periods.

The behaviour of $G_1(0, t)$ for some sample cases is shown in figures 2 and 3. One striking feature of the behaviour for $\nu = 0$ for large x_0 is the nearly total cancellation of the oscillations for an extended period of time: the atom is effectively raised to an infinite temperature. The semi-classical theory simply predicts regular sinusoidal oscillations in $F_1(0, t)$, which I have not shown on the graphs. The frequency of these

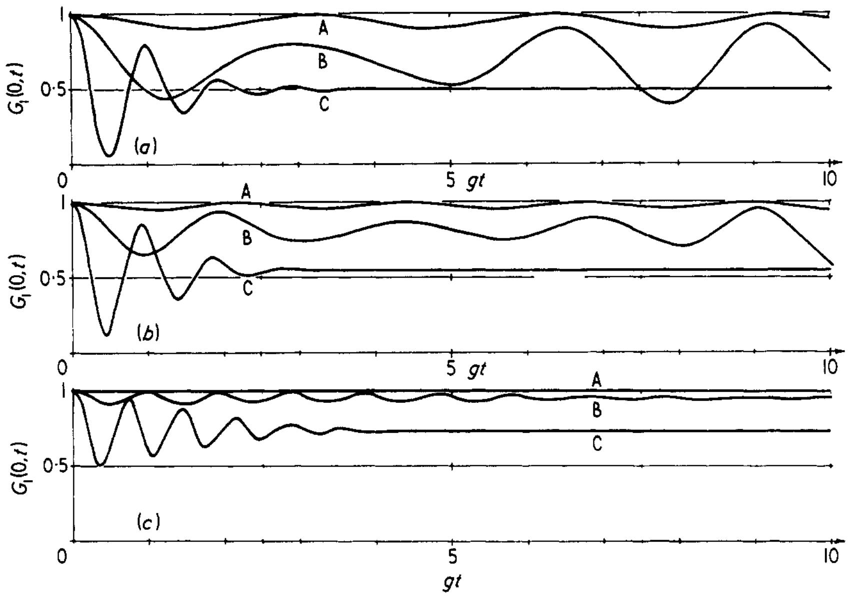

Figure 2. Behaviour, in quantum theory, of $G_1(0, t)$, the probability of finding an atom in the ground state at time t, plotted as a function of gt. The radiation field is initially in a coherent state, whose intensity (in natural units—ie, the mean photon number), x_0, is given with each curve; values of x_0 are 0·1 (curves A), 1·0 (curves B) and 10 (curves C). The three graphs are again for: (*a*) atom and cavity perfectly matched, $\nu = 0$; (*b*) atom and cavity slightly mismatched, $\nu = 2g$; (*c*) atom and cavity quite mismatched, $\nu = 6g$. See equation (18). The corresponding semi-classical behaviour is a pure sinusoidal oscillation with period T given by $gT = \pi/\sqrt{x_0}$, so that gT is 9·93 for $x_0 = 0{\cdot}1$, 3·14 for $x_0 = 1{\cdot}0$, and 0·99 for $x_0 = 10$. Note that the quantum theory predicts an almost total absence of oscillations for extended periods for large x_0, independent of ν.

oscillations is $2g\sqrt{x_0}$, which is more or less the same as that of the initial oscillations of $G_1(0, t)$ shown in the graphs.

The differences between these predictions should not be impossible to see. For a cavity of 10^2 cm^3 in volume, an atomic dipole moment of $e \times 10^{-8}$ cm, and for microwave frequencies on the order of 10^{10} s^{-1} the coupling constant g is of the order of 10^4 s^{-1}. The time scale of the figures is thus of the order of tenths of milliseconds. For fairly low intensities, corresponding to a field temperature of 10^4 K, $x_0 \sim 10^5$, and the frequency of the semi-classical oscillations is of the order of 10^7 s^{-1}; for more typical maser generated intensities (mW cm^{-2}), $x_0 \sim 10^{10}$, and the corresponding semi-classical frequency is 10^9 s^{-1}.

6. Conclusions

One of the most fruitful methods of investigating the interaction of isolated atoms with the radiation field employs atomic beam techniques†. Although such experiments are by no means the only ones that can be done, they are sufficiently general that they may

† An experimentally oriented discussion of a closely related situation is given in Silverman and Pipkin (1972). However, Silverman and Pipkin are chiefly interested in the radiation damping, which they treat according to quantum mechanics, and treat the driving field semi-classically.

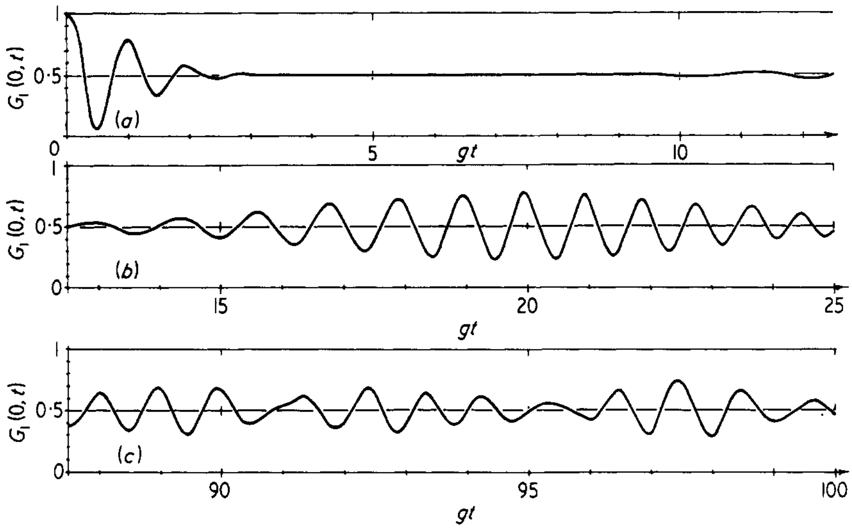

Figure 3. The long-term behaviour of $G_1(0, t)$ for an initially coherent field with dimensionless intensity $x_0 = 10$, with cavity and atom perfectly matched, $\nu = 0$. The three graphs are for: (*a*) $0 \leqslant gt \leqslant 12{\cdot}5$; (*b*) (continuation of (*a*)) $12{\cdot}5 \leqslant gt \leqslant 25$; (*c*) $87{\cdot}5 \leqslant gt \leqslant 100$. See equation (18). The period of the semi-classical oscillations is $gT = 0{\cdot}99$, which is approximately the period of the oscillations in the quantum behaviour. The behaviour for $gt > 25$ has the general character of that illustrated in the last graph.

serve as a paradigm for our discussion. In such an experiment one has a cavity filled with a radiation field prepared to be in a specified state; at $t = 0$ an atom—also in a specified state—enters the cavity; after a certain amount of time, t, which can be adjusted by varying the length of the cavity or the speed of the atom, the state of the atom is investigated by a detector. One thus measures just the probability of finding an atom in, say, the ground state at time t, given that it was initially in the ground state, and given the initial state of the field. For the quantum theory that probability is just $G_1(0, t)$; for the semi-classical theory it is $F_1(0, t)$.

The initial state of the radiation field can, in principle, be determined from *a priori* considerations or from photon-counting and interference experiments. Thus, although the functions $p_j(n)$ and $\not{p}_j(x)$ are not directly measurable, they are experimentally verifiable. If one, for example, prepares a field to exhibit the correlation and coherence properties of fields with a well defined amplitude, one may use the appropriate expressions for a coherent field from either the quantum or semi-classical theories. If one were to perform an atomic beam experiment of the sort described one should in principle be able to see whether the results obeyed equation (18) or (19).

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