Thermodynamics of two-level atoms interacting with the continuum of electromagnetic field modes

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We study the thermodynamic properties of two-level atoms interacting with all the modes of the electromagnetic field. We show that the presence of the A^2 term in the interaction Hamiltonian has two important consequences: The divergence difficulties noted previously for the all-mode problem are overcome, so that a formal thermodynamic limit exists; and the phase transition, which occurs in the single-mode case without the A^2 term, is absent.

In the last two years the concept of a phase transition in the Dicke model of superradiance was very extensively discussed.[1-5] From all of these papers a common result emerges: The phase transition occurs as long as the number of photon modes is held fixed. This conclusion is independent of the rotating-wave approximation. With Żakowicz, however, we have shown[6] that the A^2 term plays an important role in the thermodynamic properties of a system of two-level atoms, and that the presence of the phase transition in the Dicke Hamiltonian is due entirely to the neglect by previous workers of this term from the interaction Hamiltonian.

The problem becomes more complicated if more than one photon is admitted, and the continuum-of-modes case has never been solved. Furthermore, Hepp and Lieb[4] have pointed out that in the infinite-mode case there is an infrared problem and one should certainly include the A^2 term in the Hamiltonian. The results of our present paper support this opinion. The A^2 term removes, however, not only the infrared problem, but also the phase transition. Unfortunately, the result is formal. We are unable to prove rigorously the existence and the stability of the thermodynamic limit in this case. However, the important fact is that without the A^2 term the formal thermodynamic limit is divergent.[4] With the A^2 term included the formal limit exists and is finite.

The technique we will use to compute the asymptotic value of the partition function is a modification of the technique invented by Wang and Hioe.[2,3] The Hamiltonian in the case of m modes is

$$H=\frac{\hbar\omega_{ba}}{2}\sum_{j=1}^{N}\sigma_j^z+\sum_{i=1}^{m}\hbar\omega_i a_i^\dagger a_i + \frac{1}{\sqrt{N}}\sum_{j=1}^{N}(\sigma_j^+ + \sigma_j^-)\vec{\lambda}_0\sum_{i=1}^{m}\frac{\vec{\epsilon}_i}{\sqrt{\omega_i}}(a_i^\dagger + a_i) + \kappa\left(\sum_{i=1}^{m}\frac{\epsilon_i}{\sqrt{\omega_i}}(a_i^\dagger + a_i)\right)^2, \tag{1}$$

where

$$\vec{\lambda}_0=\omega_{ba}(2\pi\hbar)^{1/2}\rho^{1/2}\vec{d}_{ba}, \tag{2}$$

$$\kappa=(e^2/2m)2\pi\hbar\rho. \tag{3}$$

The vector $\vec{d}_{ba}$ is the transition dipole moment between states $|b\rangle$ and $|a\rangle$. Note that the dependence of the Hamiltonian on the frequencies of the particular modes is displayed explicitly in (1). The vectors $\vec{\epsilon}_i$ denote the polarization of ith transverse mode. After summation over all of the atomic states and integration over all of the imaginary parts of the coherent-state amplitudes for the modes, we arrive with the following expression for the canonical partition function $Z(N,T)$:

$$Z(N,T)=C\int_{-\infty}^{+\infty}dx_1\cdots dx_m\exp\left\{-\beta\left[\sum_{i=1}^{m}\omega_i x_i^2+4\kappa\left(\sum_{i=1}^{m}\frac{\vec{\epsilon}_i}{\sqrt{\omega_i}}x_i\right)^2\right]\right\}\left\{2\cosh\left(\frac{\beta\omega_{ba}\hbar}{2}\left[1+\frac{16}{\omega_{ba}^2 N}\left(\vec{\lambda}_0\sum_{i=1}^{m}\frac{\vec{\epsilon}_i}{\sqrt{\omega_i}}x_i\right)^2\right]^{1/2}\right)\right\}^N. \tag{4}$$

With a slight modification of the method of Wang and Hioe we can reduce this problem to a one-mode problem with an equivalent coupling constant Λ. To do so, we change variables in the m-fold integral (4). The new set of variables, $z_1,\ldots,z_m$, should satisfy

$$\sum_{i=1}^{m} \frac{\vec{\epsilon}_i}{\sqrt{\omega_i}} x_i = \epsilon \frac{\vec{\lambda}_0}{\lambda_0} z_1,$$

$$\sum_{i=1}^{m} \alpha_{ji} \vec{\epsilon}_i x_i = \epsilon \frac{\vec{\lambda}_0}{\lambda_0} z_j . \tag{5}$$

A detailed knowledge of the matrix α_{ij} is unimportant. All we must assure is that the quadratic form in the exponent does not contain the terms $z_1 z_j$ for $j = 2, \ldots, m$, and that the coefficient multiplying z_1^2 is equal to 1. The partition function becomes

$$Z(N,T) = C' \int_{-\infty}^{\infty} dz_1 \exp\left(-\beta z_1^2 + N \ln\left\{2\cosh\left[\frac{\beta\hbar\omega_{ba}}{2}\left(1+\frac{4\Lambda^2}{\omega_{ba}^2 N} z_1^2\right)^{1/2}\right]\right\}\right), \tag{6}$$

where

$$\Lambda^2 = \frac{4\lambda_0^2}{[(1/\lambda_0^2)\sum_{i=1}^{m}(\vec{\lambda}_0\vec{\epsilon}_i)^2/\omega_i^2]^{-1} + 4\kappa}. \tag{7}$$

This leads to the function $f_3(\rho)$ for the case considered here of m modes, and the A^2 term included in the atomic Hamiltonian,

$$f_3(\rho) = \frac{\hbar[(d_{ba})^{-2}\sum_{i=1}^{m}(\vec{d}_{ba}\vec{\epsilon}_i)^2/\omega_i^2]^{-1} + (8\pi\hbar e^2/2m)\rho}{8\pi d_{ba}^2 \omega_{ba}\rho}. \tag{8}$$

The properties of $f_3(\rho)$ may be compared with those of the corresponding functions $f_1(\rho)$ and $f_2(\rho)$ derived in Ref. 6. These previously derived functions are appropriate to the cases of one mode, no A^2 term in atomic Hamiltonian,

$$f_1(\rho) = \hbar\omega^2/8\pi d_{ba}^2\omega_{ba}\rho,$$

and of one mode with an A^2 term included in atomic Hamiltonian,

$$f_2(\rho) = \frac{\hbar\omega^2 + (8\pi\hbar e^2/2m)\rho}{8\pi d_{ba}^2\omega_{ba}\rho}.$$

Obviously, the properties of $f_3(\rho)$ are the same as the properties of $f_2(\rho)$. Therefore the phase transition cannot occur if realistic atomic parameters for d_{ba} and ω_{ba} are assumed.

What seems more important, however, is that expression (7) for the equivalent coupling constant Λ enables us to study the interaction with a continuum of modes in the limit of a very large cavity. Using the well-known relation

$$\sum_{\text{modes}} \rightarrow \frac{V}{(2\pi)^3} \sum_{\text{pol}} \int d^3k, \tag{9}$$

the relevant sum in the equation (7) can be evaluated as follows:

$$\frac{1}{d_{ba}^2}\sum_i \frac{(\vec{d}_{ba}\vec{\epsilon}_i)^2}{\omega_i^2} = \frac{1}{d_{ba}^2}\frac{V}{c^2(2\pi)^3}\int \frac{d^3k}{k^2}\sum_{\lambda=1}^{2}[\vec{d}_{ba}\cdot\vec{\epsilon}_\lambda(\vec{k})]^2$$

$$= \frac{V}{c^2(2\pi)^3}\frac{8\pi}{3}\int_0^{k_{\max}} dk = \frac{V}{c^2 3\pi^2} k_{\max}. \tag{10}$$

The cutoff[7] $k_{\max}$ is introduced at the value of the wave vector that corresponds to a wavelength of the order of a Bohr radius. We now see that for the problem of identical atoms in all space the function

$$f = \lim_{N,V\rightarrow\infty} f_3$$

in the thermodynamic limit becomes density independent and is equal to the asymptotic value of f_2 from Ref. 6,

$$f = f_{as} = \frac{\hbar e^2}{2m}\frac{1}{d_{ba}^2\omega_{ba}}. \tag{11}$$

As explained in Ref. 6, the Thomas-Reiche-Kuh sum rule requires $f_{as} > 1$, which excludes the possibility of a phase transition.

Note that without the A^2 term the equivalent coupling constant Λ, as defined by Wang and Hioe,[2] is infrared divergent in the thermodynamic limit when all of the modes are taken into account. This behavior was noted by Hepp and Lieb.[4] The contribution from the A^2 term eliminates this divergence, and leads to a finite value of Λ.

We conjecture that the phase transition in a few other examples of the model Hamiltonians worked out in Refs. 3 and 4 would also disappear if the contribution from the A^2 term were to be taken into account.[8]

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[7]One can avoid the dipole approximation for the two-level atom. The oscillating factor $\exp(i\vec{k}\cdot\vec{r})$ gives rise in this case to the natural form factor regularizing the integral (10). Its precise form depends on the transition considered; cf. J. R. Ackerhalt, J. H. Eberly, and P. L. Knight, in *Coherence and Quantum Optics*, edited by L. Mandel and E. Wolf (Plenum, New York, 1973), p. 635.
[8]For example, the model in which the atoms do not sit at the same point has the same thermodynamic properties as the one-point model. For a method to establish this result see Refs. 3 and 4.