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Abstract. Extra terms which describe the phonon absorption and emission associated with Brillouin scattering are added to the usual Dicke Hamiltonian. The general effect on the Dicke phase transition is an enhancement of the photon numbers. When an effective phonon coupling constant B exceeds a certain value, the transition is of the first-order type. The condition $\epsilon/\lambda^2 < 1$ found by Wang and Hioe to be necessary for a phase transition to occur, is no longer necessary if the constant B is large enough and in such cases the transition is again first order in type.

1. Introduction

There has been considerable interest in the discovery (Hepp and Lieb 1973) that the Dicke model of non-linear optics exhibits a phase transition.

Wang and Hioe (1973) have shown that if the partition function of the model is calculated using coherent photon states as the basis, expressions closely resembling the functional integral formulation of the thermodynamics of a superconductor are obtained (Langer 1964). It has been found that when the rotating wave approximation is relaxed, the qualitative features of the second-order transition are unchanged (Hioe 1973, Carmichael *et al* 1973). As it is comparatively easy to excite long wave phonons in matter, it is important that thermodynamic calculations based on the Dicke model should attempt to take these into account.

Hioe has proposed a modified Dicke model which seeks to include the effect of atomic motions when these may be described in terms of a vibrating harmonic lattice. A serious criticism of this Hamiltonian is that the phase factors of the interaction term are incorrectly chosen, resulting in eg a quantum transition probability for photon absorption (wavevector k) which depends on the position of the atom x as $\sin^2 k \cdot x$, a manifestly false conclusion. It is still an open question whether or not the phase transition is affected by coupling to local density fluctuations.

It is known that Brillouin scattering may be explained in terms of first-order dilation effects and the interaction energy may be found for some cases (see eg Thompson 1970). With this in mind, we may expect that if the photon number becomes large as in the Dicke model transition, then because of the stimulated Brillouin effect, the phonon number should be large too. This suggests that a phase transition, if it occurs, could be of the first-order type in some circumstances. The thermodynamics of the model discussed below shows this property. Upon replacing the exponential phase factors by unity in the usual dipole interaction and in the Brillouin energy, and retaining the rotating

wave approximation, the model Hamiltonian becomes

$$H = \sum_k \omega_k a_k^\dagger a_k + \tfrac{1}{2}\omega_0 \sum_l \sigma_z(l) + \sum_f \Omega_f c_f^\dagger c_f$$

$$+ \sum_l \sum_k \frac{\lambda_k \omega_k}{2\sqrt{N}} (a_k \sigma^{(+)}(l) + a_k^\dagger \sigma^{(-)}(l)) \left(1 + N^{-1/2} \sum_f (\kappa_f c_f + \kappa_f^* c_f^\dagger) \right). \quad (1)$$

The notation of Wang and Hioe has been followed, but here annihilation and creation operators $c_f, c_f^\dagger$ referring to phonons of wavevector f and frequency Ω_f are introduced with coefficients κ_f, κ_f^* derived from the Brillouin energy term (Thompson 1970)

$$- \sum_l \int \mu_l \cdot E(x)(u_l \cdot \nabla)\rho_l(x)\,\mathrm{d}^3 x. \quad (2)$$

In (2), $\rho_l(x)$ is an average density for the atom l, u_l is its displacement operator, μ_l the dipole operator and $E(x)$ is the transverse electric field.

The analysis of u_l into phonon operators is given by

$$u_l = N^{-1/2} \sum_f \left(\frac{\hbar}{2M\Omega_f} \right)^{1/2} (v_f c_f\, \mathrm{e}^{\mathrm{i} f \cdot l} + v_f^* c_f^\dagger\, \mathrm{e}^{-\mathrm{i} f \cdot l}) \quad (3)$$

in which v_f are polarization vectors and M is the mass of an atom. For simplicity we consider the case of a single photon mode of frequency ω and a phonon mode of frequency $\Omega = v\omega$. The extension to a finite number of modes in each field is easily made (see later).

2. Partition function and free energy

In order to calculate the partition function Z ($= \mathrm{Tr}\, \mathrm{e}^{-\beta H}$) we use the coherent photon states, $|\alpha\rangle$ where α is a complex number together with a set of coherent states $|\gamma\rangle$ for the phonons of wavevector f. The details of the calculation and an explanation of the large N approximation which applies equally to the phonon variables, are given by Wang and Hioe. The result is:

$$Z = \pi^{-2} \int\int \mathrm{d}^2\alpha\, \mathrm{d}^2\gamma \exp[-\beta\omega(|\alpha|^2 + v|\gamma|^2)](\mathrm{tr}\, \mathrm{e}^{-\beta\omega h})^N \quad (4)$$

where

$$h = \tfrac{1}{2}\epsilon\sigma_z + \frac{\lambda}{2\sqrt{N}}(\alpha\sigma^{(+)} + \alpha^*\sigma^{(-)}) \left(1 + \frac{\kappa}{\sqrt{N}}\gamma + \frac{\kappa^*}{\sqrt{N}}\gamma^* \right) \quad (5)$$

$$\epsilon = \omega_0/\omega.$$

The symbol tr in (4) stands for the trace over the states of the two-level atom. From the eigenvalues of h, this trace is readily found to be

$$2\cosh\left\{ \frac{\beta\omega_0}{2} \left[1 + \frac{4|\alpha|^2\lambda^2}{N\epsilon^2} \left(1 + \frac{2\kappa_1 x_1}{\sqrt{N}} - \frac{2\kappa_2 y_1}{\sqrt{N}} \right)^2 \right]^{1/2} \right\}$$

where

$$\kappa = \kappa_1 + \mathrm{i}\kappa_2, \qquad \gamma = x_1 + \mathrm{i} y_1.$$

A rotation in the (x_1, y_1) plane shows that the result depends only on $|\kappa|$. Upon setting

$$|\alpha|^2 = Ny \tag{6}$$

and similarly scaling the remaining 'phonon' variable we obtain:

$$Z = N^{3/2}(\pi\beta v\omega)^{-1/2} \int_0^\infty dy \int_{-\infty}^\infty dx \exp[-\beta\omega NF(x, y)] \tag{7}$$

where

$$F = y + vx^2 - (\beta\omega)^{-1} \ln 2 \cosh \frac{\beta\omega_0}{2} \left(1 + \frac{4\lambda^2 y}{\epsilon^2}(1 + 2|\kappa|x)^2\right)^{1/2} \tag{8}$$

$$v = \Omega/\omega.$$

According to Laplace's method the integral (7) can be found in terms of the minimum value of F in the region of integration. This will be either a local minimum (associated with a non-zero value of x) or else it will lie in the boundary of the region, (ie $y = 0$). It is easy to see that on the boundary, the lowest F occurs when $x = 0$. The new feature of this analysis arises from the possibility that F may have (i) two or more stationary points; (ii) a local minimum value which may be greater than, equal to or less than the boundary minimum $F(0, 0)$ at that temperature.

To make the subsequent numerical work easier three parameters A, B, C are introduced with new variables η, w as follows:

$$w = 1 + 2|\kappa|x, \qquad \eta = +(1 + 4\lambda^2 yw^2\epsilon^{-2})^{1/2} \tag{9a}$$

$$A = \epsilon\lambda^{-2}, \qquad B = \epsilon^2|\kappa|^2\lambda^{-2}v^{-1}, \qquad C = \tfrac{1}{2}\beta\omega_0 \tag{9b}$$

$$F(x, y) \equiv f(w, \eta) \tag{9c}$$

where

$$2\epsilon^{-1}f = \frac{A(\eta^2 - 1)}{2w^2} + \frac{A(w - 1)^2}{2B} - \frac{1}{C} \ln 2 \cosh C\eta. \tag{9d}$$

The conditions that f be stationary may be written in the form:

$$A\eta w^{-2} = \tanh C\eta \tag{10a}$$

$$B(\eta^2 - 1) = w^4 - w^3 \tag{10b}$$

and the boundary of the f surface is $\eta = 1$.

From the elementary theory of surfaces, saddle points of f may be detected by examining the sign of

$$\Delta = f_{\eta\eta}f_{ww} - f_{\eta w}^2 \tag{11}$$

because the Jacobian of the transformation is in general non-singular and therefore does not cause difficulties.

According to (10b), if $\eta > 1$ then $w \neq 1$ indicating that phonons and photons appear together with large occupation numbers. Furthermore, if $w \neq 1$, (10a) shows that the condition $A < 1$ is no longer necessary for an acceptable solution ($\eta \geq 1$) corresponding to the super-radiant phase transition. It is replaced by the weaker condition

$$Aw^{-2} < 1.$$

Although equations (10) must be solved numerically at each temperature and for each pair of constants (A, B) one can obtain an idea of the importance of the phonon terms by considering the zero temperature limit $C \to \infty$. Upon setting $A = 1$, we see that (10) has a solution $w = \eta = 1$ as one would expect from the work of Wang and Hioe. But at $T = 0$,

$$\Delta = \frac{A^2}{Bw^2} - \frac{A^2(\eta^2 + 3)}{w^6}$$

which indicates that $\Delta < 0$ if $B > \frac{1}{4}$. The solution therefore represents a saddle point of f and may not be used to calculate the free energy from (7). A second solution with $\eta \neq 1$ which is a local minimum of f can be found in such cases. For example, with $A = 1, B = \frac{8}{15}$, the acceptable alternative solution is $\eta = 4$.

Quite simple graphical considerations lead us to expect no more than two solutions of (10) with $w > 1$ for each set A, B and C. No acceptable solutions exist for which $0 < w < 1$ since this would mean that $\eta < 1$. Also, there can be no stationary points with $w < 0$ when $B < A^2$. To show this, assume that such roots do exist; we deduce that

$$\tanh C\eta = Aw^{-2}[1 + B^{-1}(w^4 + |w|^3)]^{1/2} < 1$$

and so, *a fortiori*, $A^2 < B$ giving a contradiction. We exclude the cases $B > A^2$ since it appears that the model becomes unsatisfactory as $B \to A^2$.

When $A < 1$ we shall see that for values of B which exceed a certain value B', dependent on A, the super-radiant transition is first order, not second order. At this point it is convenient to describe how the case of many photon modes k and phonon modes f may be incorporated. It suffices to redefine the constants A and B as follows:

$$A = \frac{\omega_0}{\Sigma_k \lambda_k^2 \omega_k}, \qquad B = \frac{\omega_0^2}{(\Sigma_k \lambda_k^2 \omega_k)(\Sigma_f |\kappa_f|^2 \Omega_f^{-1})}$$

and then the one-mode theory may be used. This follows because the many-mode partition function may be reduced to the single-mode case by (i) a change of scale; (ii) a rotation of the axes labelled by the integrand variables, a device commonly used to simplify Gaussian integrals (see eg Thompson 1965, p 1438). Of course, it is no longer possible to give a simple meaning to the order parameter η in terms of the number of photons in each mode.

3. Results

Either $(\eta - 1)$ which is proportional to the photon number, or $(w - 1)$ which is proportional to the phonon number may be taken as an 'order parameter' in discussing the transition. Choosing the first of these, solutions of equations (10) are plotted against temperature in figure 1. The case $A = \frac{1}{2}$ is typical of results for the region $0 < A < 1$. Roughly, at low enough temperatures an increase in the value of B produces a larger value of η at that temperature. This actually corresponds to increasing the photon number, n, given by
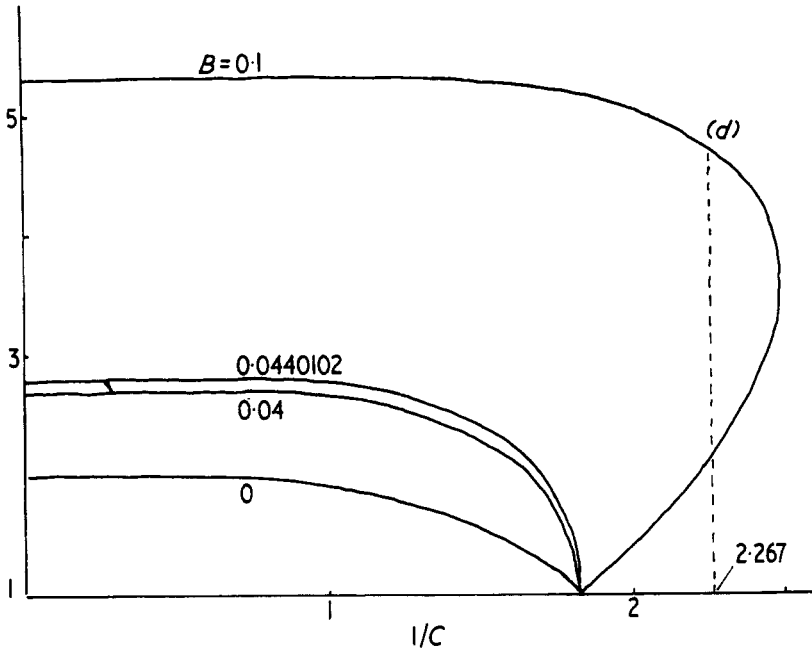
$$n = \frac{1}{4}N\epsilon A(\eta^2 - 1)w^{-2}.$$

Figure 1. Solutions for the variable η against temperature in the case $A = \frac{1}{2}$.

When $A < 1$, all the solution curves like those in figure 1, pass through the point $w = \eta = 1$ at a temperature T_0 given by

$$\frac{\epsilon}{2kT_0} = \tanh^{-1} A$$

and this is the critical temperature for values of B between 0 and B' given by

$$B' = \tfrac{1}{4}[1 + (A - A^{-1})\tanh^{-1} A]. \tag{12}$$

When $B = B'$, the curve has a vertical tangent at $w = \eta = 1$. The special value of B given by (12) may also be found by setting Δ in (11) equal to zero. For values of $B > B'$ and at temperatures greater than T_0 there appear to be two solutions. However, one is a saddle point of f and the second, which is numerically larger, is a local minimum. This minimum gives a value of f which is lower than the point of the boundary mentioned earlier, certainly for temperatures just above T_0, but as the temperature increases the local minimum of f rises above the boundary minimum and eventually the saddle point and minimum merge. At temperatures higher than this, f has no stationary points.

Contour maps of f, drawn schematically in figure 2, show why the minimum of f must be rejected in favour of the low point on the boundary for calculating the free energy. The sequence 2(*a*)–(*f*) describes the f surface at successively lower temperatures. In (*b*) the existence of an uncommon type of stationary point, ie a merging of a minimum and a saddle point, is shown by the cusp in a particular contour line. The minimum and the saddle point have separated in (*c*), but the lowest point remains on the boundary. At (*d*) we have the critical condition when the minimum and boundary low point give the same value of f. These points must be found numerically and are indicated by the vertical dashed lines in figures 1 and 3. Further reduction in temperature is described
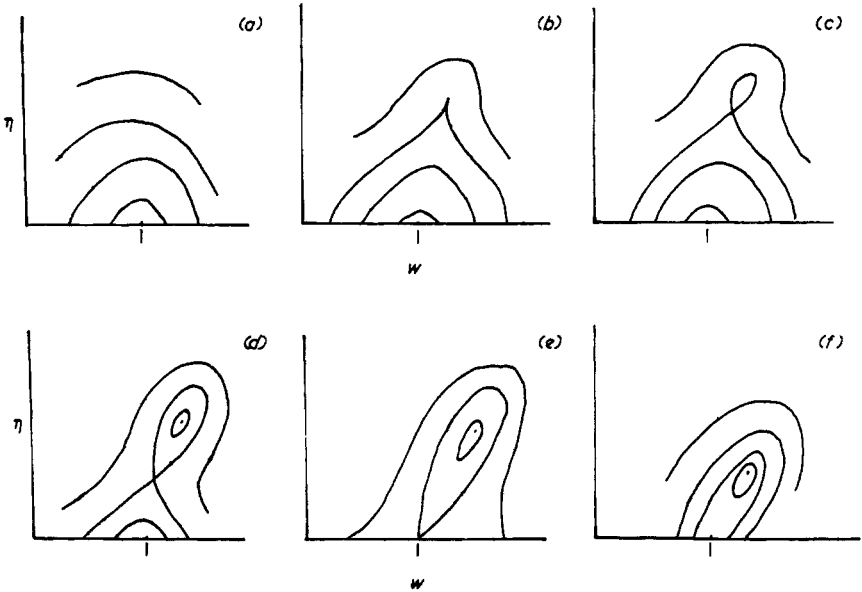
Figure 2. Schematic contour maps of the function f for decreasing temperature when $B > B'$.

by $2(e)$ (where $T = T_0$) and $2(f)$. The free energy is calculated using the coordinates of the local minimum. Since the temperature dependence of the free energy changes at $2(d)$ so that the first temperature derivative is discontinuous there, it follows that the transition is first order, being associated with a latent heat:

$$-\tfrac{1}{2}\eta_d\omega_0 \tanh \tfrac{1}{2}\beta_d\omega_0\eta_d + \tfrac{1}{2}\omega_0 \tanh \tfrac{1}{2}\beta_d\omega_0 + \frac{1}{\beta_d} \ln\left(\frac{\cosh \tfrac{1}{2}\beta_d\omega_0\eta_d}{\cosh \tfrac{1}{2}\beta_d\omega_0}\right).$$

As mentioned earlier, in the presence of the phonon interaction a super-radiant transition is possible even when A exceeds unity. An example is illustrated in figure 3
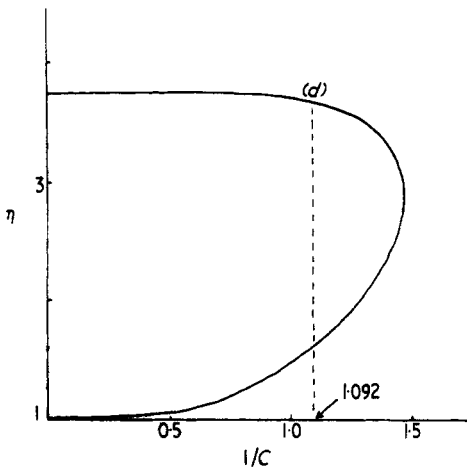

Figure 3. Solutions for the variable η against temperature. $A = 1.01$, $B = \tfrac{8}{15}$.

where $A = 1.01$, $B = \frac{8}{15}$. The transition is first order and in terms of the f surface, the situation described by figure 2(e) is not reached even at absolute zero. Finally, it must be said that as B approaches the value A^2, the minimum point of f recedes further from (1, 1) and at zero temperature approaches infinity in the limit $B = A^2$. Although one might expect a dissociation of the lattice under certain experimental conditions, it is felt that the present modified Dicke model is intrinsically unable to describe such an effect.

4. Conclusion

At zero temperature, the condition for a phase transition, ie $A < 1$, may also be derived for the multi-atom model (Swain 1972) by considering the dependence of the ground state energy on the 'excitation number' in the linear optics limit (Thompson 1972). The effect of the phonon terms upon this variational calculation of the ground state energy is now being studied. It emerges that in the case $A = 1$ the behaviour depends on whether B exceeds $\frac{1}{4}$ or not in accord with the finite temperature result of this article.

The Dicke model is widely held to be of no practical importance. However, the modified form described here is theoretically interesting in that it provides a simple mathematical mechanism for a first-order phase transition which goes over smoothly to describe a second-order transition at appropriate values of the coupling parameters. As far as I know, this mathematical mechanism has not been described in the literature.

Acknowledgment

References

Carmichael H J, Gardiner C W and Walls D F 1973 *Phys. Lett.* **46A** 47–8
Hepp K and Lieb E H 1973 *Ann. Phys., NY* **76** 360
Hioe F T 1973 *Phys. Rev.* A **8** 1440–6
Langer J S 1964 *Phys. Rev.* **134** 553–65
Swain S 1972 *J. Phys.* A: *Gen. Phys.* **5** L3–6
Thompson B V 1965 *Phys. Rev.* **138** 1433–41
—— 1970 *J. Phys.* C: *Solid St. Phys.* **3** L147–9
—— 1972 *J. Phys.* A: *Gen. Phys.* **5** 1453–60
Wang Y K and Hioe F T 1973 *Phys. Rev.* A **7** 831–6