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The super-radiant phase transition in the Dicke model

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Abstract. The exact results for the super-radiant phase transition in the Dicke model are obtained by a variational method for the free energy used to study the cooperative Jahn–Teller effect in crystals. By transforming the Hamiltonian to a representation inherent in the variational method, we show that, in the limit of infinite coupling parameter, the leading term in the Hamiltonian is an Ising interaction between the z components of spin in the rotated pseudo-spin space. Each spin interacts equally with every other spin and this provides a physical insight into the origin of the mean-field behaviour of the Dicke model.

1. Introduction

The Dicke maser model of N two-level atoms coupled to a photon mode in the rotating-wave approximation has recently been an object of considerable interest with respect to a phase transition, called the super-radiant phase transition, which the system exhibits. The exact thermodynamics of this model was obtained by Hepp and Lieb (1973a). The essential feature of this second-order phase transition is that, when the coupling parameter for interaction with the photon mode is less than a given value, there is no phase transition, the thermodynamic properties being simply those of N non-interacting two-level atoms. When the coupling parameter is larger than a certain value there is a phase transition characterized by the specific heat behaving for instance like that of a ferromagnet in the molecular field approximation. For a given value of the coupling parameter, the specific heat rises as the temperature increases. However, before the maximum of the molecular field specific heat of a ferromagnet is reached, the specific heat drops discontinuously at the super-radiant transition temperature and above this temperature the specific heat is that of a non-interacting two-level system.

Wang and Hioe (1973) calculated the exact thermodynamics using Glauber's coherent states of the photon field as a basis. Using similar methods Hioe (1973) extended the exact calculations to the particular case which does not use the rotating-wave approximation. Although they provided no justification for their method being exact, their results were proved to be rigorously correct by Hepp and Lieb (1973b). An alternative method involving a 'Bogoliubov trick' was given by Vertogen and De Vries (1974).

A mean-field variational method was used by Lee (1973) to discuss the Jahn–Teller cooperative phase transition (see for example Gehring and Gehring 1975) in a system of two-level ions interacting with the phonon field of a crystal. The essential features of the Jahn–Teller cooperative phase transition obtained show remarkable similarities to the super-radiant phase transition described above. However, the case of interaction with the phonon field is made considerably more complicated as there are a large number of phonon modes; and the different physics of the problem also requires the consideration of homogeneous strain. In the solution for this problem, the $k \to 0$ limit was taken to include homogeneous strain effects. Hence it is not obviously clear whether our variational method would yield the exact results for the Dicke model. In this paper we show that a variational calculation using the same type of trial Hamiltonian as in the spin–phonon case gives the exact results for the Dicke model. We take the simple case of one photon mode without the rotating-wave approximation. To provide some physical insight into why the exact behaviour of the model resembles that of a Weiss ferromagnet, we show by appropriately transforming the Hamiltonian that in the limit of the infinite coupling parameter, the leading term in the Hamiltonian is a spin-half Ising model with the spins interacting equally with each other.

2. Variational calculation

For easy comparison with the results given in Hioe (1973), we adopt the notation of that paper. The model Hamiltonian for N two-level atoms interacting with one photon mode is

$$H = a^\dagger a + \epsilon \sum_{i=1}^{N} S_i^z + (2\lambda/\sqrt{N}) \sum_{i=1}^{N} (a + a^\dagger) S_i^x \tag{2.1}$$

where a, $a^\dagger$ are the annihilation and creation operators for a photon of unit energy, ϵ is the energy difference between the two levels, λ is the coupling parameter and S_i^z and S_i^x are the operators for spin-half. The counter-rotating terms $a^\dagger S^+ + aS^-$ have been added to the expression for the rotating-wave approximation to give the interaction term in (2.1).

The variational principle for the free energy can be stated as follows. If H is the Hamiltonian and H_t a trial Hamiltonian containing a set of variational parameters, then the free energy $F = -kT \ln \mathrm{Tr} \exp(-\beta H)$ satisfies the relation

$$F \leqslant F_v = F_t + \langle H - H_t \rangle_t \tag{2.2}$$

where

$$F_t = -kT \ln \mathrm{Tr} \exp(-\beta H_t) \tag{2.3}$$

and

$$\langle H - H_t \rangle_t = \frac{\mathrm{Tr}(H - H_t) \exp(-\beta H_t)}{\mathrm{Tr} \exp(-\beta H_t)}. \tag{2.4}$$

A choice for H_t using mean-field arguments was made by Lee (1973, to be referred to as BSL). Let H_{ts} be the trial Hamiltonian for the spin system and H_{tp} the trial Hamiltonian for the photon system. The total trial Hamiltonian H_t is given by

$$H_t = H_{ts} + H_{tp}. \tag{2.5}$$

Using arguments similar to that in BSL, we have

$$H_{ts} = v \sum_i S_i^z + \mu \sum_i S_i^x \tag{2.6}$$

and

$$H_{tp} = g a^\dagger a + f(a + a^\dagger) \tag{2.7}$$

where μ, v, f and g are variational parameters. The rest of the calculations closely follow the steps in BSL and we refer the reader to this paper for details. The diagonalizing canonical transformations for H_{ts} are

$$H'_{ts} = RH_{ts}R^\dagger = (\mu^2 + v^2)^{1/2} \sum_i S_i^z \tag{2.8}$$

where the unitary operator R with $R^\dagger R = RR^\dagger = 1$ is defined by

$$\left.\begin{aligned} RS_i^z R^\dagger &= S_i^z \cos\theta - S_i^x \sin\theta \\ RS_i^x R^\dagger &= S_i^z \sin\theta + S_i^x \cos\theta \end{aligned}\right\} i = 1, 2, \ldots, N \tag{2.9}$$

and

$$\tan\theta = \frac{\mu}{v}, \qquad \sin\theta = \frac{\mu}{\sqrt{(\mu^2 + v^2)}}, \qquad \cos\theta = \frac{v}{\sqrt{(\mu^2 + v^2)}}. \tag{2.10}$$

H_{tp} can be diagonalized by a c number shift of the photon operators a and $a^\dagger$ which is a canonical transformation generated by the unitary operator U (i.e. $U^\dagger U = UU^\dagger = 1$).
Hence

$$H'_{tp} = UH_{tp}U^\dagger = g a^\dagger a - (f^2/g) \tag{2.11}$$

where

$$UaU^\dagger = a - (f/g), \qquad Ua^\dagger U^\dagger = a^\dagger - (f/g). \tag{2.12}$$

We also have

$$H'_t = URH_tR^\dagger U^\dagger = H'_{tp} + H'_{ts}. \tag{2.13}$$

Using equations (2.3), (2.5), (2.8) and (2.11), we get

$$F_t = -(f^2/g) - kT \ln \mathrm{Tr} \exp(-\beta g a^\dagger a) - NkT \ln \mathrm{Tr} \exp(-\beta\sqrt{\mu^2 + v^2} S^z). \tag{2.14}$$

Using equations (2.1), (2.3) and (2.12) we get

$$\begin{aligned} H' &= URHR^\dagger U^\dagger \\ &= a^\dagger a + \frac{f^2}{g^2} - \frac{f}{g}(a + a^\dagger) + \epsilon \cos\theta \sum_i S_i^z - \epsilon \sin\theta \sum_i S_i^x \\ &\quad + \frac{2\lambda}{\sqrt{N}} \sum_i \left((a + a^\dagger) S_i^z \sin\theta + (a + a^\dagger) S_i^x \cos\theta - \frac{2f}{g} S_i^z \sin\theta - \frac{2f}{g} S_i^x \cos\theta \right). \end{aligned} \tag{2.15}$$

Hence

$$\langle H \rangle_t = \langle H' \rangle' = \langle a^\dagger a \rangle' + \frac{f^2}{g^2} + N\epsilon \cos\theta \langle S^z \rangle' - \frac{4\lambda f}{g} \sqrt{N} \langle S^z \rangle' \sin\theta \tag{2.16}$$

where

$$\langle \cdots \rangle' = \frac{\mathrm{Tr} \cdots \exp(-\beta H'_t)}{\mathrm{Tr} \exp(-\beta H'_t)} \tag{2.17}$$

with H'_t given in equation (2.13). We have used the fact that the averages $\langle S_i^z\rangle' = \langle S^z\rangle'$ are independent of the index i and that $\langle a\rangle' = \langle a^\dagger\rangle' = \langle S_i^x\rangle' = 0$.

Note that $\langle S^z\rangle'$ is given by

$$\langle S^z\rangle' = -\tfrac{1}{2}\tanh(\tfrac{1}{2}\beta\sqrt{\mu^2+v^2}) \tag{2.18}$$

and

$$\langle a^\dagger a\rangle' = \frac{\mathrm{Tr}\, a^\dagger a \exp(-\beta g a^\dagger a)}{\mathrm{Tr}\exp(-\beta g a^\dagger a)}. \tag{2.19}$$

The upper bound for the free energy F_v in equation (2.2) is, dropping the superscripts in $\langle\cdots\rangle'$ for convenience

$$F_v = -kT \ln \mathrm{Tr}\exp(-\beta g a^\dagger a) - NkT \ln \mathrm{Tr}\exp(-\beta\sqrt{\mu^2+v^2}S^z) + (1-g)\langle a^\dagger a\rangle + \frac{f^2}{g^2}$$
$$+N\langle S^z\rangle(\epsilon\cos\theta - \sqrt{\mu^2+v^2}) - \frac{4\lambda f}{g}\sqrt{N}\langle S^z\rangle\sin\theta. \tag{2.20}$$

The minimization of F_v with respect to g and f gives us the following solutions:

$$g = 1 \tag{2.21}$$

$$f = 2\lambda\sqrt{N}\langle S^z\rangle\sin\theta \tag{2.22}$$

noting that θ is related to μ and v in equation (2.10). Minimization of F_v with respect to μ and v, following the arguments in BSL gives the equations

$$\frac{v\epsilon}{\sqrt{(\mu^2+v^2)}} - \sqrt{\mu^2+v^2} - \frac{4\lambda f}{g\sqrt{N}}\frac{\mu}{\sqrt{(\mu^2+v^2)}} = 0 \tag{2.23}$$

$$\epsilon\mu + (4\lambda f v/g\sqrt{N}) = 0. \tag{2.24}$$

The solutions of equations (2.23) and (2.24) using equations (2.21) and (2.22) are

$$v = \epsilon \tag{2.25}$$

$$\mu = 0 \tag{2.26}$$

or

$$\sqrt{(\mu^2+\epsilon^2)} = -8\lambda^2\langle S^z\rangle. \tag{2.27}$$

Equation (2.27) can also be written as

$$\mu = \pm(64\lambda^4\langle S^z\rangle^2 - \epsilon^2)^{1/2}. \tag{2.28}$$

For real solutions of μ the following condition must be satisfied:

$$64\lambda^4\langle S^z\rangle^2 \geqslant \epsilon^2. \tag{2.29}$$

The maximum value of $\langle S^z\rangle^2 = \frac{1}{4}$. For a given ϵ, to satisfy condition (2.29) would require for the maximum value of $\langle S^z\rangle^2$, the smallest value of λ as $4\lambda^2 = \epsilon$. As $\langle S^z\rangle^2$ decreases in value we would require a larger value of λ to satisfy (2.29). Hence we can write condition (2.29) as

$$4\lambda^2 \geqslant \epsilon \tag{2.30}$$

which includes all values of λ satisfying (2.29) for a given ϵ.

When $4\lambda^2 \leqslant \epsilon$, the only solution for μ is given by equation (2.26), i.e. $\mu = 0$. With $\eta = \epsilon$ given by equation (2.25) we can verify by substitution in equation (2.20) that

$$F_v/N = -kT \ln(2 \cosh \tfrac{1}{2}\beta\epsilon) \qquad (2.31)$$

neglecting the free energy of the single photon mode of $O(1/N)$. This is the unperturbed solution and there is no phase transition.

When $4\lambda^2 \geqslant \epsilon$ the equation which determines $\langle S^z \rangle$ is given by substituting equation (2.27) into equation (2.18). We get

$$\langle S^z \rangle = \tfrac{1}{2} \tanh(4\beta\lambda^2 \langle S^z \rangle) \qquad (2.32)$$

an equation for $\langle S^z \rangle$ which resembles that for the Weiss ferromagnet. As T increases from $T=0$, $\langle S^z \rangle$ decreases from the maximum value $\frac{1}{2}$ until it reaches a value at temperature T_c where condition (2.29) becomes an equality. This defines the critical point for the super-radiant phase transition. Since at $T = T_c$, $\langle S^z \rangle = \epsilon/8\lambda^2$ we get using equation (2.32), the equation which determines $\beta_c = 1/kT_c$ as

$$\frac{\epsilon}{4\lambda^2} = \tanh(\tfrac{1}{2}\beta_c\epsilon). \qquad (2.33)$$

Above T_c the condition (2.27) is violated and we have the unperturbed solution given by equation (2.30). The free energy F_v in (2.20) becomes, using (2.10), (2.21), (2.22), (2.25) and (2.27)

$$\frac{F_v}{N} = -kT \ln[2 \cosh(4\beta\lambda^2 \langle S^z \rangle)] + 4\lambda^2 \langle S^z \rangle^2 - \frac{\epsilon^2}{16\lambda^2}. \qquad (2.34)$$

To compare our results with that given in Hioe (1973) we note that $a = 2\lambda$ as defined in that paper. Also, we identify σ in that paper with $\langle S^z \rangle$ here. We note that equations (2.30), (2.31), (2.32), (2.33) and (2.34) agree with equations (25), (26), (27) and (28) of his paper. Hence our variational calculation gives us the exact thermodynamics of the Dicke model. Strictly we have not proved that our method gives the exact thermodynamics but it is nevertheless surprising that the variational method based on mean-field arguments for the choice of the trial Hamiltonian does give us the exact answer. We note that in our calculation the order parameter $\langle S^z \rangle$ appearing in equation (2.32) has a simple physical meaning. Since the effective temperature-dependent splitting of the two levels is given by $(\mu^2 + \epsilon^2)^{1/2}$, equation (2.27) shows that the temperature-dependent level separation is directly proportional to $\langle S^z \rangle$. The order parameter σ appearing in Hioe (1973) does not appear to have a physical meaning which can be deduced easily from his calculations.

We can also readily verify that if we apply our method using the *ansatz* given in equations (2.5), (2.6) and (2.7) to the model Hamiltonian with the rotating-wave approximation as originally discussed by Hepp and Lieb (1973a) and Wang and Hioe (1973) we get the same phase transition behaviour.

3. The Ising model limit

The fact that the exact thermodynamics of the Dicke Hamiltonian leads to molecular-field-type solutions suggests that long range forces exist in the system. In fact Hepp and Lieb (1973a) pointed out that their results are typical of the van der Waals limits in systems with a long range interaction except that their mean field appears to be off diagonal. In our *ansatz* for H_{ts} in equation (2.6) we are actually considering a mean field in the z direction of the rotated pseudo-spin space and the diagonalization of H_{ts} diagonalizes the off-diagonal mean field acting on the S^x components. By analogy with spin–phonon problems (Gehring and Gehring 1975) we expect that the interaction of the independent spins with the photon mode will induce an effective spin–spin interaction of a long range nature and this will be responsible for producing the molecular-field-type behaviour. In this section we demonstrate, by making a transformation of the Hamiltonian in equation (2.1) directly related to the variational method, that in the limit $\lambda \to \infty$ the leading term in the Hamiltonian is an Ising term with the spins interacting equally with each other. As is well known (see for example Stanley 1971) the exact solution of this Ising model with an infinite range interaction is the molecular-field solution.

First, we note from equations (2.32) and (2.33) that as λ increases for a fixed value of ϵ, the transition temperature T_c increases and $\langle S^z \rangle$ approaches the behaviour of a Weiss ferromagnet more, being closer to zero at T_c.

It was shown in BSL that in the limit $T \to 0$, our variational calculation for the free energy reduces to the following variational principle for the ground state energy E_0,

$$E_0 \leqslant E_t = \langle 0|URHR^\dagger U^\dagger|0\rangle = \langle 0|H'|0\rangle \tag{3.1}$$

with R, U and H' given in equations (2.9), (2.12) and (2.15) respectively. The normalized vacuum state $|0\rangle$ is defined by $a|0\rangle = 0$, $S_i^z|0\rangle = -\frac{1}{2}|0\rangle$ for all i and $\langle 0|0\rangle = 1$. From equation (2.15) we get

$$E_t = \frac{f^2}{g^2} - \tfrac{1}{2}N\epsilon \cos\theta + \frac{2\lambda f N}{g\sqrt{N}} \sin\theta \tag{3.2}$$

noting that $\langle 0|a^\dagger a|0\rangle = \langle 0|S^x|0\rangle = \langle 0|(a+a^\dagger)|0\rangle = 0$. Minimization of E_t with respect to θ and f/g gives

$$\frac{f}{g} = -\lambda\sqrt{N}\left(1 - \frac{\epsilon^2}{16\lambda^4}\right)^{1/2} \tag{3.3}$$

and

$$\left.\begin{aligned} &\theta = 0 \\ \text{or}\quad & \\ &\cos\theta = \epsilon/4\lambda^2 \end{aligned}\right\} \tag{3.4}$$

We assume that $4\lambda^2 \geqslant \epsilon$ so that the second solution in (3.4) is taken. Substituting the quantities in (3.3) and (3.4) into equation (2.15) we get

$$H' = H_1 + H_2 \tag{3.5}$$

where

$$H_1 = a^\dagger a + 4\lambda^2 \sum_i S_i^z + \frac{2\lambda}{\sqrt{N}}\left(1 - \frac{\epsilon^2}{16\lambda^4}\right)^{1/2} \sum_i (a+a^\dagger)(S_i^z + \tfrac{1}{2}) \tag{3.6}$$

$$H_2 = \frac{\epsilon}{2\sqrt{N}\lambda} \sum_i (a+a^\dagger) S_i^x. \tag{3.7}$$

Note that H_2 is of $O(1/\lambda)$ whereas H_1 is $O(\lambda^2)$ and $O(\lambda)$. Let us take λ very large, so that H_2 becomes very small and can be neglected as a first approximation. Then we get

$$H' = H_1 + O(1/\lambda). \tag{3.8}$$

Now since all the z components of spin in H_1 commute with each other we can diagonalize H_1 exactly to give

$$H_1' = U_1 H_1 U_1^\dagger = a^\dagger a + \frac{\epsilon^2}{4\lambda^2}\sum_i S_i^z - \frac{4\lambda^2}{N}\left(1 - \frac{\epsilon^2}{16\lambda^4}\right)\sum_{i=1}^N \sum_{j=1}^N S_i^z S_j^z \tag{3.9}$$

where

$$U_1 a U_1^\dagger = a + f_1, \qquad U_1 a^\dagger U_1^\dagger = a^\dagger + f_1 \tag{3.10}$$

and

$$f_1 = -\frac{2\lambda}{\sqrt{N}}\left(1 - \frac{\epsilon^2}{16\lambda^4}\right)^{1/2} \sum_i (S_i^z + \tfrac{1}{2}). \tag{3.11}$$

Consistent with neglecting terms of $O(1/\lambda)$ in equation (3.8) we must also neglect terms of $O(1/\lambda^2)$ in (3.9). This gives,

$$H_1' = a^\dagger a - \frac{4\lambda^2}{N}\sum_{i=1}^N \sum_{j=1}^N S_i^z S_j^z. \tag{3.12}$$

The terms with $i = j$ in (3.12) merely give constant terms since $(S_i^z)^2 = \frac{1}{4}$. Hence we have a leading term which is an Ising interaction, each spin interacting equally with each other. This has an exact solution (Stanley 1971, p 91) given by

$$y = \lambda\sqrt{2\beta}\tanh(\sqrt{2\beta}\lambda y) \tag{3.13}$$

where y is an order parameter. If we let $y = 2\lambda\sqrt{2\beta}\langle S^z\rangle$, then equation (3.13) becomes

$$\langle S^z\rangle = \tfrac{1}{2}\tanh(4\beta\lambda^2\langle S^z\rangle) \tag{3.14}$$

which agrees with equation (2.32) except that in this limit $\lambda \to \infty$, condition (2.29) is not necessary.

4. Conclusion

The exact solution of the Dicke model obtained by a mean-field-type variational calculation for the free energy is, apart from being another derivation of the exact thermodynamics, an important test of the similar variational method that was applied to a spin–phonon problem with a similar structure for the Hamiltonian where the problem is more complicated because of the interaction of the spins with an infinite number of phonon modes and the presence of phase factors depending on the site of the two-level ion. Although we have no direct proof of the fact that the variational method here is exact at present, we hope to investigate this question in future. We believe the transformation of the Hamiltonian inherent in the variational method, to display a leading term which is an Ising interaction between the z components of spin in the rotated pseudo-spin space where each spin interacts equally with each other in the limit $\lambda \to \infty$, provides physical insight into the fact that long range effective interactions between the spins, induced by their interaction with the photon field, are responsible for the mean-field behaviour found for the super-radiant phase transition.

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