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A.Klemm, V.A.Zagrebnov

A COMPRESSIBLE DICKE MODEL (EXACT SOLUTION)

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A.Klemm,* V.A.Zagrebnov

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* On leave of absence from Technical University Dresden, GDR.

Клемм А., Загребнов В.А.

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Сжимаемая модель Дикке (точное решение)

Рассмотрена модель Дикке с фононными степенями свободы. Показано, что взаимодействие с пространственно неоднородным электромагнитным полем может привести к фазовому переходу первого рода. Плотность свободной энергии при $|\Lambda|$, $N \to \infty$ вычислена точно.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований
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Klemm A., Zagrebnov V.A.

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A Compressible Dicke Model
(Exact Solution)

The thermodynamic properties of a generalized Dicke model including: (i) the spatial variation of electromagnetic field, (ii) classical Debye vibrations of atoms around their equilibrium positions, are investigated in the thermodynamic limit exactly and rigorously. Contrary to ordinary case our model may have a transition of the first-order type accompanied by Bose-condensation of a phonon mode.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. Introduction

The interaction of an ultraviolet cut-off quantized radiation field in a box Λ with a system of N atoms is described by the following Hamiltonian [1]

$$H_\Lambda = \sum_{j=1}^{N} \{ \frac{1}{2m} (\mathbf{p}_j - \frac{e}{c} \mathbf{A}_\Lambda(\mathbf{x}_j))^2 + U_j(\mathbf{x}_j) \} + H_{phot}(\Lambda), \quad (1.1)$$

where $\mathbf{A}_\Lambda(\mathbf{x})$ can be expressed by the boson operators $b^*(\mathbf{k},\kappa)$:

$$\mathbf{A}_\Lambda(\mathbf{x}) = \sum_{\kappa} \sum_{|\mathbf{k}|<K} \frac{1}{\sqrt{\omega_k}} \frac{\mathbf{e}(\mathbf{k},\kappa)}{\sqrt{|\Lambda|}} \{ b(\mathbf{k},\kappa) e^{i\mathbf{k}\mathbf{x}} + b^+(\mathbf{k},\kappa) e^{-i\mathbf{k}\mathbf{x}} \}. \quad (1.2)$$

Here ω_k is the spectrum of the photons in the box Λ, $|\Lambda|$ is the volume of Λ and $(\mathbf{k}, \mathbf{e}(\mathbf{k},\kappa)) = 0$, $H_{phot}(\Lambda)$ is the Hamiltonian of the free transversal photons in Λ. Momentum $\mathbf{p}_j$ corresponds to a single electron in the j-th atom, $U_j(\mathbf{x}_j)$ is the interaction potential between them and $\mathbf{A}_\Lambda(\mathbf{x}_j)$ is the vector-potential of the electromagnetic field at the position of j-th atom.

An interesting approximation of the real situation described by Hamiltonian (1.1) has been invented by Dicke [2]

$$H_{\Lambda,N} = \omega_k b^+ b + \epsilon \sum_{j=1}^{N} \sigma_j^z + \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} (\sigma_j^+ b + \sigma_j^- b^+), \quad (1.3)$$

where σ_j^{α} $(\alpha = x, y, z)$ are spin-1/2 operators, $\sigma_j^{\pm} = \sigma_j^x \pm i\sigma_j^y$.

(i) Here only one mode of electromagnetic field with the energy ω_k and wave-vector k is retained.

(ii) Hamiltonian (1.3) corresponds to N two-level atoms having energy spacing $\epsilon > 0$.

(iii) The interaction with electromagnetic field has been simplified according to the "rotating wave approximation", namely, terms like $\sigma_j^+ b^+$ and $\sigma_j^- b$ have been omitted.

(iv) The atoms are considered to be at fixed positions, without any interaction between them.

(v) The spatial variation of the radiation field has been neglected, i.e., coupling constant λ is independent of j.

(vi) The $\mathbf{A}^2(x_j)$-terms are supposed to be negligible and the linear $\mathbf{A}(x_j)$ -terms are investigated in the dipole approximation.

The procedure of transition from (1.1) to (1.3) with conditions (i)-(vi) was described in detail by Haken [1].

As has been shown by different methods in papers [3, 4] and [5,6] for the system (1.3) one can calculate the free energy per atom in the thermodynamic limit $|\Lambda| \to \infty$, $N \to \infty$, $\frac{|\Lambda|}{N} = \text{const}$ exactly and rigorously. Note, that interaction discussed in these papers has a more general form than (1.3). First, the generalization to the finite multimode case, to which the methods of [3-6] can be applied, was considered. Therefore the restriction (i) is irrelevant. The difficulties arising in the infinite mode cases were discussed in [4]. Second, the methods of [4, 5], were shown to work if the "rotating wave approximation" (iii) was violated. At last, the generalization to multilevel atoms can be done in the framework of the methods [4, 5] without any difficulties (compare (ii)) and $\mathbf{A}^2(x_j)$ -terms can be taken into account [7] (compare (vi)). Recently, in paper [8] some nonlinear generalizations of Dicke model (1.3) have been proposed.

The most unsatisfactory restriction in (1.3) is (v) (see discussion in [4]). The thermodynamic properties of the model (1.1), (1.3) can be evaluated exactly only in the thermodynamic limit, thus (v) corresponds to an interaction with the electromagnetic field only of wave-vector $k = 0$. This is an unrealistic situation, because the electromagnetic field in a macroscopic cavity may have $|k|^{-1}$ comparable with the separations between atoms of matter.

In papers [4, 9-12] (see also Appendix) it was shown that restriction (v) can be violated, in this case one can also calculate the free energy per atom in the thermodynamic limit exactly. The thermodynamic properties of a system with the spatial variation of the radiation field $(k \neq 0)$ are similar to those with $k = 0$ (see, e.g., Appendix).

The important generalization is $k \neq 0$ and violation of (iv). In this case one has an interaction between photons with $k \neq 0$ and phonons. Such a generalization for a finite length cavity has been considered by Hioe [10] (see also [12]). The atoms were assumed to make small classical motions about their equilibrium positions (Einstein phonons). The thermodynamic properties of such a system, as was stated by Hioe [10], coincide with the ones of a system without vibrations of atoms *.

In this paper we also consider a Dicke model with atoms, which are not held rigidly in their equilibrium positions. But we correct the model described by Hioe [10] in the two important points:

a) in contrast to the Einstein vibrations we consider a collective motion of the atoms, described by the classical Debye phonons,

b) instead of the cavity finite in the thermodynamic limit, we consider the infinite one (see fig. 1 and fig. 2,

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*Linear extra terms which describe the phonon absorption and emission associated with the Brillouin scattering are added to the usual Dicke model by Thompson [11]. In this case the transition may be of the first-order type. The rigorous treatment of analogous classical case leads to the same result.

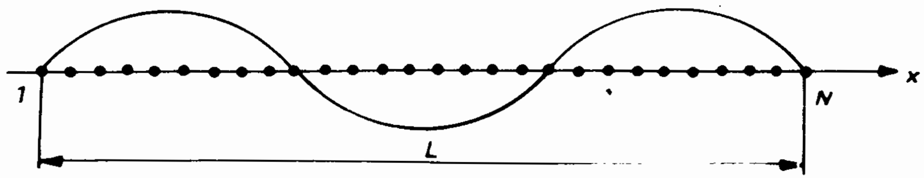

Fig. 1. Spatial dependence of the electromagnetic field amplitude in the Hioe model C [10]. *Here* L *- the length of the cavity.*

fig. 7). Then photons with wave-vector k interact strongly only with those longitudinal phonons (acoustic or optic) which wave-vectors q are collinear and comparable with k (see [13, 14]). This is the reason for taking into consideration the interaction with only one longitudinal harmonic phonon mode $q = k$. Therefore the physical picture of the interaction is quasi one-dimensional because in two other directions there is a translation invariance. We show that the properties of such a model can be examined in the thermodynamic limit by the method described previously in papers [5, 6] (see also Appendix). They are different from the thermodynamic properties of the previous generalization of the Dicke model [10, 12]. In our model a Bose-condensation of classical phonons $q = k$, accompanied by macroscopic lattice-distortions [15], is possible. This leads to a first order phase transition (in contrast to [10, 12]) into the superradiant state accompanied by the structural distortion of the lattice.

In section 2 we explicitly describe the conventional Hamiltonian of the system under consideration. It is the

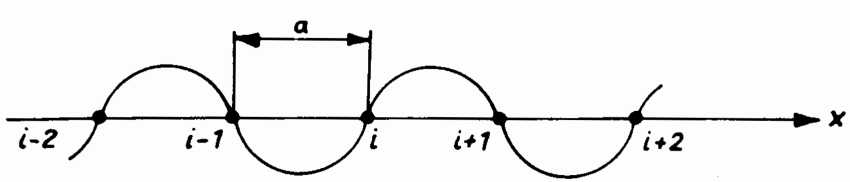

Fig. 2. Spatial dependence of the electromagnetic field amplitude in our model for the case $Q = \pi / a$, $\phi = 0$.

simplest one-mode generalization to the compressible Dicke model with spatial variation of the radiation field. We use the generalized Bogolubov (Jr.) method developed in [5, 6] (see also the applications of this method in [16, 17]) for the proof that the free energy per atom can be calculated for our model in the thermodynamic limit exactly and rigorously.

In section 3 we analyze the thermodynamic properties of the compressible Dicke model and show the possibility of the first order phase transition into the superradiant state accompanied by the Bose condensation of phonons (structural phase transition, compare [15, 16]).

We conclude this paper (section 4) with some remarks about the thermodynamic properties and the admissible generalization of the model described in section 2.

2. *The Hamiltonian*

As was pointed out in section 1 the assumption that all atoms of the system interacting with radiation see exactly the same field even in the thermodynamic limit is unrealistic. We relax this restriction (see (v) in section 1) by considering the spatial variation of the electromagnetic field in one direction, which coincides with axis 0X, i.e. k is collinear to 0X. We consider the interaction with the sinusoidal standing electromagnetic wave (the running-wave case is equivalent to the original Dicke model (1.3), see [3] and Appendix). This corresponds to a system placed in a macroscopic rectangular cavity with one axis being parallel to 0X. The system is supposed to be an N-particle compressible crystal with two-level atoms in the sites of the lattice, thus we relax the restriction (iv) (see section 1). Therefore this system is a quasi-one-dimensional compressible Dicke model with sinusoidal spatial variation of the electromagnetic field of given phase ϕ.

So consider the Hamiltonian of the system to be given by (cf. (1.3))

$$H = \omega_k b^+ b + \epsilon \sum_{j=1} \sigma_j^z + \frac{1}{\sqrt{N}} \sum_{j=1} \lambda_j (\sigma_j^+ b + \sigma_j^- b^+) + H_{ph} , \tag{2.1}$$

where

$$\lambda_j = \lambda \sin(kR_j + \phi) . \tag{2.2}$$

Here $R_j = l_j + u_j$ is the position of the j-th atom of mass m, u_j denotes its displacement from the lattice equilibrium position l_j and $kl_j = kja e_x$, where e_x is the unit vector of the axis 0X, a is the lattice constant of the crystal. The Hamiltonian of the classical harmonic lattice is denoted by H_{ph}:

$$H_{ph} = \sum_{j=1}^{N} \frac{p_j^2}{2m} + \frac{1}{2} \sum_{i,j=1}^{N} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta , \tag{2.3}$$

where $\Phi_{ij}^{\alpha\beta}$ are the elements of the force constant matrix of the solid $(\alpha, \beta = x, y, z)$.

Let us represent the displacements $\{u_j\}$ as superpositions of the classical harmonic modes q:

$$u_j^\alpha = \frac{1}{\sqrt{N}} \sum_q e^{iql_j} u_q^\alpha . \tag{2.4}$$

As was pointed out in section 1, the strongest interaction between classical vibrations and electromagnetic field (2.2) occurs if $q = k = Q$. Therefore in (2.1), (2.2) we can restrict ourselves to the one-mode approximation:

$$u_j^\alpha = \frac{1}{\sqrt{N}} (e^{iQl_j} u_Q^\alpha + e^{-iQl_j} u_{-Q}^\alpha) = \frac{2}{\sqrt{N}} |u_Q| \cos(Ql_j + \psi) e_Q^\alpha , \tag{2.5}$$

e_Q^α are the components of the unit phonon polarization vector.

Using the method of papers /5, 6/ it can be shown (see Appendix), that for any fixed set of parameters $\{u_j, \phi\}$ the Hamiltonian (2.1) is thermodynamically equivalent to the following one:

$$H_0(\bar\eta, \bar\eta^*, \{u_j, \phi\}) = \omega_Q (b^+ + \frac{1}{\omega_Q} \sqrt{N} \bar\eta^*)(b + \frac{1}{\omega_Q} \sqrt{N} \bar\eta) + \epsilon \sum_{j=1}^{N} \sigma_j^z - \frac{1}{\omega_Q} \sum_{j=1}^{N} \lambda_j (\bar\eta^* \sigma_j^- + \bar\eta \sigma_j^+) + \frac{N}{\omega_Q} |\bar\eta|^2 + H_{ph} , \tag{2.6}$$

where $\bar\eta, \bar\eta^*$ realize for fixed $\{u_j, \phi\}$ the absolute minimum of the free energy per particle:

$$f_N [H_0(\eta, \eta^*, \{u_j, \phi\})] = -\frac{\theta}{N} \ln \mathrm{Tr} \exp(-\beta H_0), \tag{2.7}$$

here β is the inverse temperature, $\beta = \theta^{-1}$. This means (see (A.6)), that

$$|f_N[H(\{u_j, \phi\})] - f_N[H_0(\bar\eta, \bar\eta^*, \{u_j, \phi\})]| < \epsilon_N$$
$$\lim_{N \to \infty} \epsilon_N = 0 \tag{2.8}$$

uniformly with respect to $\{u_j^\alpha, \phi\}$, because in this case the coupling constants λ_j (2.2) satisfy (A.2). Therefore in the thermodynamic limit the free energy per particle of the compressible Dicke model (2.1)-(2.3) (one-mode approximation $q = Q$) is rigorously expressed (see Appendix) as

$$g(\theta) = \lim_{N \to \infty} \{ -\frac{\theta}{N} \ln [\int_0^\infty d\xi_Q \sqrt{N} \int_0^{2\pi} d\psi \exp\{-\beta N (f_N[H_0(\xi_Q, \psi)] + \frac{\Omega_Q^2}{2} \xi_Q^2)\}]\} + f_N[H'_{ph}] ,$$

$$\xi_Q = \frac{|u_Q|}{\sqrt{N}} , \tag{2.9}$$

$g(\theta)$ is obtained by averaging the partition function

$$Z_N[H_0(\xi_Q, \psi)] \equiv$$
$$\equiv \exp(-\beta N f_N[H_0(\bar{\eta}(\xi_Q,\psi), \bar{\eta}^*(\xi_Q,\psi), \{\xi_Q \psi, \phi\})])$$

with a Gaussian-type weight function $\exp(-\beta N \frac{\Omega_Q^2}{2}\xi_Q^2)$ (compare (A.7)). In (2.9) H'_{ph} coincides with the Hamiltonian of harmonic lattice (2.3) from which the contribution of one longitudinal mode $|\mathbf{q}| = Q$ with polarization $\mathbf{e}_Q^{a} = \mathbf{e}_Q^{x}$ is subtracted. This contribution is equal to $N\frac{\Omega_Q^2}{2}\xi_Q^2$, where Ω_Q is the corresponding frequency and $\xi_Q = \frac{|\mathbf{u}_Q|}{\sqrt{N}}\mathbf{e}_Q^x$ (2.5). Thus $f[H'_{ph}]$ is a smooth function of the temperature θ.

In the thermodynamic limit $N \to \infty$, $|\Lambda| \to \infty$, $\frac{|\Lambda|}{N} = v$ the integral (2.9) can be calculated exactly by the steepest descent method, therefore

$$g(\theta, v) = \lim_{N\to\infty} f_N[H_0(\bar{\xi}_Q, \bar{\psi})] + \frac{\Omega_Q^2}{2}\bar{\xi}_Q + f[H'_{ph}], \qquad (2.10)$$

where $\bar{\xi}_Q$ and $\bar{\psi}$ imply the absolute minimum of the function $f_N[H_0(\bar{\eta}(\xi_Q,\psi), \bar{\eta}^*(\xi_Q,\psi), \xi_Q,\psi)] + \frac{\Omega_Q^2}{2}\xi_Q^2$. Let us denote

$$\tilde{H}_0(\eta,\eta^*,\xi_Q,\psi) = H_0(\eta,\eta^*,\xi_Q,\psi) + \frac{\Omega_Q^2}{2}\xi_Q^2. \qquad (2.11)$$

Then the solutions of the equations

$$\frac{\partial}{\partial\eta} f_N[\tilde{H}_0(\eta,\eta^*,\xi_Q\,\psi)] = 0; \quad \frac{\partial}{\partial\eta^*} f_N[\tilde{H}_0(\eta,\eta^*,\xi_Q,\psi)] = 0;$$
$$\frac{\partial}{\partial\xi_Q} f_N[\tilde{H}_0(\eta,\eta^*,\xi_Q,\psi)] = 0; \quad \frac{\partial}{\partial\psi} f_N[\tilde{H}_0(\eta,\eta^*,\xi_Q,\psi)] = 0, \qquad (2.12)$$

corresponding to abs-min $f_N[\tilde{H}_0(\eta,\eta^*,\xi_Q,\psi)]$ give us an exact and rigorous solutions the problem of the compressible Dicke model (2.1) in the one-mode approximation $\mathbf{q} = \mathbf{Q}$ (2.5).

3. *Thermodynamics*

The thermodynamic properties of the system (2.1)-(2.5) can be investigated in the limit $N \to \infty$, $|\Lambda| \to \infty$, $\frac{|\Lambda|}{N} = v$ from the free energy per particle (2.10) and equations (2.12).

A. In this paper we analyse, at first, an important case $k = q = Q = \frac{\pi}{a}$ and $\phi = 0$ (2.2). This choice of the electromagnetic field parameters corresponds to the highly "unstable model", because for the rigid lattice there is no interaction between field and atoms.(see fig. 2). Thus for such a system the restrictions (iv) and (v) (see section 1) are the most critical: Interaction appears only if we relax point (iv). A consequence is the strong correlation between macroscopic lattice distortions with $\langle\xi_Q\rangle \neq 0$ and superradiant phase transition in the atomic system with $\langle\sigma_j^{\pm}\rangle \neq 0$ *. In the particular case $Q = \frac{\pi}{a}$, $\phi = 0$ the equations (2.12) take the form (see (2.6) and Appendix)

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*Here $\langle\dots\rangle$ is the thermodynamic average with Hamiltonian (2.1) or with equivalent one (2.11).

$$|\eta| = |\eta| \frac{\lambda^2 \sin^2(2Q\xi_Q \cos\psi)}{\omega_Q} \frac{\operatorname{th}\frac{\beta}{2}E}{E},$$

$$\frac{\operatorname{th}\frac{\beta}{2}E}{E} \frac{|\eta|^2 \lambda^2 Q\cos\psi}{\omega_Q^2} \sin(4Q\xi_Q \cos\psi) = \frac{\Omega_Q^2}{2}\xi_Q,$$

$$\frac{\operatorname{th}\frac{\beta}{2}E}{E} \frac{|\eta|^2 \lambda^2 Q\xi_Q \sin\psi}{\omega_Q^2} \sin(4Q\xi_Q \cos\psi) = 0, \qquad (3.1)$$

where

$$E = \sqrt{\epsilon^2 + 4|\eta|^2 \frac{\lambda^2}{\omega_Q^2} \sin^2(2Q\xi_Q\cos\psi)}\ . \qquad (3.2)$$

Now the free energy per particle (2.10) becomes:

$$g(\theta) = -\theta \ln 2\operatorname{ch}\frac{\beta}{2} E(|\bar\eta|, \bar\xi_Q, \bar\psi) + \frac{1}{\omega_Q}|\bar\eta|^2 + $$
$$+ \frac{\Omega_Q^2}{2}\bar\xi_Q + f[H'_{ph}]\ . \qquad (3.3)$$

We see the solutions of (3.1) are degenerate $\eta = |\eta| e^{i\chi}$, this corresponds to the rotating invariance of Hamiltonian (2.1) in X–Y-plane. Except for the trivial solutions, when the order parameters

$$\bar\eta = \frac{1}{N}\sum_{j=1}\lambda_j \langle\sigma_j^-\rangle_{\bar H_0}, \quad \bar\eta^* = \frac{1}{N}\sum_{j=1}\lambda_j \langle\sigma_j^+\rangle_{\bar H_0},$$

$$\bar\xi_Q = \langle\xi_Q\rangle_{\bar H_0} \qquad (3.4)$$

equal zero, the equations (3.1) give some nontrivial ones. The thermodynamic averages above are calculated with Hamiltonian

$$\bar H_0 = \tilde H_0(\bar\eta, \bar\eta^*, \bar\xi_Q, \bar\psi). \qquad (3.5)$$

If we adopt now for the atomic subsystem the new order parameter σ, corresponding to the mean value of the spin variables $\{\sigma_j^\pm\}$ in the X–Y plane (see Appendix):

$$\bar\sigma = |\langle\sigma_j^\pm\rangle_{\bar H_0}| = |\lambda \sin(2Q\xi_Q\cos\psi)|^{-1}\ |\bar\eta|,$$

$$\bar\sigma \leq \frac{1}{2}, \qquad (3.6)$$

then the equations (3.1) take the form:

$$\sigma = \sigma \frac{\lambda^2 \sin^2(2Q\xi_Q\cos\psi)}{\omega_Q} \frac{\operatorname{th}\frac{\beta}{2}E}{E},$$

$$\frac{\operatorname{th}\frac{\beta}{2}E}{E} \frac{\lambda^4 Q\cos\psi}{\omega_Q^2}\sigma^2 \sin^2(2Q\xi_Q\cos\psi)\sin(4Q\xi_Q\cos\psi) = \frac{\Omega_Q^2}{2}\xi_Q$$

$$\frac{\operatorname{th}\frac{\beta}{2}E}{E} \frac{\lambda^4 Q\xi_Q \sin\psi}{\omega_Q^2}\sigma^2 \sin^2(2Q\xi_Q\cos\psi)\sin(4Q\xi_Q\cos\psi) = 0. \qquad (3.7)$$

Note, that we are interested in such nontrivial or trivial solutions of (3.1) or (3.7), that

$$f_N[\bar H_0] = \underset{(\eta,\eta^*,\xi_Q,\psi)}{\text{abs min}}\ f_N[\tilde H_0(\eta,\eta^*,\xi_Q,\psi)]. \qquad (3.8)$$

But equations (3.1), (3.7) (or (2.12)) contain the solutions corresponding to all the extremal points of the function $f_N[\tilde H_0(\eta,\eta^*,\xi_Q,\psi)]$.

If $|\bar\eta| \neq 0$ and $\bar\xi_Q \neq 0$, from the third equation (3.7) and the explicit from of $f_N[\tilde H_0(|\eta|,\xi_Q,\psi)]$ (see (3.3)), we get

$$\bar\psi = n\pi, \quad n = 0, \pm 1, \pm 2, \ldots\ . \qquad (3.9)$$

If $\psi = \frac{\pi}{2} + n\pi$ then we have only the trivial solutions

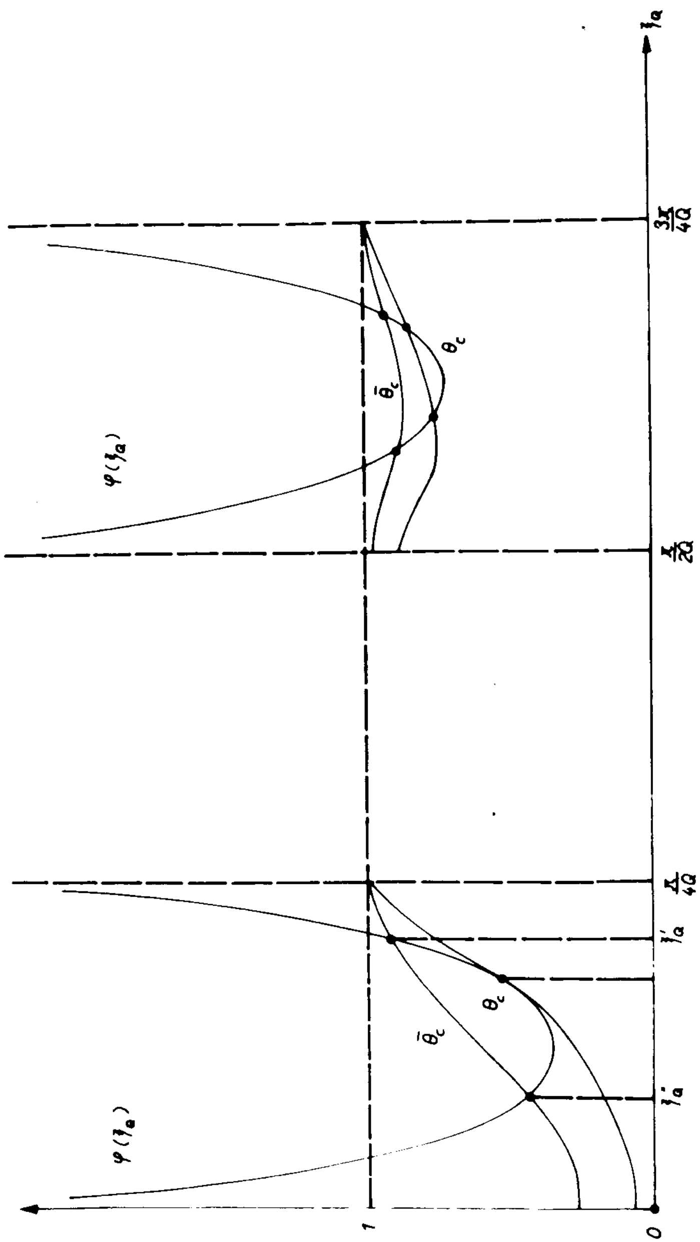

Fig. 3. Left- and rigth-hand sides of the first equation (3.10) plotted against order parameter ξ_Q *at the temperatures* $\theta = \theta_c$ *and* $\theta = \bar{\theta}_c$.

for $|\eta|$ and ξ_Q. From (3.7), (3.9) we get for $\bar{\sigma} \neq 0, \bar{\xi}_Q \neq 0$ the following equations:

$$\phi(\xi_Q) \equiv \frac{\omega_Q \sqrt{\epsilon^2 + 2\frac{\lambda^2 \Omega_Q^2}{\omega_Q Q} \sin^4(2Q\xi_Q) \frac{\xi_Q}{\sin(4Q\xi_Q)}}}{\lambda^2 \sin^2(2Q\xi_Q)} = \mathrm{th}\,\frac{\beta}{2} \sqrt{\epsilon^2 + 2\frac{\lambda^2 \Omega_Q^2}{\omega_Q Q} \sin^4(2Q\xi_Q) \frac{\xi_Q}{\sin(4Q\xi_Q)}},$$

$$\sigma^2 = \frac{\Omega_Q^2 \omega_Q \xi_Q}{2\lambda^2 Q \sin(4Q\xi_Q)}. \qquad (3.10)$$

The left-hand side of the first equation (3.10) is a concave function of ξ_Q defined on the intervals $(l\frac{\pi}{2}, \frac{\pi}{4Q} + l\frac{\pi}{2})$, $l = 0, 1, 2, \ldots$. Then it is clear, that if

$$\min_{\xi_Q \in (0, \frac{\pi}{4Q})} \phi(\xi) \leq 1, \qquad (3.11)$$

there is some critical temperature $\theta_c = \beta_c^{-1}$ (see fig. 3) such that for $\theta < \theta_c$ equations (3.10) have two nontrivial solutions and in the opposite case $\theta > \theta_c$ only a trivial one (see figs. 4 and 5).

Therefore the analysis of the problem (3.8), (3.10) for $\theta > \theta_c$ is simple: $f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]$ is a smooth function of ξ_Q on its domain (see (3.3) and (3.10)), thus the trivial solution corresponds to absolute minumum of $f_N[\tilde{H}_0]$, , i.e.;

$$\bar{\xi}_Q(\theta > \theta_c) = 0, \quad \bar{\sigma}(\theta > \theta_c) = 0. \qquad (3.12)$$

For $\theta < \theta_c$ in addition to the trivial solution of (3.7) we have two nontrivial ones (see figs. 3-5). Now we have

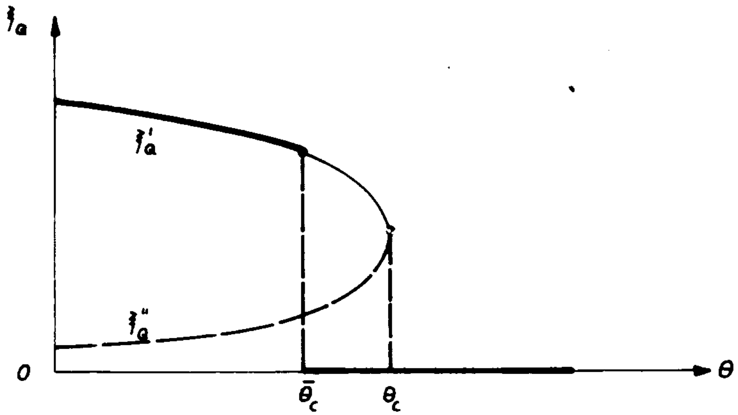

Fig. 4. The solutions of the first equation (3.10) versus temperature θ. *The bold-faced lines correspond to abs-min* $f_N[\tilde{H}_0(\bar{\sigma}(\xi_Q), \xi_Q)]$.

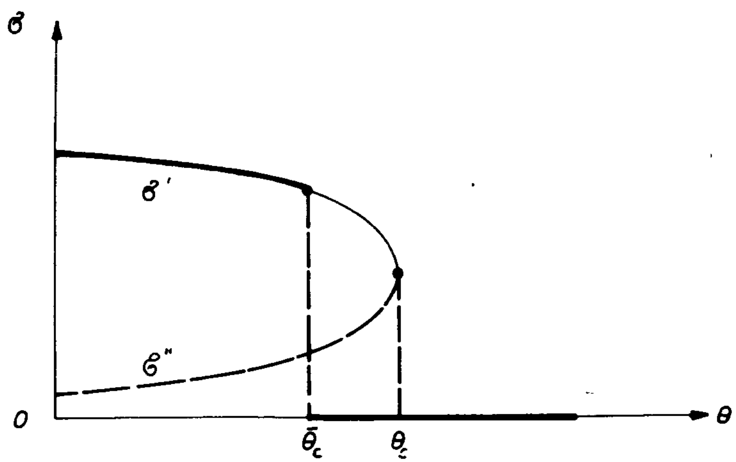

Fig. 5. The solutions of the second equation (3.10) versus temperature θ. *The bold-faced lines correspond to abs-min* $f_N[\tilde{H}_0(\sigma, \bar{\xi}_Q(\sigma))]$.

to check which of them corresponds to the solution of the abs-min problem (3.8). In this range of temperatures, $\theta < \theta_c$, the function $f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]$ has except for $\xi_Q = 0$, a local minimum at ξ'_Q, while at ξ''_Q a local maximum lies (see figs. 3, 4 and 6). Note that $\theta = \theta_c$ is the bifurcation point for the nontrivial solutions of equations (3.10), where $\xi'_Q(\theta_c) = \xi''_Q(\theta_c)$. From the smoothness of $f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]$ we have

$$f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]\Big|_{\substack{\theta = \theta_c \\ \xi_Q = 0}} < f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]\Big|_{\substack{\theta = \theta_c \\ \xi'_Q = \xi''_Q}}. \quad (3.13)$$

Thus, there is a critical temperature $\bar{\theta}_c$, that for $\bar{\theta}_c \leq \theta \leq \theta_c$

$$f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]\Big|_{\xi_Q = 0} \leq f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)]\Big|_{\xi_Q = \xi'_Q} \quad (3.14)$$

equality takes place only at $\theta = \bar{\theta}_c$ (see fig. 6), i.e.,

$$\bar{\xi}_Q(\bar{\theta}_c < \theta) = 0, \quad \bar{\sigma}(\bar{\theta}_c < \theta) = 0. \quad (3.15)$$

Therefore $\theta = \bar{\theta}_c$ is the temperature of the first order phase transition. For $\theta < \bar{\theta}_c$ functions $\bar{\xi}_Q(\theta)$, $\bar{\sigma}(\theta)$ jump to their non-zero values (see figs. 4-6):

$$\bar{\xi}_Q(\theta < \bar{\theta}_c) = \xi'_Q(\theta), \qquad \bar{\sigma}(\theta < \bar{\theta}_c) = \sigma'(\theta). \quad (3.16)$$

B. The second case we analyse here is the $\phi = \frac{\pi}{2}$, $k = q = \frac{\pi}{a}$ (2.2) (see fig. 7). Then our model is expected to be stable with respect to the lattice distortions. The reason lies in a maximal interactions amplitude between

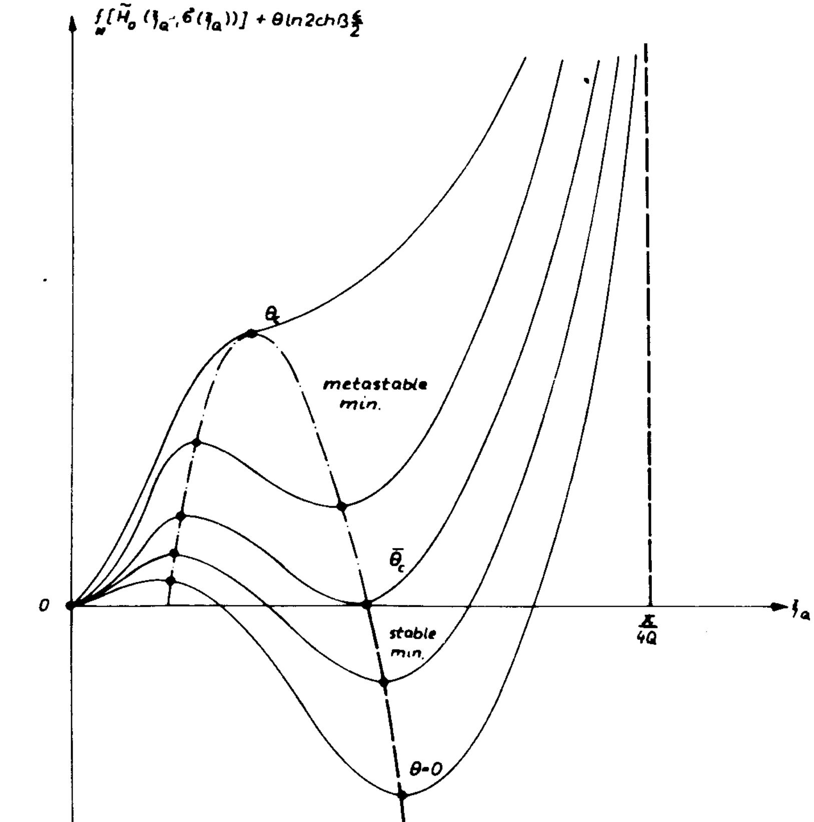

Fig. 6. The function $f_N[\tilde H_0(\sigma(\xi_Q), \xi_Q)] + \theta \ln 2\mathrm{ch}\beta\frac{\epsilon}{2}$ *plotted against order parameter* ξ_Q *at different temperatures. Here* $\sigma(\xi_Q)$ *is taken from the second equation (3.10).*

field and atoms at $u_j^\alpha = 0$ (rigid lattice). Now the interaction parameters have the values $\lambda_j = (-1)^j \lambda \cos(2Q\xi_Q \cos\psi)$. Difficulties according to the opposite signs do not arise (see (A.2)) and the free energy per particle can be also calculated in the thermodynamic limit exactly and rigorously (3.3). The equations (2.12) lead now to

$$\sigma = \sigma \frac{\lambda^2 \cos^2(2Q\xi_Q \cos\psi)}{\omega_Q} \frac{\mathrm{th}\frac{\beta}{2}E}{E},$$

$$\frac{\mathrm{th}\frac{\beta}{2}E}{E} \frac{\lambda^4 Q \cos\psi}{\omega_Q^2} \sigma^2 \cos^2(2Q\xi_Q \cos\psi) \sin(4Q\xi_Q \cos\psi) = -\frac{\Omega_Q^2}{2}\xi_Q,$$

$$\frac{\mathrm{th}\frac{\beta}{2}E}{E} \frac{\lambda^4 Q\xi_Q \sin\psi}{\omega_Q^2} \sigma^2 \cos^2(2Q\xi_Q \cos\psi) \sin(4Q\xi_Q \cos\psi) = 0, \tag{3.17}$$

where

$$E = \sqrt{\epsilon^2 + 4\sigma^2 \frac{\lambda^4 \cos^4(2Q\xi_Q \cos\psi)}{\omega_Q^2}},$$

$$\sigma = |\lambda \cos(2Q\xi_Q \cos\psi)|^{-1} |\eta|. \tag{3.18}$$

From the third equation (3.17) $\psi = \frac{\pi}{2} + n\pi$ $(n = 0, 1, 2, \ldots)$ leads to $\xi_Q = 0$. For the nontrivial solution $\xi_Q \neq 0$ we have $\psi = n\pi$ $(n = 0, 1, 2, \ldots)$ and

$$\phi(\xi_Q) \equiv \frac{\omega_Q \sqrt{\epsilon^2 - 2\frac{\lambda^2\Omega_Q^2}{Q\omega_Q}\cos^4(2Q\xi_Q)}\,\frac{\xi_Q}{\sin(4Q\xi_Q)}}{\lambda^2 \cos^2(2Q\xi_Q)} =$$

$$= \mathrm{th}\frac{\beta}{2}\sqrt{\epsilon^2 - 2\frac{\lambda^2\Omega_Q^2}{Q\omega_Q}\cos^4(2Q\xi_Q)}\,\frac{\xi_Q}{\sin(4Q\xi_Q)},$$

$$\sigma^2 = -\frac{\Omega_Q^2 \omega_Q \xi_Q}{2\lambda^2 Q \sin(4Q\xi_Q)}. \tag{3.19}$$

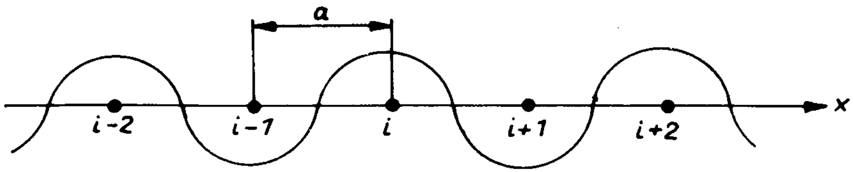

Fig. 7. Spatial dependence of the electromagnetic field amplitude in our model for the case $Q = \pi/a$, $\phi = \pi/2$.

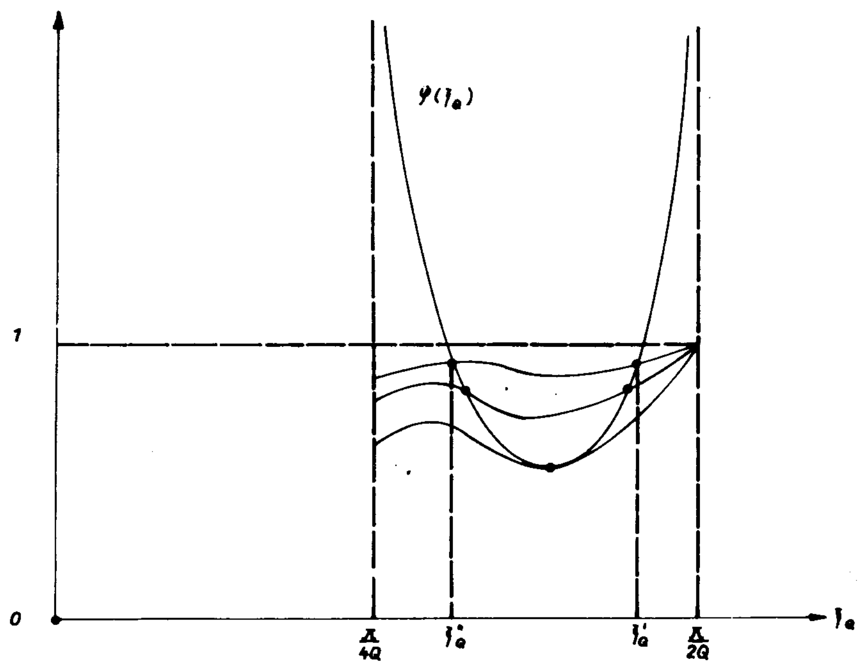

Fig. 8. The left- and rigth-hand sides of the first equation (3.19) plotted against order parameter ξ_Q *at different temperatures.*

Due to the positive definiteness of σ^2 and ξ_Q we find from (3.19), that there is no solution in domains $(\frac{\pi}{2Q}n\,,\ \frac{\pi}{2Q}n + \frac{\pi}{4Q})$, , $n = 0, 1, 2, \ldots$ (see fig. 8). The absolute minimum of the free energy per particle

$$f_N[\tilde{H}_0(\sigma, \xi_Q)] = -\theta \ln 2\,\mathrm{ch}\frac{\beta}{2}\sqrt{\epsilon^2 + 4\sigma^2\frac{\lambda^4}{\omega_Q^2}\cos^4(2Q\xi_Q)} + \sigma^2\frac{\lambda^2\cos^2(2Q\xi_Q)}{\omega_Q} + \frac{\Omega_Q^2}{2}\xi_Q^2 \qquad (3.20)$$

for fixed σ takes place at $\xi_Q = 0$. The same is true if we take into account (3.19) (see fig. 9). Thus we conclude,

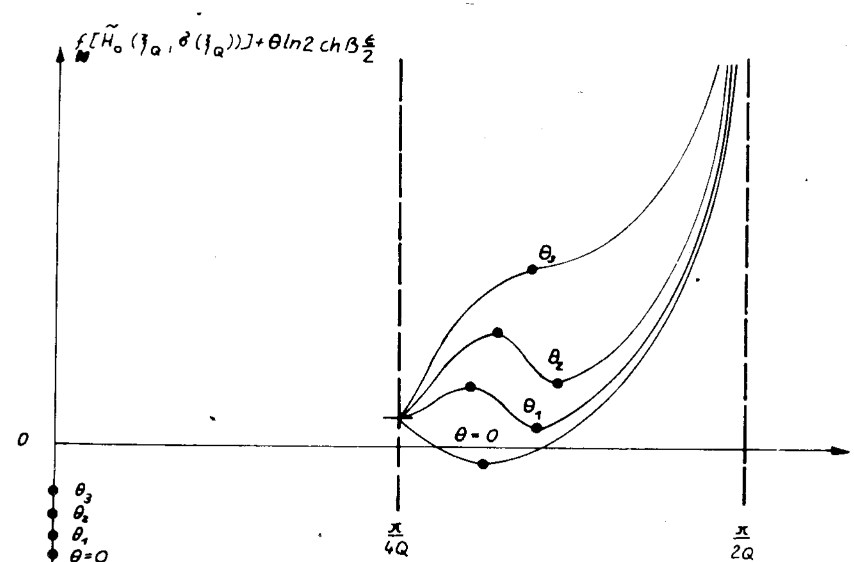

Fig. 9. The function $f_N[\tilde{H}_0(\sigma(\xi_Q), \xi_Q)] + \theta \ln 2\,\mathrm{ch}\,\beta\frac{\epsilon}{2}$ *plotted against order parameter* ξ_Q *at different temperatures.*

that the only possible solution of the abs-min problem (3.8) for $\phi = \frac{\pi}{2}$ is $\bar{\xi} = 0$ and $\bar{\sigma}$ satisfies the equation:

$$\sigma = \sigma \frac{\lambda^2}{\omega_Q} \frac{\mathrm{th}\frac{\beta}{2}E}{E}, \quad E = \sqrt{\epsilon^2 + \frac{4\sigma^2\lambda^4}{\omega_Q^2}} . \tag{3.21}$$

This result agrees with that solution, found for the ordinary Dicke model in /3-6/ with a second order phase transition to superradiant state, i.e.,

$$\begin{aligned} &\text{for } \theta \geq \theta_c \quad \bar{\xi}_Q(\theta) = 0, \ \bar{\sigma}(\theta) = 0 \\ &\text{for } \theta < \theta_c \quad \bar{\xi}_Q(\theta) = 0, \ \bar{\sigma}(\theta) > 0 \end{aligned} \qquad \theta_c = \frac{1}{2}|\epsilon|\{\mathrm{arc\,th}\frac{|\epsilon|\omega_Q}{\lambda^2}\}^{-1} . \tag{3.22}$$

4. *Conclusion*

In our paper we have investigated a generalized Dicke model, in which we take into account the spatial dependence of the electromagnetic field and classical lattice vibrations on the equilibrium positions of the atoms. As we have used Debye phonons instead of Einstein-type vibrations /10, 12/, we find for $k = q = Q$ and $\phi = 0$ (2.2), (2.5) strong correlation between vibrations and superradiant phase transitions. This leads to a first order phase transition accompanied by a macroscopic structural distortion: $\bar{\xi}_Q(\theta < \bar{\theta}_c) = \lim_{N\to\infty} \frac{|u_Q|}{\sqrt{N}} \neq 0$, , i.e., the Bose-condensation of the phonon mode $q = Q$. This behaviour shows some parallels to a metal-insulator phase transition in the case of half-filled tight-binding bands /16/ . The lattice instability of such systems leads to a structural transition driving a second-order metal-insulator one.

Setting $\phi = 0$ corresponds to absence of any interaction between field and atoms if $u_j^\alpha = 0$ (rigid lattice). Thus the high instability of the lattice is due to "sucking" of the atoms to the regions with non-zero radiation field* . Due to Debye phonons and infiniteness of the cavity ($|\Lambda| \to \infty$) this is a collective macroscopic effect in contrast to the Hioe model C /10/ (see also fig. 1).

Note that there is a region of temperature $\bar{\theta}_c \leq \theta \leq \theta_c$ (see figs. 4-6), where the free energy per atom (3.3), (3.8) has a minimum at order parameters nonequal zero: ξ'_Q, σ', but the absolute minimum lies at zero. So, for $\bar{\theta}_c \leq \theta \leq \theta_c$ we have a metastable branch of order parameters $\xi_Q(\theta) = \xi'_Q$, $\sigma(\theta) = \sigma'$, here a small distortion is able to cause their falling down to zero, i.e., to the stable state. This behaviour is obviously hysteresis like.

The case $\phi = \frac{\pi}{2}$ is shown to have the absolute minimal free energy per particle at a nondistorted lattice: $\bar{\xi}_Q(\theta) = 0$. Therefore the lattice vibrations do not effect the second order phase transition of the ordinary Dicke model /3-6, 9/. It is clear because now the "sucking" effect is absent. Comparing the free energies per particle of both the cases, we find that

$$f_N[\bar{H}_0(\phi = \frac{\pi}{2})] < f_N[\bar{H}_0(\phi = 0)] .$$

Thus we can conclude that examples for $0 \leq \phi \leq \frac{\pi}{2}$ correspond to gradual transition between these extremal cases.

Note that our model (2.1), (2.2) can be straightforward generalized to the finite-mode case and the antiresonant terms in the interaction. The thermodynamic properties of the system will be unchanged. The free energy per

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*For Einstein-type vibrations "sucking" effect creates the atom displacements from their equilibrium positions. It can be easily verified that for our model ($Q = \pi/a$, $\phi = 0$) substitution of Debye classical phonons by Einstein ones leads to a second order phase transition because there is no collective effect (see also Hioe /10/).

particle can be also exactly calculated in the thermodynamic limit if we take into account the classical phonons of the lattice.

The consideration of our model for intermediate case

$0 < \phi < \frac{\pi}{2}$ and other generalizations will be published elsewhere.

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Appendix: Dicke model with N *coupling constants*

We give here a sketch of the proof of the statement employed in section 2. To avoid unnecessary complications we shall consider a one-mode two-level Dicke Hamiltonian with N different coupling constants:

$$H_D = \omega_k b^+ b + \epsilon \sum_{j=1}^{N} \sigma_j^z + \frac{1}{\sqrt{N}} \sum_{j=1}^{N} (\lambda_j \sigma_j^- b^+ + \lambda_j^* \sigma_j^+ b). \quad (A.1)$$

This operator is defined on the Hilbert space $\mathcal{H} = \mathcal{H}_B \otimes \mathcal{H}_S$, here $\mathcal{H}_B$ is the Fook space of the boson mode ω_k and $\mathcal{H}_S$ is the 2^N-dimensional space of the spin subsystem. Let us introduce the operators

$$J^+ = \sum_{j=1}^{N} \lambda_j^* \sigma_j^+ , \qquad J^- = \sum_{j=1}^{N} \lambda_j \sigma_j^-$$

then if for arbitrary $j = 1, 2, \ldots$ and independently of N

$$|\lambda_j| \le \lambda , \quad (A.2)$$

the operators J^+, J^- and $S^z = \sum_{j=1}^{N} \sigma_j^z$ satisfy all conditions of the main Theorem in paper /6/:

$$\frac{1}{N} \| J^{\pm} \|_{\mathcal{H}_S} \le \lambda ; \qquad \frac{1}{N} \| [H_D , J^{\pm}]_- \|_{\mathcal{H}_S} \le C . \quad (A.3)$$

Therefore Hamiltonian (A.1) in thermodynamically equivalent to

$$H_0 (\bar{\eta}, \bar{\eta}^*) = \omega_k (b^+ + \frac{1}{\omega_k} \sqrt{N} \bar{\eta}^*)(b + \frac{1}{\omega_k} \sqrt{N} \bar{\eta}) - \frac{1}{\omega_k} (J^- \bar{\eta}^* + J^+ \bar{\eta}) + N \frac{1}{\omega_k} |\bar{\eta}|^2 + \epsilon S^z , \quad (A.4)$$

where $\bar{\eta}, \bar{\eta}^*$ are the solutions of the abs-min equation

$$\operatorname*{abs\,min}_{(\eta,\eta^*)} f_N [H_0 (\eta, \eta^*)] = f_N [H_0 (\bar{\eta}, \bar{\eta}^*)] . \quad (A.5)$$

Now, as follows from /5/, the estimate

$$[f_N [H_D] - f_N [H_0 (\bar{\eta}, \bar{\eta}^*)] | \le \sqrt{\theta} (\max |\lambda_j|)^{3/2} \epsilon_N$$

$$\lim_{N \to \infty} \epsilon_N = 0 \quad (A.6)$$

is uniform for the temperature θ and the coupling constants $|\lambda_j|$ from the finite interval of the positive real axis R^1_+. Consequently, if we integrate $Z_N [H_D (\lambda_1, \ldots, \lambda_N)] = \exp\{ -\beta N f_N [H_D (\lambda_1, \ldots, \lambda_N)] \}$ and $Z_N [H_0 (\bar{\eta}, \bar{\eta}^*, \lambda_1, \ldots, \lambda_N)] = \exp\{ -\beta N \times f_N [H_0 (\bar{\eta}, \bar{\eta}^*, \lambda_1, \ldots, \lambda_N)] \}$ with some weight function $g(\lambda_1, \ldots, \lambda_N)$ in the finite region $\{ |\lambda_j| < \lambda \}$:

$$\tilde{Z}_N [H_D] = \int_{-\lambda}^{\lambda} \ldots \int_{-\lambda}^{\lambda} d|\lambda_1| \ldots d|\lambda_N| \, Z_N [H_D] \, g(\lambda_1, \ldots, \lambda_N) ,$$
$$\tilde{Z}_N [H_0] = \int_{-\lambda}^{\lambda} \ldots \int_{-\lambda}^{\lambda} d|\lambda_1| \ldots d|\lambda_N| \, Z_N [H_0] \, g(\lambda_1, \ldots, \lambda_N) , \quad (A.7)$$

then

$$\lim_{N\to\infty} |\tilde{f}_N[H_D] - \tilde{f}[H_0]| = 0 \quad \text{(A.8)}$$

uniformly for the temperature θ from the finite interval of the R^1_+.

For $H_0(\bar{\eta}, \bar{\eta}^*)$ (A.4) the free energy per particle can be easily calculated in the explicit form:

$$f_N[H_0(\bar{\eta}, \bar{\eta}^*)] = -\frac{\theta}{N}\sum_{j=1} \ln 2\,\mathrm{ch}\frac{\beta}{2}E_j + \frac{1}{\omega_k}|\bar{\eta}|^2 + $$

$$+ \frac{\theta}{N}\ln(1 - e^{-\beta\omega_k}), \quad \text{(A.9)}$$

$$E_j = \sqrt{\epsilon^2 + 4\frac{|\lambda_j|^2}{\omega_k^2}|\bar{\eta}|^2}.$$

The order parameters $\bar{\eta}, \bar{\eta}^*$ satisfy the equations

$$\eta = \langle \frac{\bar{J}}{N} \rangle_{H_0(\eta,\eta^*)} = \frac{1}{N}\sum_{j=1}^{N} \frac{\mathrm{th}\frac{\beta}{2}E_j}{E_j}\, \frac{|\lambda_j|^2}{\omega_k}\eta^*$$

$$\eta^* = \langle \frac{J^+}{N} \rangle_{H_0(\eta,\eta^*)} = \frac{1}{N}\sum_{j=1}^{N} \frac{\mathrm{th}\frac{\beta}{2}E_j}{E_j}\, \frac{|\lambda_j|^2}{\omega_k}\eta. \quad \text{(A.10)}$$

References

1. H.Haken. Handbuch der Physik XXV, 2C, Springer Verlag, Berlin, Heidelberg, New York, 1970.
2. R.H.Dicke. Phys.Rev., 93, 99 (1954).
3. K.Hepp and E.H.Lieb. Ann. of Phys., 76, 360 (1973).
4. K.Hepp and E.H.Lieb. Phys.Rev., A8, 2517 (1973).
5. J.G.Brankov, V.A.Zagrebnov and N.S.Tonchev. Preprint JINR, P4-7735, Dubna, 1974; Teor. i Mat. Fiz., 22, 20 (1975).
6. V.A.Zagrebnov, J.G.Brankov and N.S.Tonchev. Preprint JINR, E4-8818, Dubna, 1975; Dokl. Acad. Nauk USSR, 225, 71 (1975).

7. K.Rzazewski, K.Wodkiewicz and W.Zakowicz. Phys. Rev.Lett., 35, 432 (1975).
8. P.J.Gambardella. Physica, 80A, 550 (1975).
9. Y.K.Wang and F.T.Hioe. Phys.Rev., A7, 831 (1973)
10. F.T.Hioe. Phys.Rev., A8, 1440 (1974).
11. B.V.Thompson. J.Phys., A8, 126 (1975).
12. B.M.Pimental and A.H.Zimerman. Nuovo Cimento, 30B, 43 (1975).
13. C.H.Kittel. Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, 1971.
14. J.M.Ziman. Principles of the Theory of Solids, Cambridge Univ. Press, London, 1972.
15. W.Kohn and D.Sherrington. Rev.Mod.Phys., 42, 1 (1970).
16. J.G.Brankov, N.S.Tonchev and V.A.Zagrebnov. Physica, 79A, 125 (1975).
17. J.G.Brankov, A.S.Shumovsky and V.A.Zagrebnov. Physica, 78, 183 (1974).

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