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Effect of spin–spin interaction on the super-radiant phase transition for the Dicke Hamiltonian

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Abstract. The thermodynamic equilibrium properties of the Dicke Hamiltonian for a collection of spin-$\frac{1}{2}$ particles interacting via magnetic dipole interaction with a single mode of the radiation field and with each other by spin–spin interaction are analysed and the conditions for the existence of a super-radiant phase transition are derived. It is shown, using the approximate long-range spin–spin interaction (MI), in the Dicke Hamiltonian, that the conditions for the existence of the super-radiant phase transition are invariant with respect to isotropic MI whether or not the A^2 term is included. If the counter-rotating terms in the spin–radiation field interaction are dropped from the Hamiltonian, the MI lowers the transition temperature. For anisotropic MI, the transition temperature is raised or lowered depending specifically upon the anisotropy. The conditions for the existence of the super-radiant phase transition are independent of the Curie temperature. These results easily generalise to finite many modes of the radiation field.

1. Introduction

There has been much recent interest in the phase transition in thermodynamic equilibrium of the Dicke model Hamiltonian (Dicke 1954) in its various 'dressed' forms. This has been stimulated by the proof (Hepp and Lieb 1973a) that Dicke's Hamiltonian predicts the existence of a second-order phase transition for a certain range of values for the coupling constants. Since the work of Wang and Hioe (1973) and Hepp and Lieb (1973b) which simplified the calculational aspects of the Hepp and Lieb procedure and that of Gilmore and Bowden (1976a) which produced further simplification and facilitated ease of calculation of the conditions for the existence of phase transitions for various 'dressed' forms of the Dicke Hamiltonian, much published work has appeared dealing with various ramifications of Dicke's original Hamiltonian (Carmichael *et al* 1973, Kudenko *et al* 1975, Thompson 1975, Rzażewski *et al* 1975).

The importance of the atomic interaction in the discussion of the thermodynamic equilibrium properties of the Dicke Hamiltonian is obvious. The condition for the existence of a phase transition in the Dicke model Hamiltonian is enhanced by higher density, but the atomic interaction, which in itself may cause a phase transition even in the absence of the electromagnetic field, becomes increasingly important. However, to our knowledge, none of the authors of previous work have considered the effect of direct interaction among the atoms, except for Kudenko *et al* (1975) who treated the effect of interatomic Coulomb interaction. In their work they use the molecular field

approximation, and the Coulomb contribution to their Hamiltonian gives only diagonal terms.

In this paper we analyse the effect of the atomic interaction on the super-radiant phase transition in the Dicke model Hamiltonian in thermodynamic equilibrium. For the purpose of simplified mathematical manipulation we introduce a simple form for the magnetic atomic interaction (MI), namely, that the interaction is independent of the interatomic distance. This is a good approximation for the long-range dipole–dipole interaction among the atoms contained in a volume smaller than a wavelength of the electromagnetic field. Although it is a poor approximation for the short-range force like the Heisenberg exchange interaction, this approximation for the atomic interaction is necessary for the Dicke model which has no spatial dependence, i.e. it is a point model†. The results of our calculation are therefore readily applicable to a system of magnetic moments contained, say, in a microwave cavity. For this reason and for simplicity we restrict our treatment to that for one mode of the radiation field, although the calculation easily generalises to finite many modes.

In the next section we discuss the modified Dicke Hamiltonian and introduce a canonical transformation which simplifies subsequent calculations. The method of Gilmore and Bowden (1976a, b) is used to obtain a linearised thermodynamically equivalent Hamiltonian for the modified Dicke model in § 3, and the corresponding free energy as a function of variational parameters is derived. In § 4 we minimise the free energy in the variational parameters which results in a set of coupled non-linear equations from which the gap equations for the super-radiant phase transition are derived. The results of the calculations are discussed in § 5 in terms of conditions on the parameters in the model for the existence of a super-radiant phase transition in the atom–radiation field interaction.

2. The modified Dicke model

The Dicke Hamiltonian in one radiation field mode including the A^2 term (Rżazewski *et al* 1975, Gilmore and Bowden 1976b) and MI denoted by J^α is

$$\mathcal{H} = \tfrac{1}{2}\omega(a^\dagger a + aa^\dagger) + \kappa(a + a^\dagger)^2 + \epsilon \sum_j \tfrac{1}{2}\sigma_j^z + \frac{\lambda}{\sqrt{N}} \sum_j (a^\dagger \sigma_j^- + a\sigma_j^+ + ra^\dagger \sigma_j^+ + ra\sigma_j^-)$$

$$- u_B H \sum_j \tfrac{1}{2}\sigma_j^z - \tfrac{1}{2} \sum_{g,f,\alpha} J^{(\alpha)} S_g^\alpha S_f^\alpha \tag{2.1}$$

where $r = 0, 1$ labels the contributions from the counter-rotating terms in the atom–field interaction, and

$$S_g^\alpha = \tfrac{1}{2}\sigma_g^\alpha \tag{2.2}$$

is the αth component of the gth spin. Here, and throughout, we set $\hbar = 1$. We also assume that $J_\parallel, J_\perp > 0$ in the following discussion. Furthermore, we have assumed in (2.1) that the collection of spins is contained in a volume much smaller than a wavelength of the radiation field. This assumption is consistent with the usual form for the Dicke model Hamiltonian.

† The spin wave theory, which is a mean-field approach in momentum space, should of course be used to discuss the thermodynamic equilibrium properties of an extended ferromagnet. The model with spatial consideration involves a more involved calculation and will appear in a subsequent publication.

It is convenient to perform a canonical transformation of (2.1) to get

$$\mathscr{H}' = \omega' a^\dagger a + \epsilon \sum_j \tfrac{1}{2}\sigma_j^z + \frac{\lambda'}{\sqrt{N}} \sum_j [a^\dagger \sigma_j^- + a\sigma_j^+ + r(a^\dagger \sigma_j^+ + a\sigma_j^-)] + \mathscr{H}_S, \quad (2.3)$$

where

$$\mathscr{H}_S = \tfrac{1}{2}(\epsilon - u_B H) \sum_j \sigma_j^z - \tfrac{1}{4} J_\parallel \sum_{q,p} \sigma_q^z \sigma_p^z - \tfrac{1}{2} J_\perp \sum_{q,p} (\sigma_q^- \sigma_p^+ + \sigma_q^+ \sigma_p^-) \quad (2.4),$$

and (Gilmore and Bowden 1976b)

$$\omega' = \omega \sqrt{f} \quad (2.5a)$$

$$\lambda' = \tfrac{1}{2}\lambda[(1+r)f^{-1/4} + (1-r)f^{1/4}] \quad (2.5b)$$

$$r' = \frac{1 - [(1-r)/(1+r)]\sqrt{f}}{1 + [(1-r)/(1+r)]\sqrt{f}} \quad (2.5c)$$

$$f = 1 + 4\frac{\kappa}{\omega}. \quad (2.5d)$$

There are at least three methods that can be used to calculate the gap equations associated with the equilibrium statistical mechanics of (2.1). They are: (*a*) the Green function approach to calculate the coupled non-linear equations for $\langle \sigma^+ \rangle$, $\langle \sigma^- \rangle$, $\langle a \rangle$ and $\langle a^\dagger \rangle$, and $\langle \sigma^z \rangle$; (*b*) the method of Wang and Hioe (1973); and (*c*) the linearisation procedure of Gilmore and Bowden (1976a, b). All three methods result in the same expressions for the gap equations†.

The set of Green functions (Zubarov 1960) which should be used to derive the coupled non-linear equations is

$$G_{gf}(t-t') = -i\theta(t-t')\langle [\sigma_g^-(t), \sigma_f^+(t')]_+ \rangle \quad (2.6)$$

and

$$G_{gf}^z(t-t') = -i\theta(t-t')\langle [\sigma_g^z(t), \sigma_f^+(t')]_+ \rangle. \quad (2.7)$$

If the corresponding equations of motion are solved using standard decoupling approximations (Fetter and Walecka 1971, Hubbard 1959)†, the desired coupled non-linear equations are derived.

The solution to the resulting equations leads to identical conditions for the existence of a phase transition that one obtains from the functional integration method (Wang and Hioe 1973), as well as that obtained from the linearisation procedure (Gilmore and Bowden 1976a, b). In our opinion, the latter procedure is by far the simplest of these methods to apply; therefore, we restrict our calculation to the linearisation procedure in the next section to determine the gap equations and corresponding conditions for the existence of a phase transition and critical temperature.

† The equivalence of the structure of (2.1) to the BCS model should be noted, and both can be solved in the thermodynamic limit. The equivalence of the mean-field approach, the Green function method, and the functional integral method in the BCS model is given by Fetter and Walecka (1971) and Hubbard (1959).

3. Linearisation of the Hamiltonian

The linearisation method has been developed and applied to selected cases in earlier publications (Gilmore and Bowden 1976a, b); therefore, we simply outline the procedure in what follows. The equilibrium thermodynamics of (2.3) can be completely determined if the free energy F is known:

$$e^{-\beta F} = \mathrm{Tr}\, e^{-\beta \mathscr{H}'}. \tag{3.1}$$

As it stands, the bilinear combination of operators in (2.3) precludes the actual performance of the operation on the right-hand side of (3.1). However, the Hamiltonian $\mathscr{H}'$, i.e. (2.3), can be linearised (Gilmore and Bowden 1976a) to give a thermodynamically equivalent Hamiltonian $\mathscr{H}'_{\mathrm{L}}$ such that the associated linearised free energy F_{L} satisfies the condition (Gilmore and Bowden 1976a, b),

$$\lim_{N\to\infty} \frac{F - F_{\mathrm{L}}(u, \nu_j, \eta_j)}{N} \to 0, \tag{3.2}$$

where u, ν_j, and η_j are adjustable parameters chosen variationally. These parameters are introduced by replacing a, σ_j^-, and σ_j^z in the interaction part of (2.3) by the following:

$$a = (a-u)+u, \tag{3.3a}$$

$$\sigma_j^- = (\sigma_j^- - \nu_j)+\nu_j, \tag{3.3b}$$

$$\sigma_j^z = (\sigma_j^z - \eta_j)+\eta_j. \tag{3.3c}$$

The result is that (2.3) can be written in the equivalent form

$$\mathscr{H}' = \mathscr{H}'_{\mathrm{F}} + \mathscr{H}'_{\mathrm{m}} + \mathscr{H}'_{\mathrm{mo}} + \mathscr{H}'_{\mathrm{LO}} + \mathscr{H}'_{\mathrm{BL}}, \tag{3.4}$$

where

$$\mathscr{H}'_{\mathrm{F}} = \omega' a^\dagger a + \frac{\lambda'}{\sqrt{N}} \sum_j [a^\dagger \nu_j + a\nu_j^* + r'(a^\dagger \nu_j^* + a\nu_j)], \tag{3.5a}$$

$$\mathscr{H}'_{\mathrm{m}} = \tfrac{1}{2}(\epsilon_0 - \eta J_\parallel)\sum_j \sigma_j^z - J_\perp \sum_j (\sigma_j^- \nu^* + \sigma_j^+ \nu) + \frac{\lambda'}{\sqrt{N}} \sum_j [u^* \sigma_j^- + u\sigma_j^+ + r'(u^*\sigma_j^+ + u\sigma_j^-)], \tag{3.5b}$$

$$\mathscr{H}'_{\mathrm{LO}} = -\frac{\lambda'}{\sqrt{N}} \sum_j [u^* \nu_j + u\nu_j^* + r'(u^*\nu_j^* + u\nu_j)], \tag{3.5c}$$

$$\mathscr{H}'_{\mathrm{mo}} = \tfrac{1}{4} J_\parallel \sum_{\substack{i,j \\ i\neq j}} \eta_i \eta_j + J_\perp \sum_{\substack{i,j \\ i\neq j}} (\nu_i \nu_j^* + \nu_i^* \nu_j), \tag{3.5d}$$

$$\begin{aligned}\mathscr{H}'_{\mathrm{BL}} = {} & -\tfrac{1}{4} J_\parallel \sum_{\substack{i,j \\ i\neq j}} [(\sigma_i^z - \eta_i)(\sigma_j^z - \eta_j)] - J_\perp \sum_{\substack{i,j \\ i\neq j}} [(\sigma_i^- - \nu_i)(\sigma_j^+ - \nu_j^*) + (\sigma_i^+ - \nu_i^*)(\sigma_j^- - \nu_j)] \\ & + \frac{\lambda'}{\sqrt{N}} \sum_j \{(a^\dagger - u^*)(\sigma_j^- - \nu_j) + (a-u)(\sigma_j^+ - \nu_j^*) \\ & + r'[(a^\dagger - u^*)(\sigma_j^+ - \nu_j^*) + (a-u)(\sigma_j^- - \nu_j)]\}. \end{aligned} \tag{3.5e}$$

Here we have written

$$\epsilon_0 = \epsilon - u_{\mathrm{B}} H. \tag{3.6}$$

If the adjustable parameters in (3.3) are chosen variationally to minimise the free energy, the procedure developed by Gilmore and Bowden (1976a, b) can be used to show that the contribution to the free energy per particle $f = F/N$ of the bilinear part of (3.4), i.e. (3.5*e*), vanishes in the limit (3.2). The choice of the parameters in (3.3) which does this is

$$u = \langle a \rangle, \tag{3.7a}$$

$$\nu_j = \nu = \langle \sigma^- \rangle, \tag{3.7b}$$

$$\eta_j = \eta = \langle \sigma^z \rangle. \tag{3.7c}$$

The adjustable parameters introduced in (3.3) are therefore seen to be order parameters for the system. Thus, the Hamiltonian $\mathscr{H}_L$ thermodynamically equivalent to (3.4) is

$$\mathscr{H}_L = \mathscr{H}'_F + \mathscr{H}'_m + \mathscr{H}'_{mo} + \mathscr{H}'_{LO} \tag{3.8}$$

where the terms on the right in (3.8) are given by (3.5). The linearised free energy is then calculated from

$$e^{-\beta F_L} = \mathrm{Tr}\, e^{-\beta \mathscr{H}_L}, \tag{3.9}$$

and in the limit (3.2)

$$f_L = F_L/N \tag{3.10}$$

is an exact result. It is to be noted that the last two terms in (3.8) are c-numbers and can therefore be dropped as far as the calculation of thermal averages is concerned. They do, however, contribute to the linearised free energy F_L.

From (3.9), (3.10), and (3.5) the free energy per particle f_L is

$$f_L = \tfrac{1}{4}J_\parallel \eta^2 + J_\perp |\nu|^2 - \lambda'[u'^* \nu + u' \nu^* + r'(u'^* \nu^* + u' \nu)]$$
$$- \frac{\lambda'^2}{\omega'} |(\nu + r' \nu^*)|^2 - \frac{1}{\beta} \ln 2 - \frac{1}{\beta} \ln \cosh \beta\theta \tag{3.11}$$

where

$$\theta = [(\tfrac{1}{2}\epsilon_0 - \tfrac{1}{2}J_\parallel \eta)^2 + |\lambda'(u' + r' u'^*) - J_\perp \nu|^2]^{\frac{1}{2}} \tag{3.12}$$

and we have written in (3.11)

$$u' \equiv u/\sqrt{N}. \tag{3.13}$$

In the next section we use (3.11) to develop the coupled non-linear equations from which the gap equations are derived.

4. Calculation of the gap equations

We now require that the free energy $f_L(u', \nu, \eta)$ be a minimum in the parameters (3.7). It is necessary that the following three normal equations be satisfied:

$$\partial f_L / \partial u' = 0, \tag{4.1a}$$

$$\partial f_L / \partial \nu = 0, \tag{4.1b}$$

$$\partial f_L / \partial \eta = 0. \tag{4.1c}$$

Explicitly, from (3.11) and (3.12)

$$\frac{\partial f_L}{\partial u'} = -\lambda'(\nu^* + r'\nu) - \lambda'^2\left[r'\left((u' + r'u'^*) - \frac{J_\perp}{\lambda'}\nu\right) + \left((u'^* + r'u') - \frac{J_\perp}{\lambda'}\nu^*\right)\right]\frac{\tanh\beta\theta}{2\theta} = 0, \tag{4.2a}$$

$$\frac{\partial f_L}{\partial \nu} = J_\perp\nu^* - \lambda'(u'^* + r'u') - \frac{\lambda'^2}{\omega'}[(\nu + r'\nu^*)r' + (\nu^* + r'\nu)]$$

$$+ J_\perp[\lambda'(u'^* + r'u') - J_\perp\nu^*]\frac{\tanh\beta\theta}{2\theta} = 0 \tag{4.2b}$$

$$\frac{\partial f_L}{\partial \eta} = \eta + (\epsilon_0 - J_\parallel\eta)\frac{\tanh\beta\theta}{2\theta} = 0. \tag{4.2c}$$

It is to be noted that equation (4.2*c*) gives an immediate expression for the magnetisation:

$$\frac{\tanh\beta\theta}{2\theta} = \frac{-\eta}{(\epsilon_0 - J_\parallel\eta)}, \tag{4.3}$$

which is the standard result if the order parameters (3.7*a*) and (3.7*b*) are set equal to zero.

Equations (4.2*a*) and (4.2*b*) have the solution $\nu = u' = 0$. This corresponds to the chaotic branch of the free energy (Gilmore and Bowden 1976a, b). These two equations and their complex conjugates combine to eliminate ν and ν^* to give the following equations:

$$(u' + u'^*)\left[1 - \left(\frac{\lambda'^2}{\omega'}(1 + r')^2 + J_\perp\right)\frac{\tanh\beta\theta}{2\theta}\right] = 0. \tag{4.4}$$

$$(u' - u'^*)\left[1 - \left(\frac{\lambda'^2}{\omega'}(1 - r')^2 - J_\perp\right)\frac{\tanh\beta\theta}{2\theta}\right] = 0. \tag{4.5}$$

The non-trivial solutions to (4.4) and (4.5) give, respectively, the equations

$$\frac{\tanh\beta\theta}{(1 + |g|^2)^{1/2}} = (\epsilon_0 - J_\parallel\eta)\left(\frac{\lambda'^2}{\omega'}(1 + r')^2 + J_\perp\right)^{-1} \tag{4.6}$$

$$\frac{\tanh\beta\theta}{(1 + |g|^2)^{1/2}} = (\epsilon_0 - J_\parallel\eta)\left(\frac{\lambda'^2}{\omega'}(1 - r')^2 - J_\perp\right)^{-1} \tag{4.7}$$

where we have used (3.12) to write θ in the denominators in (4.4) and (4.5) in the form

$$\theta = \tfrac{1}{2}(\epsilon_0 - J_\parallel\eta)(1 + |g|^2)^{1/2} \tag{4.8}$$

where

$$|g|^2 = \frac{4|\lambda'(u' + r'u'^*) - J_\perp\nu|^2}{(\epsilon_0 - J_\parallel\eta)^2}. \tag{4.9}$$

If (4.3) is used to eliminate η from the right-hand side of (4.6) and (4.7), the results are

$$\frac{\tanh\beta\theta}{(1 + |g|^2)^{1/2}} = \epsilon_0\left(\frac{\lambda'^2}{\omega'}(1 + r')^2 + J_\perp - J_\parallel\right)^{-1} \tag{4.10}$$

and

$$\frac{\tanh \beta\theta}{(1+|g|^2)^{1/2}} = \epsilon_0\left(\frac{\lambda'^2}{\omega'}(1-r')^2 - (J_\parallel + J_\perp)\right)^{-1} \tag{4.11}$$

where we have used (4.3) together with (4.8) to get

$$\frac{\tanh \beta\theta}{(1+|g|^2)^{1/2}} = -\eta. \tag{4.12}$$

For $u' = \nu' = 0$, then $|g|^2 = 0$, and, provided a solution exists, (4.10) and (4.11) each correspond to a gap equation which represents a bifurcation of the free energy at the respective critical temperatures (Gilmore and Bowden 1976a, b). We have explicitly

$$\tanh \beta_c^{(1)}\theta_c = \epsilon_0\left(\lambda^2 \frac{(1+r)^2}{\omega + 4\kappa} + J_\perp - J_\parallel\right)^{-1} \tag{4.13}$$

and

$$\tanh \beta_c^{(2)}\theta_c = \epsilon_0\left(\frac{\lambda^2}{\omega}(1-r)^2 - (J_\parallel + J_\perp)\right)^{-1} \tag{4.14}$$

where

$$\theta_c = \tfrac{1}{2}(\epsilon_0 - J_\parallel \eta) \tag{4.15}$$

and we have used (2.5) to transform back to the original parameters in the Hamiltonian (2.1).

The magnetisation is determined by (4.12) which requires that

$$-1 < \eta < 0. \tag{4.16}$$

The minimum branch in the free energy is determined by examination of the eigenvalues of the free energy stability matrix (Gilmore and Bowden 1976b) $|f_{Lij}|$. The branch corresponding to (4.10) or (4.11) with the higher transition temperature given by (4.13) or (4.14) respectively, is the minimum, and the one with lower transition temperature is not stable.

5. Conclusions

We have verified that three methods, that of Wang and Hioe (1973), a Green function technique (Zubarov 1960), (2.6) and (2.7), and the linearisation method of Gilmore and Bowden (1976a, b) all lead to the same equations, (4.13) and (4.14). In this paper we used the linearisation procedure to derive these results.

Consider the special case of isotropic MI, $J_\perp = J_\parallel$ and the counter-rotating terms in the atom–radiation field interaction present, i.e. from (2.5*c*), $r' = r = 1$. A solution to (4.14) in this case does not exist, and there can be only one bifurcation of the free energy corresponding to (4.13). Examination of the eigenvalues of the free energy stability matrix (Gilmore and Bowden 1976b) shows that the ordered branch, if it exists, is indeed a minimum. The isotropic MI has no effect on the condition for the existence of a phase transition which is explicitly

$$\epsilon_0 \omega'/4\lambda'^2 < 1. \tag{5.1}$$

The only effect of the MI in this case is to raise the critical temperature (4.13) and (4.15). If the counter-rotating terms in the atom–field interaction are dropped, i.e. $r = 0$, then (4.14) may correspond to the minimum branch in the free energy depending upon whether or not the term $J_{\parallel}+J_{\perp}$ in the denominator is weak enough to produce a crossover (Gilmore and Bowden 1976b) of the bifurcation point with that given by (4.13) to give a higher critical temperature. Even if it does, the magnetic interaction causes more stringent requirements to be placed on the other parameters in the Hamiltonian for a phase transition to exist, i.e. (5.1) is now replaced by

$$\frac{\epsilon_0\omega'}{\lambda'^2} < 1 - \frac{J_{\parallel}+J_{\perp}}{\lambda'^2}\omega'. \tag{5.2}$$

For the case where $J_{\parallel} = 0$, $J_{\perp} \neq 0$, and $r = 1$, there is again only one bifurcation of the free energy from the chaotic branch given by (4.13). In this case the MI enhances the condition for a phase transition to exist, namely,

$$\frac{\epsilon_0\omega'}{4\lambda'^2} < 1 + \frac{J_{\perp}\omega'}{4\lambda'^2} \tag{5.3}$$

so that λ'^2/ω' can be smaller than the requirement corresponding to (5.1). In this case MI increases the critical temperature.

From the form of (4.13) and (4.14), it is recognised that $J_{\perp}$ can enhance the condition for a phase transition to exist, whereas $J_{\parallel}$ always tends to destroy the possibility for a phase transition. Putting this in a different light, $J_{\perp}$ can aid to induce a macroscopic transverse polarisation, but $J_{\parallel}$ tends to prevent this by producing a 'rigidity' in the direction of the DC magnetic field H.

It is to be noted that the right-hand side of (4.13) and (4.14) is independent of the magnetisation parameter η. Therefore, the conditions for the existence of a super-radiant phase transition are independent of any ferromagnetic transition temperature dictated by (4.3). The super-radiant phase transition temperature does, however, increase with the magnetisation as seen by using (4.15) in (4.13) or (4.14). The super-radiant gap equations (4.13) and (4.14) are valid below as well as above the Curie temperature.

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