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IRREVERSIBLE BEHAVIOUR OF A SIMPLE QUANTUM MODEL IN THE THERMODYNAMIC LIMIT

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The irreversible behaviour of a simple Wigner-Weisskopf system in the thermodynamic limit (of the form proposed by Stey and Gibberd) is investigated. The system exhibits irreversible behaviour in that the Boltzmann entropy increases monotonically with time and the spectrum of created photons tends to the Lorentzian distribution.

It is well known that for systems described by the Hamiltonian having the discrete spectrum the motion of the elements of the time evolution operator, due to the existence of Poincaré recurrences, is quasi-periodic. However, certain limiting procedures, such as the infinite-volume or thermodynamic limit, allow us to remove the oscillations to the infinite future.

The problem of the temporal behaviour of various kinds of the Wigner-Weisskopf models in the infinite-volume limit was widely discussed in the paper of Stey and Gibberd [1]. These authors have shown that in order to avoid the non-unitarity of the evolution operator of the infinite system a certain limiting procedure should be carried out. In this work we have analyzed the behaviour of a simple infinite system obtained by this procedure. We have computed the Boltzmann entropy and examined the time evolution of the number of photons at different frequencies. The irreversible decay of the excited state leads to the creation of a photon field with the Lorentzian spectrum.

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1. The model

Consider a model of Wigner-Weisskopf kind [2], consisting of a two-level atom and a photon field. The Hamiltonian has a form

$$H = |E\rangle E\langle E| + \sum_n |n\rangle \varepsilon_n \langle n| + \frac{V}{\sqrt{l}} \sum_n (|E\rangle\langle n| + |n\rangle\langle E|), \tag{1}$$

where $|E\rangle$ is the excited state of the atom, $|n\rangle$ is the state of a photon of the frequency n, l can be regarded as the "length" of the system. We assume that the interaction V does not depend on the frequency n. The vectors $|E\rangle$ and $|n\rangle$ form the complete orthonormal basis

$$\langle E|E\rangle = 1, \quad \langle n|n'\rangle = \delta_{nn'},$$
$$\langle E|n\rangle = \langle n|E\rangle = 0, \quad |E\rangle\langle E| + \sum_n |n\rangle\langle n| = 1, \tag{2}$$

and the Hamiltonian (1) conserves the number of particles, in the sense that the destruction of a photon excites the atom and the creation of a photon deexcites the atom. A transition between two distinct states $|n\rangle$ and $|m\rangle$ can occur only by intervention of the state $|E\rangle$.

For the above system, Stey and Gibberd [1] have solved the energy-eigenvalue problem and computed exactly the elements of the time evolution operator $U(t) = \exp(-itH)$:

$$U_{EE}(t, l) = e^{-(iE+V^2)t} + \sum_{n=0}^{\infty}\left[\left(-\frac{2V^2}{n}\right)(t-2nl)L_{n-1}^{(1)}[2V^2(t-2nl)]\right.$$
$$\left.\times e^{-(iE+V^2)(t-2nl)}\theta(t-2nl)\right],$$

$$U_{nE}(t, l) = \frac{V}{i\sqrt{l}}\{e^{-i\varepsilon_n t}B_0(t, \gamma_n) + \sum_{r=1}^{\infty}\sum_{v=0}^{\infty}[A_{r,v}B_{r-v}(t-2rl, \gamma_n)e^{-i\varepsilon_n(t-2rl)}$$
$$\times\theta(t-2rl)]\} = U_{En}(t, l),$$

$$U_{mn}(t, l) = \delta_{mn}e^{-i\varepsilon_m t} - \frac{V^2}{l}\left[\sum_{\mu=1}^{\infty}\frac{(-\gamma_n)^{\mu-1}}{\mu!}B_\mu(t, \gamma_m)e^{-i\varepsilon_m t}\right.$$
$$\left.+\sum_{r=1}^{\infty}\sum_{v=0}^{\infty}\sum_{\mu=r-v+1}^{\infty}(r-v)!A_{r,v}\frac{(-\gamma_n)^{\mu+r-v-1}}{\mu!}B_\mu(t-2rl, \gamma_m)e^{-i\varepsilon_m(t-2rl)}\theta(t-2rl)\right], \tag{3}$$

$$\theta(x) = \begin{cases} 0 \text{ for } x < 0 \\ 1/2 \text{ for } x = 0 \\ 1 \text{ for } x > 0; \end{cases}$$

$$\gamma_n = i\varepsilon_n - (V^2 + iE),$$

$$A_{r,v} = (-2V^2)^{r-v}\binom{r-1}{v}[(r-v)!]^{-1},$$

$$B_k(t, \alpha) = k!e^{\alpha t}(-\alpha)^{-k-1} \sum_{m=k+1}^{\infty} \frac{(-\alpha t)^m}{m!},$$

and $L_n^{(\alpha)}$ is the generalized Laguerre polynomial.

The motion of the elements of the evolution operator $U(t, l)$ is quasi-periodic in time and without a limit in an ordinary sense as $t \to \infty$. When one takes an infinite-volume or thermodynamic limit, the exact quasi-periodic evolutions pass to decaying evolution. This fact is associated with the appearance of a continuum part in the spectrum of the Hamiltonian in the above limits [3, 4]. However, when we take the $l \to \infty$ limit of the elements of $U(t, l)$, the operator becomes non-unitary. Apart from this fact, the quasi-periodic motion is displaced to the infinite future, so that we cannot analyze the long time behaviour in this limit (see Appendix). These difficulties can be avoided if we first re-define the states in such a way that a new state is

$$|\omega\rangle = (l\pi^{-1})^{1/2}|n\rangle$$

and then take the $l \to \infty$ limit. We have

$$\langle\omega|E\rangle = \langle E|\omega\rangle = 0,$$
$$\langle\omega|\omega'\rangle = l\pi^{-1}\delta_{nn'} \xrightarrow[l\to\infty]{} \delta(\omega-\omega'). \tag{5}$$

We assume that the energy $\varepsilon_n = n\pi l^{-1}$.

The $l \to \infty$ limit is taken in the distributive sense [5], i. e., for functions $f(n\pi l^{-1})$ we assume

$$f(\omega) = \sum_{n'} \langle n|n'\rangle f(n'\pi l^{-1}) \xrightarrow[l\to\infty]{} \int_{-\infty}^{\infty} d\omega' \delta(\omega-\omega') f(\omega'). \tag{6}$$

The Hamiltonian (1) formally becomes, for $l \to \infty$,

$$H = |E\rangle E\langle E| + \int_{-\infty}^{\infty} d\omega|\omega\rangle\omega\langle\omega| + V\pi^{-1/2} \int_{-\infty}^{\infty} d\omega(|E\rangle\langle\omega| + |\omega\rangle\langle E|) \tag{7}$$

and it can be shown that $U(t)$ remains unitary and

$$U_{EE}(t) = \lim_{l\to\infty} U_{EE}(t, l) = e^{-(iE+V^2)t}, \tag{8}$$

$$U_{E\omega}(t) = \lim_{l\to\infty} \left(\frac{l}{\pi}\right)^{1/2} U_{En}(t, l) = -\frac{iV}{\sqrt{\pi}} \frac{e^{-i\omega t} - e^{-(iE+V^2)t}}{V^2 - i(\omega-E)}, \tag{9}$$

$$U_{\omega\omega'}(t) = \lim_{l\to\infty} \left(\frac{l}{\pi}\right) U_{nn'}(t, l) = \delta(\omega-\omega')e^{-i\omega' t}$$

$$-\frac{V^2}{\pi} \sum_{\mu=1}^{\infty} \sum_{\nu=\mu+1}^{\infty} \frac{[V^2 - i(\omega'-E)]^{\mu-1}\{[V^2 - i(\omega-E)]t\}^{\nu} e^{-(V^2+iE)t}}{\nu![V^2 - i(\omega-E)]^{\mu+1}}. \tag{10}$$

2. *Time evolution*

The density matrix at the moment t is given by

$$\varrho(t) = Z(t, t_0)\,\varrho(t_0), \tag{11}$$

where $Z(t, t_0)$ is the time evolution superoperator:

$$ZA = UAU^{+}$$

for any quantum mechanical operator A, and

$$Z_{\alpha\beta,\gamma\delta} = U_{\alpha\gamma}U^{*}_{\beta\delta}.$$

When we assume that the initial density matrix of the system has the form

$$\varrho_{\alpha\beta}(t_0) = \delta_{\alpha E}\delta_{\beta E}, \tag{12}$$

i. e., we have initially the excited atom in the photon vacuum, all the initial correlations being equal to 0, we obtain:

$$\varrho_{EE}(t) = |U_{EE}(t)|^2,$$

$$\varrho_{E\omega}(t) = \varrho^{*}_{\omega E}(t) = U_{EE}(t)U^{*}_{\omega E}(t),$$

$$\varrho_{\omega\omega'}(t) = U_{\omega E}(t)U^{*}_{\omega' E}(t).$$

We can apply these formulas for the computation of various dynamical properties of the system.

The entropy of the system can be defined as the Boltzmann entropy, $S_B = -k\sum_{\alpha}\varrho_{\alpha\alpha}\ln\varrho_{\alpha\alpha}$, or the Gibbs entropy, $S_G = -k\,\mathrm{Tr}(\varrho\ln\varrho)$. For systems described by the unitary evolution operators the Gibbs entropy has a constant value. The Boltzmann entropy for a system described by the Hamiltonian (7) and with the initial conditions (12) has the form:

$$S_B = -k\Bigg\{2\ln(1-e^{-2V^2t})+e^{-2V^2t}\Bigg[\ln 2\pi-2V^2t$$

$$-2e^{V^2t}\Bigg(2\ln(1-e^{-2V^2t})ch(V^2t)+2\sum_{k=1}^{E(t)}k^{-1}e^{-kV^2t}sh[V^2(t-k)]$$

$$-\frac{V^2}{\pi}\int_{-\infty}^{\infty}d\omega\,\frac{\cos[(\omega-E)t]\ln[V^4+(\omega-E)^2]}{V^4+(\omega-E)^2}\Bigg)\Bigg]-\ln(4\pi V^2)\Bigg\},$$

$$\lim_{t\to\infty} S_B = k\ln(4\pi V^2). \tag{13}$$

We analyzed numerically the time dependence of the S_B obtaining (for $E = 0$, $V = 1$) the monotonic increase with time, without any oscillations.

When the excited state decays in time, the total number of photons increases respectively. Instead of the total number of photons we can consider the proportional to it quantity $P(t) = \int_{-\infty}^{\infty} d\omega\, \varrho_{\omega\omega}(t)$. Because Tr $\varrho = 1$, we have

$$P(t) = 1-\varrho_{EE}(t) = 1-e^{-2V^2t}. \tag{14}$$

However, when we take into account only the number of photons having the frequency ω, $P_\omega(t)$, we obtain a damped oscillatory behaviour around the equilibrium value of ω:

$$P_\omega(t) = \{\pi V^2[1+V^{-4}(\omega-E)^2]\}^{-1}\{1+e^{-2V^2t}-2e^{-V^2t}\cos[(\omega-E)t]. \tag{16}$$

For $t = \to\infty$ we obtain the Lorentzian distribution of photons:

$$P_\omega(\infty) = \{\pi V^2[1+V^{-4}(\omega-E)^2]\}^{-1}. \tag{17}$$

The exact solutions of various quantum models showing the irreversible behaviour were obtained explicitly by many authors (cf. e. g. [6, 7]). However, it would be of interest to investigate the asymptotic time behaviour of quantum systems in a more general way, e. g. by means of the asymptotic master equations. Fuliński and Kramarczyk [8] obtained equilibrium in the double limit $t\to\infty$, $t_0\to-\infty$ (being the analogy of the equilibrium solution (17)). The problem of constructing the asymptotic expansions for "master quantities" in the long time approximation remains open and will be the subject of further investigations.

APPENDIX

If we take the infinite-volume limit of the matrix elements of $U(t, l)$, their quasi-periodic behaviour will be displaced in to the infinite future. However, if we investigate the behaviour of these elements by taking simultaneously the $t\to\infty$ and $l\to\infty$ limits, we may obtain various asymptotic values depending on relations between t and l.

We will analyze the asymptotic behaviour of $U_{EE}(t, l)$. For $t < 21$ all the Heaviside functions vanish and $U_{EE}(t, \infty)$ has the form (8).

The generalized Laguerre polynomials have an asymptotic form [9]

$$L_n^{(m)}(x) = \pi^{-1/2}\exp(x/2-1/4)x^{-m/2-1/4}n^{m/2-1/4}\cos[2n^{1/2}x-\pi/2(m-1/2)]$$
$$+0(m/n^2-3/4), \quad (m \text{ real}, x > 0). \tag{A.1}$$

Thus

$$L_{n-1}^{(1)}(x) \approx \cos[2(n-1)^{1/2}x-3\pi/4]\exp(x/2)x^{-3/4}(n-1)^{1/4}, \quad x = 2V^2(t-2nl). \tag{A.2}$$

The term

$$\pi^{-1/2}\exp[-iE(t-2nl)]\cos[2(n-1)^{1/2}x-3\pi/4]$$

in (3) is finite, as the product of trigonometric functions, so it is sufficient to analyze the behaviour of

$$K(t, l) = \sum_{n=1}^{\infty} x^{1/4} \frac{(n-1)^{1/4}}{n}. \tag{A.3}$$

For $n = 1$ and/or $x = 0$, $K(t, l) = 0$. Thus $K(t, l) = 0$ only for $t-4l > 0$, i. e. $t > 4l$.

For $n = 2$ and $x > 0$ either $t-4l \to c$ (constant value, finite) or $t-4l \to \pm \infty$. In the first case we can obtain the finite value of $K(t, l)$ $(t, l \to \infty)$. In the second case the limit of $K(t, l)$ does not exist $(t-4l \to \infty)$ or is equal to 0 $(t-4l \to -\infty)$. If for $n > 2$ $x \neq 0$, $K(t, l)$ will be divergent.

From the above analysis we can draw following conclusions:

For $t, l \to \infty$ the first term of the series (A.3) vanishes. The second term can be finite — in that case all the following terms are equal to 0. When a term of order greater than 2 is finite, all the preceding terms are infinite and all the following terms are equal to 0.

For systems which for long times expand linearly in time,

$$l = 1/4\, t - c \; (c > 0), \tag{A.4}$$

the element $U_{EE}(t, l)$ has an asymptotic form

$$U_{EE}^{as}(t, l) = e^{-(iE+V^2)t} + V^2 c e^{-(iE+V^2)c}. \tag{A.4}$$

In this case we do not obtain the complete decay of state $|E\rangle$.

REFERENCES

[1] G. C. Stey, R. W. Gibberd, *Physica* **60**, 1 (1972).
[2] V. Weisskopf, E. Wigner, *Z. Phys.* **63**, 54 (1930); **65**, 18 (1930).
[3] J. L. Pietenpol, *Phys. Rev.* **162**, 1031 (1967).
[4] K. Friedrichs, *Commun. Pure Appl. Math.* **1**, 361 (1948).
[5] J. P. Marchand, *Distributions*, North-Holland, Amsterdam 1962.
[6] C. Favre, J. P. Marchand, *Helv. Phys. Acta* **39**, 5 (1966).
[7] A. Lopez, *Z. Phys.* **192**, 63 (1966).
[8] A. Fuliński, W. Kramarczyk, *Physica* **45**, 575 (1968).
[9] I. Gradshteyn, I. Ryzhik, *Tables of Integrals, Series and Products*, Academic Press, New York 1965.