Weak Mixing in a Quantum System

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An analytical solution to the Wigner-Weisskopf problem (an excited two-level atom in interaction with a radiation field), obtained for both finite- and infinite-length boxes, is re-examined in terms of the qualitative behavior implied. As the equations and the plots of the solutions show, there is a major difference between the behavior of the finite system (with discrete spectrum) and that obtaining in the large-system limit. In the first case, a pulse-shaped wave "travels down the line" and comes back (and is sent off again) many times, completely "losing its shape" in the process (and subsequently re-gaining it on a much longer time scale infinitely often, due to the presence of a Poincaré recurrence). In the large-system limit, on the other hand, a delta-impulse-like wave travels down the line only once (in finite time), and there is also no loss of shape upon its return after infinite time. Thus, there is no longer any even temporary "smearing out" of the initially sharply localized energy, and hence no "mixing" in the intuitive sense of the word. Nonetheless a dense spectrum is found (similarly as in the distribution theoretical case of an isolated delta-impulse in an infinite domain), and hence weak mixing in the sense of Lebowitz. The contradiction can be resolved at the expense of having to abandon some symmetry: by assuming the atom adjacent to two cavities of incommensurate lengths. Then the infinite system limit is unchanged (no return in finite time), but the transition is characterized by intuitive mixing of increasing effectiveness.

1. Introduction

Recently, considerable interest has been directed toward the problem of understanding the qualitative behavior and properties of finite versus infinite quantum and classical systems; see the proceedings of the Volta Memorial Conference [1] for many pertinent papers. As emphasized by Lebowitz and Penrose [2b], a finite quantum system can never exhibit any of the properties higher than simple ergodicity since the spectrum of such a system is necessarily discrete; in fact, the system will in general not even be ergodic (that is, for almost all initial conditions trace out the whole energy surface). On the other hand, very little is known in the way of rigorous results about the qualitative properties of infinite quantum systems, a fact which is unfortunate inasmuch as it is only for infinite systems that one can expect to find strictly irreversible behavior in quantum systems. The purpose of this communication is to draw attention to a theoretical problem which arises in constructing the

large-system limit (as well as the thermodynamic limit) of a certain exactly solved model in quantum statistics — namely, that of an excited two-level atom in interaction with a field of radiation. The significance of this issue is that the "kind" of ergodic behavior one finds in constructing the limit may depend on usually ignored subtleties in the formulation of the problem (like the relative position of the atom in the field). We conjecture that the very possibility of having such subtleties interfere may be of general importance in constructing the thermodynamic limit in both quantum and linear classical mechanical systems.

2. The Analytical Problem

In a recent series of papers [3-10], the dynamics of a two-level atom in interaction with a one-dimensional field of electromagnetic radiation has been studied. Consider a Hamiltonian having the structure

$$H = \varepsilon_{1} \alpha \alpha^{*} + \varepsilon_{2} \alpha \alpha^{*}$$

$$+ \sum_{\lambda} \left| \frac{1}{2} \hbar \omega_{\lambda} (a_{\lambda}^{*} a_{\lambda} + 1) \right|$$

$$+ \sum_{\lambda} \left(h_{\lambda}^{*} \alpha^{*} a_{\lambda} + h_{\lambda} \alpha a_{\lambda}^{*} \right),$$
(1)

where ε_1 and ε_2 are the energies of the ground state $|1\rangle$ and excited state $|2\rangle$ of the two-level atom, and

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$$\alpha = |1\rangle\langle 2|, \quad \alpha^* = |2\rangle\langle 1|,$$

and

$$\begin{aligned} & \langle n_{\lambda} | a_{\lambda} | m_{\lambda} \rangle \\ &= |2(n_{\lambda} + 1)|^{1/2} \delta^{Kr} (m_{\lambda} - n_{\lambda} - 1) \\ &= \langle m_{\lambda} | a_{\lambda}^{*} | n_{\lambda} \rangle. \end{aligned}$$

Here the state $|n_{\lambda}\rangle$ is that which has $n_{\lambda} (=0,1,2,...)$ photons in the 1th mode of the radiation field, and $\delta^{\rm Kr}(...)$ is the Kronecker delta. Further, $\hbar \omega_{\lambda}$ is the energy of a photon in the 1th mode of the field, $\hbar E = \varepsilon_2 - \varepsilon_1$ is the energy separating the two levels of the atom, and the function h_{λ} gives the coupling between the atom and the radiation field. The exact dynamics of a system governed by the Hamiltonian (Eq. (1)) of the problem has been determined from the time-dependent Schroedinger equation of the problem, both for the case of discrete and continuous spectra, first for the case that a field is assumed to be re-excited initially [6, 7] (the spontaneous-emission case), and then for the case that there is present initially an extra photon in the radiation field [9, 10] (the induced-emission case). In this note we wish to focus first on the discrete spectrum case (which derives mathematically from considering the atom to be in interaction with a radiation field confined to a box of length L [6, 9]), considering explicitly the behavior found in systems of ever-increasing size and then, in the subsequent Section, we consider the results obtained in the thermodynamic limit.

3. The Discrete Spectrum Case

We wish to focus first on the discrete spectrum case, the situation which arises when one considers the excited two-level system to be confined to a box of finite length L. The exact eigenfrequencies of the atom-radiation problem were determined, first for the case of a field initially de-excited (in [6]) and then for the case where one mode of the field is excited at time t=0 (in [9]). The number of eigenfrequencies needed to ensure that the normalization condition for the probability density be satisfied at the initial time, viz. $\varrho(\tau=0)=1$, was found to be a strong function of the length of the cavity: increasing the length of the cavity by a factor of 10 increased the number of eigenfre-

quencies needed to achieve (comparable) accuracy in the determination of ϱ (τ =0), by at least an order of magnitude. Qualitatively speaking, the spectrum of eigenvalues of the problem quickly becomes "dense" with increase in the length of the radiation cavity (while in the mathematical sense it does so only in the limit).

In representative (numerically implemented) analytical calculations of the probability $\varrho(t)$ that at time t the atom be in its excited state, the explicit consideration of a finite statistical-mechanical system leads to the phenomenon of "major reexcitations" in the evolution of the system, and it is the structure and pattern of these reexcitations that is one of the main concerns of this note. To simplify the following discussion, let us specify a dimensionless set of temporal and spatial variables; let

$$\tau = \alpha E t \tag{2a}$$

and

$$\sigma^2 = \alpha \ EL/c. \tag{2b}$$

In these equations, α is a coupling constant which scales the interaction of the atom with the field, and c is the phase velocity of the bosons (the speed of light). Then the parameter τ may be regarded as the (dimensionless) time required for a wave to cross the system of length L, and σ^2 is the corresponding reduced length of the system.

In Figs. 1-3 (adapted from [6, 9]) we record the behavior of the excitation probability of $\rho(\tau)$ versus τ for specific choices of parameters, α , σ^2 and f(x) $=x^{-\varrho}$; here f is a dimensionless coupling function whose argument $x = c |k_{\nu}|/E$ involves k_{ν} , the wave number of the yth mode of the field. The parameter choices relevant to Figs. 1 and 2 are similar (except for a difference in coupling function). In Figure 3, the reduced length σ^2 is 10 times larger. In each figure, the solid line corresponds to the field being deexcited at time t=0 while the dotted line corresponds to one extra photon in the field at t=0. We emphasize that the profiles displayed in Figs. 1-3 represent the time evolution generated via the exact solution to the Schroedinger equation for the problem described previously [6, 9]. We now discuss Figs. 1—3 in light of the observed reexcitations.

We begin by noticing that the profiles displayed are characterized by an initial decay over a rather short time scale followed at later times, determined by the size σ^2 of the system, by large and rapid

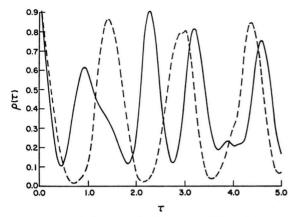


Fig. 1. Plot of the re-excitation probability of the atom, $\varrho(\tau)$, versus reduced time, τ . Parameters chosen: $\alpha=0.1$, $\sigma^2=1$, and $f(x)=x^{-1/2}$. (See text for explanations.) The solid line describes the time evolution of $\varrho(\tau)$ assuming the field is de-excited at time $\tau=0$. For comparison, the dashed line displays the time evolution of $\varrho(\tau)$ assuming the presence of an excitation in the field at time $\tau=0$.

fluctuations. It is these fluctuations that one may call a (major) "reexcitation". (We avoided the word "recurrence" because the first Poincaré recurrence is inobservable in physically and numerically accessible finite times.) It is with respect to these "reexcitations" that the behavior displayed in Figs. 1 and 2 versus Fig. 3 is especially interesting. These figures show that as the length σ^2 (or L) of the box becomes longer, the time for a high probability of the atom to be reexcited increases; and in fact it was shown explicitly (in [7, 10]) that in the infinite-system limit the first such reexcitation is displaced to infinite time.

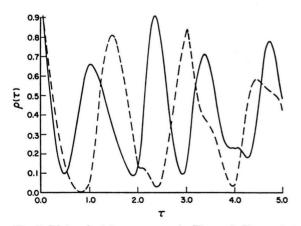


Fig. 2. Plots of $\varrho(\tau)$ versus τ as in Figure 1. Parameters: as in Fig. 1, except $f(x) = x^{-1/4}$. (A different coupling function.)

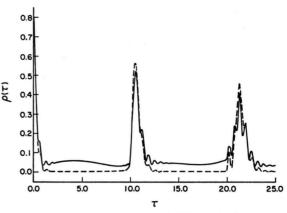


Fig. 3. Plots of $\varrho(\tau)$ versus τ as in Figure 1. Parameters: as in Fig. 1 except $\sigma^2 = 10$. (A ten times larger box.)

Interestingly, the qualitative understanding of the difference between solid and dotted lines in Figures 1, 2, 3 (the former lines corresponding to the field de-excited at initial time, the latter to the presence of an excitation in the field at that time) is simply that the initially greater intensity of radiation in the latter case leads to a somewhat more rapid initial decay of the excited state, to more frequent recurrences of high values of this probability of excitation, and to a raising of the values of this probability. However, the remarkable similarity between the two profiles displayed in Figure 3 (the profiles for the longer cavity) suggests that the observed "re-excitations" may be attributed to a common qualitative mechanism.

This qualitative interpretation is as follows: if one imagines the excited atom giving up an excitation (a photon) to the field (this due to the coupling between the atom and the field), and then one describes the subsequent history of the emitted photon in a wave language, one gets the picture of a wave travelling to the end of the cavity and then, upon reflection, returning to the atom, with an attendant probability of the atom's being re-excited.

The longer the box, the longer the distance to be travelled by the wave, and hence the longer a time interval required for re-excitation. On first encounter with the reflected wave, the atom does not regain its initial state with unit probability; moreover the subsequent decay of the first fluctuation takes place on a time scale somewhat longer than the initial decay. As is seen clearly in Fig. 3, the fluctuation following the first "re-excitation" is even more diffuse, and in fact the pattern of the

second fluctuation breaks up into several "fingers" clustered together at a value of $\tau \approx 22.0$. In the subsequent evolution, this decoupling of the initial pattern continues, with the number of "fingers" in each new re-excitation increasing, and with the overall height of the fluctuations decreasing, until (when one reaches $\tau \approx 100$ for the case $\sigma^2 = 10$) the initial decay pattern has been broken down into a more or less random sequence of fluctuations, with only a remote suggestion of the initial pattern (that is, fluctuations separated by regimes of apparent quiescence) remaining.

4. The Continuous Spectrum Case

It is of interest to consider the results obtained in the present atom-radiation problem if one constructs the so-called thermodynamic limit of statistical mechanics. In the present case, this corresponds to allowing the number of modes of the field and also the length of the cavity to tend separately to infinity while insisting that their ratio remain constant. This procedure is reflected, in the underlying analytical structure of the problem, in the following way: in the contour integral representation for the quantity $\rho(\tau)$, the set of eigenfrequencies comprising the discrete spectra of the problem is now replaced by a continuum, a situation realized mathematically in the analysis by introducing a "branch cut" along the real axis of the complex plane. The contour intergration is then carried out and the result obtained for $\rho(\tau)$ can then be studied in a variety of dynamical regimes. (See [10], especially, for details.)

In the calculation described in the previous Section, the large-system limit was constructed by identifying a set of eigenvalues which became countably infinite with increase in length of the radiation cavity (see [9]). In contrast, the procedure described in the preceding paragraph to construct the thermodynamic limit of the same problem results in a spectrum which has the measure of the real line.

The qualitative difference found in constructing $\varrho(\tau)$ via these two procedures is that in the former case there will always be a return of a high probability of re-excitation, albeit one at a point in time infinitely distant from the initial de-excitation, whereas in the second procedure the possibility of an (even eventual) return is strictly excluded. For

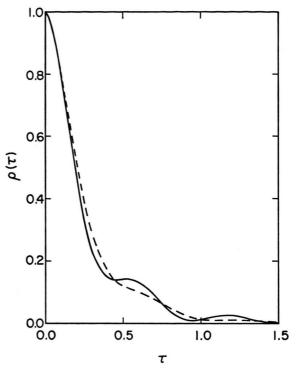


Fig. 4. Plots of $\varrho(\tau)$ versus τ as in Figure 1. Parameters as in Fig. 1 except $\sigma^2 \to \infty$. (An infinite-length box.)

a graphical example of this point, see Fig. 4 (adapted from [7]) in which is plotted the time evolution of $\varrho(\tau)$ for the choice of coupling constant $\alpha = 0.1$, in the infinite-system limit.

5. Discussion

It is interesting to consider what the results presented in the previous Sections mean in light of the well-known classical mechanical notions of ergodicity, weak mixing, and so forth (see, for example, Reference [11]). There is general agreement that finite quantum mechanical systems can (in light of their close relationship to a set of harmonic oscillators) not be expected to be even ergodic (which is the weakest of all the statistically-mechanically interesting qualitative notions); only in the infinite-mode-number limit can these systems possibly become ergodic and mixing; see Lebowitz and Penrose [2b].

In the classical mechanical system studied by Cukier and Mazur [12], a single heavy particle in a one-dimensional harmonic crystal causes the whole linear system to become (at least) weakly mixing, and by implication ergodic, in the infinite system limit (cf. [2a]). Casati and Ford [13] give as another example of a (presumably) weakly mixing system the right triangle used as a billard table: if the other two angles are incommensurate, a hard ball moving without friction will for almost all initial conditions fill the triangle densely with its path, and there is a polynomial (nonexponential) decay of correlation. In the classical mechanical literature, the presence of a (homogeneously) dense spectrum (no isolated eigenvalue other than zero) is considered both necessary and sufficient for having weak mixing; cf. [2a, p. 50] and, for the original definition, [14].

The Wigner-Weisskopf problem (an atom in a radiation field) as treated in the preceding three Sections is closely analogous to the Cukier-Mazur system (cf. [10]). In both cases, an initial de-excitation of the singular constituent (atom or heavy mass, respectively) spreads in the form of a wave until, upon reaching the end of the system (crystal or cavity, respectively), it returns, thereby initiating another round. If the system is finite, in either case the reflections back and forth after a while "degenerate" into a highly complex pattern (see Figs. 1-3); nonetheless, the fact that the system has only a finite number of modes ensures that the resulting complicated motion is still quasiperiodic, that is, analogous to a smooth motion with irrational winding number on a torus. (As a consequence, there is a Poincaré recurrence toward every once occupied state up to any arbitrarily small preassigned neighborhood radius ε .) Making the length of the box (or chain) infinite in either case generates a dense spectrum (no localized modes).

If it is true that possessing a dense spectrum suffices for weak mixing, the infinite quantum mechanical system of Sect. 3 does possess this property. The intuitive interpretation introduced (a traveling, and later returning, light wave) nonetheless suggests that things are a little bit more complicated: a dense spectrum can, evidently, be associated with a type of behavior that only very weakly (if at all) resembles a mixing process in the intuitive sense of the word. For as we saw, even the first returns of the light wave would now never take place. (An analogous observation was in a classical context made by Lanford [15]; Joseph Ford, personal communication 1981).

But how can one understand that this trivial behavior (a single wave, with respect to the whole infinite-length box infinitely-sharply-located, is traveling down the line) possesses a dense spectrum? Without going into the (distribution theoretic) details, one can rationalize this by comparing this pulse to a delta impulse. A single delta impulse is indeed well-known to possess a "continuous" (in fact, dense) spectrum; see, for example, Bracewell [16]. If this delta-function analogy is valid (which has yet to be shown in detail), this would mean that two kinds of weak mixing would have to be distinguished: simple weak mixing (due to the presence of a single delta impulse-like wave that does not exhibit any kind of visible "mixing" behavior) and nontrivial weak mixing.

The question that necessarily presents itself at this point is whether or not nontrivial weak mixing is likewise possible in the Wigner-Weisskopf problem in the limit.

Before closing, we would like to indicate where we think it might be possible to look for such an answer. The scenario we have in mind is the following: imagine an "excentric" Wigner-Weisskopf situation where the atom is not placed at one "end" (or, equivalently, into the "middle") of the one-dimensional radiation field, but rather is displaced somewhat away from the middle. This "two-adjacent-cavities problem" has yet to be studied quantitatively. But it appears already that its behavior will be much more intuitive supposing that the length (now of both cavities) is increased progressively as before, with their (incommensurate) ratio maintained.

While formerly the elongation only impeded the smearing-out process (a continual impulse-broadening brought about by the fact that the supporting medium was not truly continuous), now two processes can be expected to be at work simultaneously: (1) the same impulse-broadening effect as before (disappearing again in the limit), and (2) a new, impulse-splitting effect: each "half wave" returns after a different time, and each, upon with a certain probability re-exciting the atom, generates two new half waves (and so forth, until effect (1) takes over finally).

If the second predicted property indeed applies (which is likely in view of the analogy to the Cukier-Mazur problem where it is easier to establish), the main consequence will be a quantitative one: a

"scissors shaped" divergence between the increase in the life-time of an impulse (first "full submersion" time) under an increase of length on the one hand, and the simultaneous increase in its (much shorter) one-time travelling time (first "re-excitation" time) on the other. After writing down the ratio between these two times as a function of length close to the limit, it will be possible to arrive at a new, more sensible definition of the thermodynamic limit which is based on this ratio becoming infinite. While hereby nothing will be changed quantitatively (infinity is infinity), the new definition will be insensitive to an (in the limit) infinite rescaling of time (such that the former infinity becomes unity), thereby revealing (after an analogous rescaling of length) the true dynamical prototype of the present class of systems: a heavy resonator (linear o.d.e) coupled in a nonrotation-symmetric fashion to a linear continuum

- [1] G. Casati and J. Ford, eds., Stochastic Behavior in Classical and Quantum Hamiltonian Systems, Volta Memorial Conference, Como, 1977, Springer-Verlag, New York 1979.
- [2a] J. L. Lebowitz, Hamiltonian Flows and Rigorous Results in Non-equilibrium Statistical Mechanics, IUPAP Conf. Statistical Mechanics, University of Chicago Press, Chicago, 1972, pp. 41—63.
- [2b] J. L. Lebowitz and O. Penrose, Physics Today (2) 1973, 23.
- [3] R. Davidson and J. J. Kozak, J. Math. Phys. 11, 189 (1970).
- [4] R. Davidson and J. J. Kozak, J. Math. Phys. 11, 1420
- [5] R. Davidson and J. J. Kozak, J. Math. Phys. 12, 903 (1971).
- [6] R. Davidson and J. J. Kozak, J. Math. Phys. 14, 414 (1973).
- [7] R. Davidson and J. J. Kozak, J. Math. Phys. 14, 423 (1973).

(p.d.e.) — Max Planck's original metaphor giving rise to the Jeans-Rayleigh law (cf. [17]).

To conclude, calculations on an explicit quantum system have made possible a closer look at its infinite limits. It appears that not all approaches to the (same) limit are physically equally meaningful. Preference should be given to such physical setups where the transition process can be followed intuitively — so that (continuity of) convergence can be assured.

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- [8] J. J. W. Yang, R. Davidson, and J. J. Kozak, J. Math. Phys. 15, 491 (1974).
- [9] R. Davidson and J. J. Kozak, J. Math. Phys. 16, 1013 (1975).
- [10] R. Davidson and J. J. Kozak, J. Math. Phys. 19, 1074 (1978).
- [11] V. I. Arnold and R. Avez, Ergodic Problems of Statistical Mechanics, Benjamin, New York 1968.
- [12] R. I. Cukier and P. Mazur, Physica 53, 157 (1971).
 [13] G. Casati and J. Ford, J. Computational Phys. 20, 9
- [13] G. Casati and J. Ford, J. Computational Phys. 20, 97 (1976).
- [14] P. R. Halmos, Lectures on Ergodic Theory, Chelsea, New York 1956.
- [15] O. E. Lanford, in: The Boltzmann Equation, E. G. D. Cohen, and W. Thirring, eds. Springer-Verlag, Wien 1973, p. 619.
- 1973, p. 619.
 [16] R. N. Bracewell, The Fourier Transform and its Applications, 2nd edition, McGraw-Hill, London 1978.
- plications, 2nd edition, McGraw-Hill, London 1978.

 [17] T. S. Kuhn, Black Body Theory and the Quantum Discontinuity 1894—1912, Oxford University Press, Oxford 1978.