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Superradiant phase transition in some generalized Dicke models

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Abstract. It is shown that a superradiant phase transition occurs for some generalized Dicke models containing a quadratic term in the vector potential. A possible physical interpretation of some aspects of the transition is suggested.

I. Introduction and summary

In reference ([1]), Hepp and Lieb showed for the first time the existence of a second-order phase transition in a model of a system of two-level atoms interacting with the radiation field invented by Dicke ([2]). The model was described by the following Hamiltonian:

$$H_N^1 = \nu a^* a + \varepsilon \sum_{i=1}^N S_i^3 + \frac{\lambda}{\sqrt{N}} \sum_{i=1}^N (S_i^+ a + S_i^- a^*) \quad (I.1)$$

defined on the Hilbert space $\mathcal{H}_N \equiv \mathcal{F} \otimes \mathcal{H}_N^a$, where \mathcal{F} is Fock space for one Boson (photon) and

$$\mathcal{H}_N^a = \bigotimes_{i=1}^N \mathbb{C}_i^2$$

is the Hilbert space for the assembly of N two-level atoms. The two-level atom or molecule at the i th site is described (see, e.g. ([13])) by spin operators $s_i^\pm = s_i^1 \pm i s_i^2$ and $s_i^3 (s_i^{(\alpha)}) = \frac{1}{2} \sigma_i^{(\alpha)}$, $\sigma_i^{(\alpha)}$, $\alpha = 1, 2, 3$, being the Pauli matrices), and a^* and a are the standard photon creation and annihilation operators. They called the phase transition 'superradiant', for reasons expounded at length in reference ([13]).

Hamiltonian equation (I.1) may be obtained by performing a number of approximations on the following 'exact' non-relativistic Hamiltonian describing the

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interaction of an ultraviolet cut-off quantized radiation field in a box with a system of N atoms:

$$H_N = \sum_{i=1}^N \left[\left(\mathbf{P}_i - \frac{e}{c} \mathbf{A}_\lambda(\mathbf{x}_i) \right)^2 / 2m_i + V(\mathbf{x}_i) \right] + \sum_{\mathbf{k}, \lambda} |\mathbf{k}| a^*(\mathbf{k}, \lambda) a(\mathbf{k}, \lambda) + W. \quad (I.2)$$

Above, $\mathbf{A}_\lambda(\mathbf{x})$ is the cut-off vector potential in the Coulomb gauge for a box of volume V , and W denotes the interaction between the atoms (see [1] or [9]). If on equation (I.2) we introduce the approximation of considering the atoms as two-level systems, and consider in addition only M photon modes, we obtain the Hamiltonian

$$\begin{aligned} H_N^2 \equiv & \sum_{m=1}^M v_m a_m^* a_m + \varepsilon \sum_{n=1}^N s_n^3 + \frac{1}{\sqrt{N}} \sum_{n=1}^N \sum_{m=1}^M |\lambda_{mn}(\mathbf{k}_m)| (a_m s_n^+ + a_m^* s_n^-) \\ & + \mu_{mn}(\mathbf{k}_m) (a_m s_n^- + a_m^* s_n^+) \} \\ & + \frac{e^2 \pi}{m} \sum_{n=1}^N \left[\sum_{m=1}^M \frac{1}{\sqrt{v_m}} (a_m e^{i\mathbf{k}_m \cdot \mathbf{x}_n} + a_m^* e^{-i\mathbf{k}_m \cdot \mathbf{x}_n}) \right]^2 + W \end{aligned} \quad (I.3)$$

defined on $\mathcal{H}_N^{(M)} \equiv \mathcal{F}^{(M)} \otimes \mathcal{H}_N^a$, $\mathcal{F}^{(M)}$ being now Fock space for M photon modes. To each mode is associated a wave vector \mathbf{k}_m , and $v_m = |\mathbf{k}_m|$ is the photon energy. Expressions for λ_{mn} , μ_{mn} , and ε are given in Appendix A.

It follows from these that

$$\mu_{mn}(\mathbf{k}_m) = \lambda_{mn}^*(-\mathbf{k}_m).$$

The dipolar approximation ([1], [8], [9]) consists in replacing the factor $e^{i\mathbf{k}_m \cdot \mathbf{x}_n}$ in equations (A.2) and (A.3) by one, whereby λ_{mn} and μ_{mn} become independent of n . Neglecting further ‘retardation effects’ (that is, replacing $d_{ba}(\mathbf{k}_m)$ in the expressions for λ_{mn} and μ_{mn} by $d_{ba}(\mathbf{0})$), and taking the wave functions in equations (A.2) and (A.3) to be real, one obtains

$$\mu_m = \lambda_m^* = \lambda_m.$$

The terms multiplying each λ_{mn} in equation (I.3) are called ‘rotating terms’, and those multiplying each μ_{mn} are called ‘counterrotating terms’. The approximation of putting all $\mu_{mn} = 0$ is referred to as ‘rotating-wave approximation’, and its meaning is discussed for instance in reference ([13]).

We see then that Hamiltonian H_N^1 is obtained from H_N^2 by the following successive approximations:

- one photon mode approximation;
- dipolar approximation;
- neglect of ‘retardation effects’;
- rotating-wave approximation;
- neglect of the quadratic term in the vector potential;
- neglect of the interaction W between atoms.

We remark that f) is not expected to be a good approximation because the atomic densities involved are very high (of the order of 10^{24} cm^{-3} ([10])).

In reference [2] (see also [3]), Hepp and Lieb proved that model (I.3) exhibits a phase transition of the same kind as model equation (I.1), provided approximations

b), c), e) and f) are retained. Rzażewski *et al.* ([5]) analysed the model with one photon mode, retaining b), c) and f), but relaxing e) and considering equal coupling constant coefficients of the rotating (λ) and counterrotating (μ) terms, and showed that the phase transition found in ([2], [3]) disappeared. They further extended this result to an arbitrary number of photon modes ([6]) as well as (non-rigorously, however) to the continuum limit. Their results showed the importance of the A^2 term, as it qualitatively alters the thermodynamic properties of the system. It is also expected to be of crucial importance in removing infrared divergences in the continuum limit, a fact shown heuristically in [6] and which had already been predicted in [2].

In this paper we study the following generalized Dicke model (as well as its multimode analogue):

$$H_N^3 \equiv \varepsilon s_N^3 + v a^* a + \lambda \sqrt{N(s_N^+ a + s_N^- a^*)} + \mu \sqrt{N(s_N^+ a^* + s_N^- a)} + \kappa(a + a^*)(a + a^*), \quad (I.4)$$

where $\mu = t\lambda$; $0 \leq t \leq 1$, ε , v and κ being real positive constants, and

$$s_N^{\pm, 3} \equiv \sum_{i=1}^N s_i^{\pm, 3}$$

This model differs from the one considered in [5] in that we do not require $\lambda = \mu$. It cannot strictly be obtained by performing approximations a), b), c), and f) on Hamiltonian H_N^2 , because it corresponds to taking \mathbf{A} Hermitian in the A^2 term, and non-hermitian in the $\mathbf{p} \cdot \mathbf{A}$ term. It is a perfectly reasonable model, however, both in view of the number of approximations listed above and because the roles played by the vector potential in the terms \mathbf{A}^2 and $\mathbf{p} \cdot \mathbf{A}$ are of an entirely different nature. Hence, making the rotating-wave approximation (or, in general, taking $\lambda \neq \mu$) and keeping \mathbf{A}^2 are viewed here as two independent effects, unrelated to each other.

The results, which we present in Section II, are the following: for fixed ρ there is an interval $[0, \alpha)$, $\alpha < 1$, of values of t where the model exhibits a superradiant phase transition, while for $t \in [\alpha, 1]$ one has the situation reported in [5], where no phase transition occurs. In Section II we prove that the phase transition persists with an arbitrary but finite number M of photon modes, provided approximations b), c), d) and f) are retained. In Section IV we suggest a possible physical interpretation for some aspects of the transition.

Finally, some results of this paper were also obtained independently by Gilmore and Bowden, by different (and more general) methods ([7]). There has also been a recent but not very detailed discussion of these and related questions in reference [12]: in particular, their treatment obscures the remarkable fact that the free energy becomes independent of κ in the cases where there is a phase transition.

II. Results for one photon mode

We now consider Hamiltonian H_N^3 . As in reference [2], one may prove that the free energy f_β per atom in the thermodynamic limit corresponding to H_N^3 , defined as usual by

$$f_\beta \equiv -\beta^{-1} \lim_{N \rightarrow \infty} (N^{-1} \log \text{tr}_{\mathcal{H}_N} e^{-\beta H_N^3}) \quad (II.1)$$

is equal to

$$f_\beta = -\beta^{-1} \lim_{N \rightarrow \infty} (N^{-1} \log Z_{N\beta}^{cl}) \quad (II.2)$$

where

$$Z_{N\beta}^{cl} \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \exp\{-\beta[v(x_1^2 + x_2^2) + 4\kappa x_1^2]\} \cdot \left[2 \cosh \left\{ \frac{\beta\varepsilon}{2} \left(1 + \frac{4}{N\varepsilon^2} [(\lambda + \mu)^2 x_1^2 + (\lambda - \mu)^2 x_2^2] \right) \right\} \right]^N \quad (II.3)$$

is the partition function with the photon operators ‘made classical’ by substituting the trace on \mathcal{F} by an integration over the coherent photon states, see ([2]). Introducing new constants

$$a \equiv \frac{v + 4\kappa}{(\lambda + \mu)^2} \quad b \equiv \frac{v}{(\lambda - \mu)^2} \quad (II.4)$$

and changing to polar coordinates

$$x_1 = \frac{r \cos \theta}{\lambda + \mu} \quad x_2 = \frac{r \sin \theta}{\lambda - \mu}$$

and putting $y = r^2/N$, we obtain

$$Z_{N\beta}^{cl} \equiv \int_0^{\infty} dy \int_0^{2\pi} d\theta \exp[-Nf(\theta, y)], \quad (II.5a)$$

where

$$f(\theta, y) \equiv \beta y(a \cos^2 \theta + b \sin^2 \theta) - \log [q(y)], \quad (II.5b)$$

$$q(y) \equiv 2 \cosh \left[\frac{\beta\varepsilon}{2} (1 + 4y/\varepsilon^2)^{1/2} \right].$$

Using now Laplace’s method, minimizing the function f first with respect to θ , we find

$$\frac{\partial f(\theta_1 y)}{\partial \theta} = -\beta y \sin(2\theta) \cdot (a - b) \quad (II.6)$$

$$\frac{\partial^2 f(\theta_1 y)}{\partial \theta^2} = -2\beta y \cos(2\theta) \cdot (a - b). \quad (II.7)$$

If $a > b$, we see by equation (II.6, 7) that the minimum occurs at $\theta = \pi/2$, while if $a < b$, it occurs at $\theta = 0$. In any case find

$$Z_{N\beta}^{cl} \approx \frac{1}{2\sqrt{2\pi N\beta}|(a - b)/2|} \int_0^{\infty} \frac{dy}{\sqrt{y}} [q(y)]^N e^{-Nm\beta y} \quad (II.8)$$

where

$$m \equiv \min(a, b). \quad (II.9)$$

The condition for a phase transition is

$$\frac{1}{m} > \varepsilon. \quad (\text{II.10})$$

The critical temperature is given by

$$\varepsilon m = \tanh \left(\beta_c \frac{\varepsilon}{2} \right) \quad (\text{II.11})$$

and the energy per particle in the ground state in the thermodynamic limit ($\lim_{\beta \rightarrow \infty} f_\beta$) is given by

$$\varepsilon_0 = - \frac{\varepsilon}{4} \left(\frac{1}{m\varepsilon} + m\varepsilon \right) \left(\leq - \frac{\varepsilon}{2} \right). \quad (\text{II.12})$$

If $a > b$, we obtain from equation (II.8) the same free energy with $\kappa = 0$ equal to Hepp and Lieb's in ([1]). Hence two conditions are necessary and sufficient for a phase transition:

$$\rho > \rho_c^2 \equiv \frac{v^2}{2\pi\hbar^2\omega_{ba}d_{ba}^2(1-t)^2} \quad (\text{II.13})$$

which is equivalent to (II.10) ([5]) and

$$\rho > \rho_c^1 \equiv \frac{m\omega^2}{\pi e^2\hbar} \frac{t}{(1-t)^2} \quad (\text{II.14})$$

which is equivalent to $a > b$ ([5]). By the Thomas-Reiche-Kuhn sum rule ([11]) it follows that

$$d_{ba}^2\omega_{ba} < e^2\hbar/2m \quad (\text{II.15})$$

which implies $\rho_c^2 > \rho_c^1$, thereby reducing conditions (II.13) and (II.14) to condition (II.13). Clearly from (II.13) there exists for fixed ρ an interval $[0, \alpha)$, $\alpha < 1$, such that for $t \in [0, \alpha)$, $\rho > \rho_c^2$ and there is a phase transition, while for $t \in [\alpha, 1]$, $\rho < \rho_c^2$ and the phase transition disappears.

III. Case of several photon modes

In this section, we arrive at a result similar to that of Section II, but with an arbitrary but finite number of modes. The result is true for arbitrary $0 \leq \mu_m < \lambda_m$, $m = 1, \dots, M$, but we illustrate it for the simpler case $\mu_m = 0$, $m = 1, \dots, M$. The Hamiltonian is then

$$H_N^4 \equiv \sum_{m=1}^M v_m a_m^* a_m + \varepsilon s_N^3 + \frac{1}{\sqrt{N}} \sum_{m=1}^M [\lambda_m (a_m s_N^+ + a_m^* s_N^-)] + \kappa \left(\sum_{m=1}^M \frac{a_m + a_m^*}{\sqrt{v_m}} \right)^2. \quad (\text{III.1})$$

The ‘semi-classical’ partition function $Z(N, T)$ which yields by the methods of ([2]) the correct free energy in the thermodynamic limit is

$$Z(N, T) = \frac{1}{\pi^M} \int \cdots \int d^2\alpha_1 \dots d^2\alpha_M \exp \left\{ -\beta \left[\sum_{m=1}^M (a_m x_m^2 + v_m y_m^2) \right. \right. \\ \left. \left. + \sum_{i>j=1}^M a_{ij} x_i x_j \right] \right\} \\ \cdot \left\{ \cosh \left[\frac{\beta \varepsilon}{2} \left(1 + \frac{4}{N \varepsilon^2} |\lambda_1 \alpha_1 + \dots + \lambda_M \alpha_M|^2 \right)^{1/2} \right] \right\}^N \quad (\text{III.2})$$

where

$$d^2\alpha_i = dx_i dy_i \quad \alpha_i = x_i + iy_i \quad a_i = v_i + 4\kappa/v_i \\ a_{ij} \equiv 8/\sqrt{v_i v_j}. \quad (\text{III.3})$$

Through a transformation of type

$$\xi X^i \equiv \sum_j \xi_{ij} x_j \quad \lambda Y^i = \sum_j \lambda_{ij} y_j \quad (\text{III.4})$$

it is possible, in close analogy to ([3]), to make the coefficient of the new coordinates $(x^1)^2$ and $(y^1)^2$ equal to one, eliminate the cross products $x^i x^j$ and $y^i y^j$ for $j \geq 2$ and restrict the new coordinates to satisfy the following condition:

$$|\lambda_1 \alpha_1 + \dots + \lambda_M \alpha_M|^2 = \xi^2 (X^1)^2 + \lambda^2 (Y^1)^2. \quad (\text{III.5})$$

One finds

$$\lambda^2 = \sum_{i=1}^M \lambda_i^2 v_i^{-1}.$$

One need not evaluate ξ . Apart from an irrelevant term (in the thermodynamic limit) the partition function reads

$$Z(N, T) = \int_{-\infty}^{\infty} dX^1 \int_{-\infty}^{\infty} dY^1 \exp[-\beta((X^1)^2 + (Y^1)^2)] \\ \times \left[\cosh \left\{ \frac{\beta \varepsilon}{2} \left[1 + \frac{4}{N \varepsilon^2} (\xi^2 (X^1)^2 + \lambda^2 (Y^1)^2) \right] \right\} \right]^N \quad (\text{III.6})$$

Calculating the corresponding free energy in the thermodynamic limit, we find for the inverse critical temperature β_c :

I) If $\xi < \lambda$

$$\beta_c = \begin{cases} \frac{2}{3} \tanh^{-1} (\varepsilon/\lambda^2) & \text{if } \varepsilon < \lambda^2 \\ \infty & \text{if } \varepsilon \geq \lambda^2 \end{cases} \quad (\text{III.7})$$

II) If $\xi > \lambda$

$$\beta_c = \begin{cases} \frac{2}{3} \tanh^{-1} (\varepsilon/\lambda^2) & \text{if } \varepsilon < \xi^2 \\ \infty & \text{if } \varepsilon \geq \xi^2 \end{cases} \quad (\text{III.8})$$

Hence in both cases $\beta_c < \infty$ or $T_c > 0$ if $\varepsilon < \lambda^2$. This condition holds for

$$\rho > \rho_c^3 \equiv \hbar \omega_{ba} \left[\omega_{ba}^2 (2\pi\hbar) d_{ba}^2 \left(\sum_{i=1}^M v_i^{-2} \right) \right] \quad (\text{III.9})$$

IV. Physical discussion

We see that for $a > b$, which is favoured by κ large, the free energy becomes independent of κ . Physically, this must be the same effect occurring in the theory of diamagnetism (which comes from the A^2 term), where the classical partition function is not altered by the presence of the magnetic field. Also in the theory of superconductivity, if the Meissner effect is considered as perfect diamagnetism.

We now suggest an interpretation of the phase transition in more physical terms. To fix ideas, consider Hamiltonian equation (I.1). Its ground state ([1], page 382) is an atomic coherent state, which has a macroscopic dipole moment. This is easily seen from the fact ([1], page 368) that a variational Hamiltonian yielding a free energy equal to the exact free energy for $T < T_c$ is the following ‘Bogoliubov effective Hamiltonian’:

$$H_N(\alpha) \equiv b_N^* b_N + \lambda^2/2 \sum_{j=1}^N (1 - \mathbf{\sigma}_j \cdot \mathbf{e}) + N(|\alpha|^2 - \lambda^2/2) \quad (\text{IV.1})$$

where α is a complex number such that $b_N = a - \alpha/N$, and which is also related to the unit vector \mathbf{e} by

$$\mathbf{e} = \lambda^{-1}(\alpha + \alpha^*, i\lambda(\alpha - \alpha^*), -\varepsilon) \quad (\text{IV.2})$$

The vacuum state $|0\rangle_N$ of the boson operators b_N satisfies $b_N|0\rangle_N = 0$ and is therefore a coherent state for a , with an average number of photons $0(N)$. It may be shown (see [1], or ([13], page 229)) that there is indeed a ‘frozen in’ macroscopic electromagnetic field in the (infinite-volume) ground state of (I.1), and we see from (IV.2) that \mathbf{e} is determined by the alignment of the dipole moment with the ‘local field’. It seems therefore plausible that the phase transition in the generalized Dicke model be analogous to a ferroelectric phase transition, which takes place when the ‘local field’ becomes very large and the polarizability diverges (Clausius-Mosotti catastrophe). This argument would clarify the role played by the Thomas-Reiche-Kuhn sum rule ([11]) in reference ([5]) to exclude a phase transition in model (I.4) with $\lambda = \mu$: as is well known ([11]), this sum rule provides an upper bound to the polarizability. It remains an open problem to make this argument more quantitative, providing a distinction between the two cases $\lambda = \mu$ and $\lambda \neq \mu$ in model (I.4) along this line of ideas.

Appendix A

We give here the well-known explicit formulae for λ_{mn} , μ_{mn} and ε in (I.3):

$$\varepsilon = \omega_{ba} = E_b - E_a \quad (\text{A.1})$$

$$\lambda_{mn}(\mathbf{k}_m) = e\omega_{ba}d_{ba}(\mathbf{k}_m)(2\pi\rho)^{1/2}v_m^{-1/2} e^{i\mathbf{k}_m \cdot \mathbf{x}_n} \quad (\text{A.2})$$

$$\mu_{mn}(\mathbf{k}_m) = e\omega_{ba}d_{ba}^*(-\mathbf{k}_m)(2\pi\rho)^{1/2}v_m^{-1/2} e^{i\mathbf{k}_m \cdot \mathbf{x}_n} \quad (\text{A.3})$$

where

$$d_{ba}(\mathbf{k}_m) = \int d^3\xi \psi_{a,n}^*(\xi) e^{i\mathbf{k}_m \cdot \xi} (\hat{\varepsilon}_m \cdot \xi) \psi_{b,n}(\xi) \quad (\text{A.4})$$

is the matrix element of the dipole moment operator between the two atomic states of energies E_a and E_b ($E_b > E_a$), of wave functions ψ_a and ψ_b , respectively. Above, ε_m is a polarization vector, and ρ denotes the atomic density.

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