

Thermodynamics of oscillators interacting with radiation

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1979 J. Phys. A: Math. Gen. 12 2151

(<http://iopscience.iop.org/0305-4470/12/11/024>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 19:14

Please note that [terms and conditions apply](#).

Thermodynamics of oscillators interacting with radiation

K Rzażewski

Institute of Theoretical Physics, Warsaw University, 00-681, Warsaw, Poland

Received 5 December 1978, in final form 12 February 1979

Abstract. We show that a system of charged harmonic oscillators interacting with one transverse electromagnetic field mode does not undergo the super-radiant phase transition. Our proof does not make use of the multipole expansion and takes retardation into account.

1. Introduction

The dependence of the thermodynamic properties of a gas on the interaction of atoms with the transverse radiation field has been studied extensively in the last few years. For the simple Dicke Hamiltonian (Dicke 1954), Hepp and Lieb (1973a) have proved the existence of a so-called super-radiant phase transition. Above a certain critical density of the atoms and below a critical temperature a condensed phase forms with a macroscopic population of the photon states.

It turns out that this phenomenon is due to an anomaly of the spectrum of the Hamiltonian considered, an anomaly which is absent in more realistic models describing electric dipole interaction of atoms with radiation (Rzażewski *et al* 1975).

In Białynicki-Birula and Rzażewski (1979) we have shown that, in a system of atoms interacting with a finite number of electromagnetic field modes in the electric dipole approximation, the partition function is independent of the interaction with the radiation.

It follows from this result that one has to include higher multipoles or take into account an infinite number of the field modes to have a chance of finding a non-trivial dependence of the equilibrium thermodynamic properties of a gas on the coupling to radiation.

In this paper we develop a method suitable for treating higher multipoles. The method is then applied to the harmonic oscillator model. The result is negative. The system does not undergo a second-order phase transition.

The thermodynamics of a certain many-oscillator model has been studied recently by Knight *et al* (1978), but their model is *not* derived from a minimal-coupling Hamiltonian and in no sense does it deal with higher multipoles.

2. The method

Let us consider a model consisting of N identical single-electron atoms located at fixed positions \mathbf{R}_j ($j = 1 \dots N$) and interacting with a single transverse electromagnetic field

mode of frequency ω , wavevector \mathbf{k} , polarisation $\boldsymbol{\epsilon}$. The non-relativistic electro-dynamics Hamiltonian for the system reads

$$H = \sum_{j=1}^N \{ (1/2m) [\mathbf{p}_j - (e/c)\mathbf{A}(\mathbf{R}_j + \mathbf{r}_j)]^2 + V(\mathbf{r}_j) + \hbar\omega a^\dagger a \} \quad (2.1)$$

where \mathbf{r}_j and \mathbf{p}_j denote the position and the canonical momentum of the electron in the j th atom, $V(\mathbf{r}_j)$ is the Coulomb potential binding the electrons in each atom, a, a^\dagger are annihilation and creation operators of the mode and the vector potential is given by

$$\mathbf{A}(\mathbf{R} + \mathbf{r}) = (2\pi\hbar c^2/\omega V)^{1/2} \boldsymbol{\epsilon} \{ \exp[i\mathbf{k} \cdot (\mathbf{R} + \mathbf{r})] a + \exp[-i\mathbf{k} \cdot (\mathbf{R} + \mathbf{r})] a^\dagger \} \quad (2.2)$$

where V denotes the volume of the cavity. Note that in the Hamiltonian (2.1) we have ignored direct atom–atom electrostatic interactions.

To find the equilibrium thermodynamic properties of the system we must compute the partition function

$$Z(N, T) = \text{Tr}[\exp(-\beta H)]. \quad (2.3)$$

We have to compute the trace over both field and atomic variables. This task is simplified greatly by the observation (Wang and Hioe 1973) that the leading term in the thermodynamic limit ($N \rightarrow \infty, V \rightarrow \infty, \rho = N/V$ fixed) comes from the normal ordering of the field operators[†] in equation (2.3). Therefore, using the coherent state representation for the field trace, we can simply replace creation and annihilation operators a^\dagger and a by the classical c number complex amplitudes α^*, α , with respect to which an integral must be performed at the end. Hence

$$Z(N, T) \xrightarrow{N \rightarrow \infty} \int (d^2\alpha/\pi) \exp(-\beta\hbar\omega|\alpha|^2) \prod_{j=1}^N \text{Tr}[\exp(-\beta h_j(\alpha))] \quad (2.4)$$

where $h_j(\alpha)$ is now simply the Hamiltonian of the j th atom in the external classical field of the amplitude α . This Hamiltonian can be written as the sum of three terms:

$$h_j(\alpha) = h_j^{(0)} + h_j^{(1)} + h_j^{(2)} \quad (2.5)$$

where (dropping the unnecessary index j)

$$h^{(0)} = (1/2m)\mathbf{p}^2 + V(\mathbf{r}) \quad (2.6)$$

is the free atomic Hamiltonian,

$$h^{(1)} = -(e/mc)\mathbf{p} \cdot \mathbf{A}(\mathbf{R} + \mathbf{r}) \quad (2.7)$$

is the usually included ' $\mathbf{p} \cdot \mathbf{A}$ ' term, and

$$h^{(2)} = (e^2/2mc^2)\mathbf{A}^2(\mathbf{R} + \mathbf{r}) \quad (2.8)$$

is the often neglected ' \mathbf{A}^2 ' term. The importance of this term in the study of thermodynamics has been repeatedly stressed by the present author.

For $N \rightarrow \infty$, the integral (2.4) can be computed by the saddle-point method. If the only saddle-point that appears is $\alpha = 0$, then we have the normal phase. A phase

[†] This widely used substitution has been proved by Hepp and Lieb (1973b) for two-level atoms, but the basic ingredient—the fact that creation and annihilation operators are entering the Hamiltonian through $a/\sqrt{N}, a^\dagger/\sqrt{N}$ —is universal and comes from normalisation of the vector potential.

transition is indicated by a switch from positivity to indefiniteness or possibly negativity of the quadratic form:

$$\beta \hbar \omega |\alpha|^2 + \frac{1}{2} \sum_{i,j}^2 (\partial^2 F(\alpha) / \partial x_i \partial x_j) x_i x_j \quad (\alpha = x_1 + ix_2) \quad (2.9)$$

where

$$F(\alpha) = \sum_{j=1}^N f_j(\alpha) = - \sum_{j=1}^N \ln \text{Tr}[\exp(-\beta h_j(\alpha))]; \quad (2.10)$$

that is, we rewrite equation (2.4) in the form

$$Z(N, T) \xrightarrow{N \rightarrow \infty} \int (d^2 \alpha / \pi) \exp(-\beta \hbar \omega |\alpha|^2 - F(\alpha)). \quad (2.11)$$

However, to study the positivity of the quadratic form (2.9) we do not need to know the function $F(\alpha)$ beyond its quadratic term in α . In other words, we do not need the exact energy levels of equation (2.5), but only their perturbative values up to second order in $\hbar^{(1)}$ and first order in $\hbar^{(2)}$.

First-order corrections to the trace coming from $\hbar^{(1)}$ usually vanish. The base usually exists in which all the diagonal elements of $\hbar^{(1)}$ are equal to zero. Then we get

$$f(\alpha) = -\ln \text{Tr}[\exp(-\beta h(\alpha))] \\ \approx -\ln \text{Tr}[\exp(-\beta h^{(0)})] + \beta \sum_n \exp(-\beta E_n^{(0)}) E_n^{(2)}(\alpha) / \text{Tr}[\exp(-\beta h^{(0)})] \quad (2.12)$$

where $E_n^{(0)}$ are the energy levels of $h^{(0)}$ and $E_n^{(2)}$ are the appropriate perturbative corrections. The sum in the numerator of the second term in equation (2.11) consists of two parts: one coming from $p \cdot A$ and the other coming from the A^2 term.

Simple representations for the perturbative corrections can be found in the literature (e.g. March *et al* 1967):

$$\sum_n \exp(-\beta E_n^{(0)}) \langle n | h^{(2)} | n \rangle = \text{Tr}[\exp(-\beta h^{(0)}) h^{(2)}] \quad (2.13)$$

and

$$\sum_n \exp(-\beta E_n^{(0)}) \sum_{n'} \frac{\langle n | h^{(1)} | n' \rangle \langle n' | h^{(1)} | n \rangle}{E_n^{(0)} - E_{n'}^{(0)}} \\ = -\frac{1}{2} \int_0^\beta d\tau \text{Tr}[\exp[(\tau - \beta) h^{(0)}] h^{(1)} \exp[-\tau h^{(0)}] h^{(1)}]. \quad (2.14)$$

To go any further we have to specify the potential in $h^{(0)}$ at this point.

3. Harmonic oscillators

In this section we will apply the method outlined above to the harmonic oscillator problem, for which, as we show here, a complete analytical solution can be found. One can easily check that in this case all the diagonal elements of $\hbar^{(1)}$ vanish in the occupation number base, and that formulae (2.13) and (2.14) hold.

Thus

$$h^{(0)} = (1/2m)p^2 + \frac{1}{2}m\omega_0^2 r^2 \quad (3.1)$$

where ω_0 is the frequency of free oscillations.

If we choose the reference frame such that $\mathbf{k} = (k, 0, 0)$ and $\boldsymbol{\epsilon} = (0, 1, 0)$, then the oscillations along the z axis will not be affected by the coupling to radiation and we deal effectively with a two-dimensional harmonic oscillator with unperturbed energy levels

$$E_{n_x, n_y}^{(0)} = \hbar\omega_0(n_x + n_y) \quad (n_x, n_y = 0, 1, 2 \dots) \quad (3.2)$$

and corresponding states $|n_x, n_y\rangle$,

$$|n_x, n_y\rangle = [(a_x^+)^{n_x} (a_y^+)^{n_y} / \sqrt{n_x! n_y!}] |0, 0\rangle, \quad (3.3)$$

created from the ground state by appropriate creation operators

$$\begin{aligned} x &= (\hbar/2m\omega_0)^{1/2} (a_x^+ + a_x), & p_x &= i(m\hbar\omega_0/2)^{1/2} (a_x^+ - a_x), \\ y &= (\hbar/2m\omega_0)^{1/2} (a_y^+ + a_y), & p_y &= i(m\hbar\omega_0/2)^{1/2} (a_y^+ - a_y). \end{aligned} \quad (3.4)$$

The interaction Hamiltonians, when expressed in terms of $a_{x,y}$ and $a_{x,y}^+$, read

$$h^{(1)} = -i(\hbar\omega_0/2m)^{1/2} (a_y^+ - a_y) \{ \gamma \exp[i\kappa(a_x^+ + a_x)] + \gamma^* \exp[-i\kappa(a_x^+ + a_x)] \} \quad (3.5)$$

and

$$h^{(2)} = (1/2m) \{ \gamma \exp[i\kappa(a_x^+ + a_x)] + \gamma^* \exp[-i\kappa(a_x^+ + a_x)] \}^2 \quad (3.6)$$

where

$$\gamma = e(2\pi\hbar\rho/\omega)^{1/2} (\alpha/\sqrt{N}) \exp(i\mathbf{k} \cdot \mathbf{R}) \quad (3.7)$$

and

$$\kappa = k(\hbar/2m\omega_0)^{1/2}.$$

We start with the computation of the A^2 contribution (2.13):

$$\text{Tr}[\exp(-\beta h^{(0)}) h^{(2)}]$$

$$\begin{aligned} &= \sum_{n_x, n_y} \exp(-\nu n_x) \exp(-\nu n_y) (1/2m) \\ &\quad \times \langle n_x | \{ \gamma \exp[i\kappa(a_x^+ + a_x)] + \gamma^* \exp[-i\kappa(a_x^+ + a_x)] \}^2 | n_x \rangle \end{aligned} \quad (3.8)$$

$$\begin{aligned} &= [1/2m(1 - e^{-\nu})] [(\gamma^2 + \gamma^{*2}) \exp(-2\kappa^2) \\ &\quad \times \sum_{n=0}^{\infty} (L_n(4\kappa^2)/n!) \exp(-\nu n) + 2\gamma\gamma^*/(1 - e^{-\nu})] \end{aligned} \quad (3.9)$$

where $\nu = \hbar\omega_0\beta$ is the dimensionless inverse temperature.

We have used here the well-known expression for the matrix element:

$$\langle n | \exp(isa^+ + ira) | n \rangle = \exp(-sr/2) L_n(sr)/n! \quad (3.10)$$

where L_n denotes Laguerre polynomials.

But now we can perform the remaining sum in equation (3.9) by recognising the generating function for Laguerre polynomials:

$$\sum_{n=0}^{\infty} t^n L_n(x)/n! = \exp[-xt/(1-t)]/(1-t). \quad (3.11)$$

The final result takes the form

$$\begin{aligned} \text{Tr}[\exp(-\beta h^{(0)})h^{(2)}] \\ = [1/2m(1 - e^{-\nu})^2]\{2\gamma\gamma^* + (\gamma^2 + \gamma^{*2}) \exp[-2\kappa^2(1 + e^{-\nu})/(1 - e^{-\nu})]\}. \end{aligned} \quad (3.12)$$

We turn now to the $p \cdot A$ sum. First we observe that the action of $\exp(\tau h^{(0)})$ and $\exp(-\tau h^{(0)})$ is just the free evolution of creation and annihilation operators for imaginary time:

$$\exp(\tau h^{(0)})a_{x,y}^+ \exp(-\tau h^{(0)}) = \exp(\xi)a_{x,y}^+ \quad (3.13a)$$

$$\exp(\tau h^{(0)})a_{x,y} \exp(-\tau h^{(0)}) = \exp(-\xi)a_{x,y} \quad (3.13b)$$

where $\xi = \hbar\omega_0\tau$.

By making repeated use of the Baker–Hausdorff formula as well as formulae (3.10) and (3.11), and introducing the dimensionless parameter ξ as an integration variable, we obtain

$$\begin{aligned} -[1/4m(1 - e^{-\nu})^3] \int_0^\nu d\xi [\exp(\xi - \nu) + \exp(-\xi)] \\ \times \{[(\gamma^2 + \gamma^{*2}) \exp\{-\kappa^2[(1 + e^{-\nu})/(1 - e^{-\nu}) + (e^{\xi-\nu} + e^{-\xi})/(1 - e^{-\nu})]\}] \\ + 2\gamma\gamma^* \exp\{-\kappa^2[(1 + e^{-\nu})/(1 - e^{-\nu}) - (e^{\xi-\nu} + e^{-\xi})/(1 - e^{-\nu})]\}]. \end{aligned} \quad (3.14)$$

When both contributions are added we finally obtain

$$\begin{aligned} f(\alpha) = f(\alpha = 0) + (\beta/m)(\text{Re } \gamma)^2 [1 + \exp[-2\kappa^2 \coth(\nu/2)]] \\ - 2\{\exp[-\kappa^2 \coth(\nu/2)]/\sinh(\nu/2)\} \\ \times \int_0^{\nu/2} \cosh[\kappa^2 \cosh x/\sinh(\nu/2)] \cosh x \, dx \\ + (\beta/m)(\text{Im } \gamma)^2 [1 - \exp[-2\kappa^2 \coth(\nu/2)]] \\ - 2\{\exp[-\kappa^2 \coth(\nu/2)]/\sinh(\nu/2)\} \\ \times \int_0^{\nu/2} \sinh[\kappa^2 \cosh x/\sinh(\nu/2)] \cosh x \, dx \end{aligned} \quad (3.15)$$

The expression, complicated as it is, may still be analysed. Since both $\sinh y$ and $\cosh y$ are monotonically increasing positive functions when $y > 0$, we find the estimates

$$\int_0^{\nu/2} \cosh[\kappa^2 \cosh x/\sinh(\nu/2)] \cosh x \, dx \leq \sinh(\nu/2) \cosh[\kappa^2 \coth(\nu/2)] \quad (3.16)$$

and similarly

$$\int_0^{\nu/2} \sinh[\kappa^2 \cosh x/\sinh(\nu/2)] \cosh x \, dx \leq \sinh(\nu/2) \sinh[\kappa^2 \coth(\nu/2)] \quad (3.17)$$

from which it follows that both terms in shadow brackets are non-negative. Therefore $f(\alpha)$ has a non-negative quadratic form in the expansion at $\alpha = 0$.

Although, due to the phase factors $\exp(i\mathbf{k} \cdot \mathbf{R})$, the normal directions for different oscillators are in general different, the sum of non-negative quadratic forms is still

non-negative and $\alpha = 0$ remains a local maximum for the interacting system independent of the values of the parameters such as mass, frequency, electric charge, oscillators' positions, temperature or κ (which is the ratio of the size of the first orbit of the oscillator to the wavelength of the field mode). The method developed in this paper is not strong enough to rule out a possibility of the appearance of a global maximum of the integrand in equation (2.4) completely separated from the ever-present local maximum at $\alpha = 0$. If this were the case, a first-order phase transition would be encountered. This seems very unlikely, however, because this never showed up in the exactly soluble models of matter plus radiation.

The result (3.15) is in complete agreement with our 'no-go theorem' (Białynicki-Birula and Rzążewski 1979). Indeed, if κ is set equal to zero (the electric dipole approximation) then all the α dependence (to second order in the present case) of $f(\alpha)$ vanishes.

Acknowledgment

The author thanks the Swiss National Science Foundation for financial support during his visit to the Institute for Theoretical Physics of the University of Zürich where this work was done.

References

- Białynicki-Birula I and Rzążewski K 1979 *Phys. Rev. A* **19** 301
Dicke R H 1954 *Phys. Rev.* **93** 99
Hepp K and Lieb E H 1973a *Ann. Phys., Lpz.* **76** 360
— 1973b *Phys. Rev. A* **8** 2517
Knight J M, Aharonov Y and Hsieh G T C 1978 *Phys. Rev. A* **8** 1454
March N H, Young W H and Sampanthar S 1967 *The Many-Body Problem in Quantum Mechanics* (Cambridge: UP) § 9.2.1
Rzążewski K, Wódkiewicz K and Żakowicz W 1975 *Phys. Rev. Lett.* **35** 432
Wang Y K and Hioe F T 1973 *Phys. Rev. A* **7** 831