Phase transition in the multimode two- and three-level Dicke model (Green's function method)

1979 J. Phys. A: Math. Gen. 12 2273

(http://iopscience.iop.org/0305-4470/12/11/035)

J. Phys. A: Math. Gen., Vol. 12, No. 11, 1979. Printed in Great Britain

Phase transition in the multimode two- and three-level Dicke model (Green's function method)

C C Sung† and C M Bowden‡

† Department of Physics, University of Alabama in Huntsville, Alabama 35807, USA
‡ High Energy Laser and Research Laboratory, US Army Missile Research and Development Command, Redstone Arsenal, Alabama 35809, USA

Received 17 July 1978, in final form 8 February 1979

Abstract. By using the thermodynamic Green's function method, we study the phase transition of a collection of two- as well as three-level atoms interacting with the electromagnetic field and contained within a volume much smaller than the smallest resonance wavelength (Dicke model). We show for the case of three-level atoms the existence of two critical temperatures where a second-order phase transition takes place. The upper critical temperature is determined by the largest of the three coupling constants in the three-level model, whereas the lower critical temperature is a function of the remaining two coupling constants. We also show that for a collection of two- as well as three-level atoms, the critical temperature depends upon the number of atoms contained within λ_r^3 (λ_r is a resonance wavelength) rather than the density as has previously been suggested. Also, using the Green's function method, we show the formal equivalence of the Dicke model in thermodynamic equilibrium with the BCS model of superconductivity.

1. Introduction

The Dicke Hamiltonian (Dicke 1954), which models the interaction of a collection of N two-level atoms with the radiation field, has found wide and extensive use in quantum optics, including the detailed description of super-radiance and superfluorescence (Bonifacio *et al* 1971a, b, Bonifacio and Lugiato 1975, McGillivray and Feld 1976). The thermodynamic properties of the two-level Dicke model Hamiltonian have also been studied for the restriction to one mode, or finite many modes, of the radiation field and a second-order phase transition is found (Hepp and Lieb 1973a, b).

Since the work of Hepp and Lieb (1973a) in which they obtain exact closed-form results, others have introduced more tractable calculational methods for studying the equilibrium thermodynamic properties of the Dicke model (Wang and Hioe 1973, Hepp and Lieb 1973b, Lee 1976, Gilmore and Bowden 1976a, Mihalache 1977). These methods have been used to study the equilibrium thermodynamics of various ramifications of the Dicke Hamiltonian (Gilmore and Bowden 1976a, b and references contained therein, Provost *et al* 1976, Bowden and Sung 1978). Of particular relation to the work presented here, Mihalache (1977) used thermodynamic Green's functions to show the effect of an external field on the phase transition in the two-level Dicke model in only one photon mode of the radiation field.

In this paper, we use the thermodynamic Green's function method to discuss the thermodynamic properties of the spatially independent Dicke model of two- and three-level atoms, including all modes of the radiation field. Besides obtaining some

0305-4470/79/122273+14$01.00

interesting results for phase transitions, we show why this time-dependent approach is essential for the multimode model where the field frequency may be off the atomic resonance. The Green's function approach leads naturally to the explicit formal equivalence between these models and the BCS model for superconductivity (Fetter and Walecka 1971, Gorkov 1958).

Others have considered the multimode model (finite many modes), by extension of the one-mode model† (Hepp and Lieb 1973b, Wang and Hioe 1973, Hioe 1973, Gilmore and Bowden 1976a, b). In order for these calculations to be tractable one has to assume a point model, namely that the wavelength λ of all modes must satisfy the condition that $\lambda^3 \gg V_g$, where V_g is the atomic volume. This assumption is crucial for all the quoted calculations where the spatial dependence of the atomic operators is neglected.

A serious consequence of imposing the point model assumption improperly concerns the importance of the A^2 term (Rzażewski *et al* 1975). The claim was made (Rzażewski *et al* 1975) that inclusion of the A^2 term in the Dicke Hamiltonian, considering the requirements imposed by the Thomas–Reiche–Kuhn (TRK) sum rule (Merzbacher 1963), removes the possibility of the phase transition. This conclusion was arrived at by assuming a poin model: λ_r^3 (the resonance wavelength) $\gg V_g$, so that the spatial dependence of all the terms in A^2 can be neglected. The method of Wang and Hioe was used to calculate the conditions for the existence of the phase transition, and this requires the taking of the thermodynamic limit, i.e. $N/V=$ const. as $N, V \to \infty$, where N is the total number of atoms and V is the quantisation volume for the electromagnetic field. This leads to an inconsistency from the very beginning, since the point model requires that $\lambda_r^3 \gg V_g$, but in the thermodynamic limit which they implicitly assume, $V_g = V$, and this requires that $\lambda_r^3 \gg V$, which is not reasonable.

It is perhaps worth mentioning here that recently Knight *et al* (1978) have argued that the gauge-invariant Hamiltonian for a collection of bound electrons in the one-mode approximation does not support a phase transition. The fact is that they also ignore the spatial dependence of the electromagnetic field (their equation (36)) which presents the same dilemma as that cited above. In fact, if they retain the point model approximation for the atoms, keeping N constant, and take the quantisation volume V for the field to infinity, the contribution from the A^2 term vanishes and the Hamiltonian is no longer positive definite.

We shall show in § 3 that the condition for the existence of a phase transition for the two-level Dicke Hamiltonian in the point model approximation is

$$\hbar\omega_r/8\pi d^2\bar{\rho} \leqslant 1 \tag{1.1}$$

where ω_r is the frequency for the radiation field, d is the matrix element for the transition dipole moment, and

$$\bar{\rho} = N/\lambda_r^3 \tag{1.2}$$

is the number of atoms contained within a cubic resonance wavelength.

The condition (1.1) differs from the previous work (Rzażewski *et al* 1975, Hioe 1973) in replacing $\bar{\rho}_0$ by $\bar{\rho}$:

$$\bar{\rho}_0 = N/V. \tag{1.3}$$

---

† It is to be noted that the Dicke Hamiltonian in one mode with spatial dependence is unitarily equivalent to the point model Hamiltonian in the rotation wave approximation and without the A^2 term (Hepp and Lieb 1973a).

This difference is caused by our consideration of the assumption that

$$V_g \ll \lambda^3 < V \tag{1.4}$$

whereas

$$V_g \equiv V \ll \lambda^3 \tag{1.5}$$

is implicitly used throughout the works cited above. The failure to distinguish the difference between V_g and V in the Dicke model leads to an overestimation of the contribution of A^2, which is $\propto 1/V$. We will show explicitly later (Sung and Bowden 1979) why the A^2 term is not important if equation (1.4) is consistently taken into account.

We use the thermodynamic Green's function (Zubarev 1960) to treat the Dicke model for two-level and three-level atoms. In the next section we derive the effective atomic interaction which provides the mechanism for the phase transition. It is observed that this is identical, in the products of different atomic operators, with the form for the retarded dipole–dipole interaction which is responsible for collective spontaneous relaxation from an initial state of complete inversion (Bonifacio *et al* 1971a, b, Bonifacio and Lugiato 1975, Narducci and Bowden 1976). This result is a consequence of the explicit time behaviour of the atomic operators in the Green's function method and does not appear explicitly in previous methods for calculating the phase transition (Hepp and Lieb 1973a, b, Wang and Hioe 1973, Hioe 1973, Gilmore and Bowden 1976a, b), which inherently impose stationary conditions at thermodynamic equilibrium. This form of the interaction term exhibits a kind of pair correlation among the atoms via their mutual radiation field which is formally equivalent to the interaction in BCS theory (Fetter and Walecka 1971). This is not surprising, due to the well known formal similarity of this problem with the BCS model. The main difference in approach between this work and others is that we consider the full mode dependence in the radiation field, and the explicit time dependence of the expectation values is not suppressed (this is important, for instance, when the field frequency is not in resonance with the atomic energy levels).

In § 3, we obtain the results for the condition for the existence of the phase transition for two-level atoms in the point model (1.1), which differs from previous work by the definition (1.2).

The results for the effective atomic interaction and conditions for the existence of phase transitions for three-level atoms are obtained in § 4. It is shown that there are two critical temperatures, the greater of which is determined by the largest coupling constant, whereas the lower critical temperature is determined by solving a set of simultaneous equations involving the smaller coupling constants. The free energy and conditions for the phase transitions are derived.

The last section is used to summarise the results of previous sections and to discuss their implications further.

2. The effective atomic interaction

The Hamiltonian for two-level atoms in the presence of an electromagnetic field is given by $H_0 + H'$:

$$H_0 = \sum \omega_k a_k^\dagger a_k + \sum_i \sum_{n=1,2} \epsilon_n C_{n,i}^\dagger C_{n,i} \tag{2.1}$$

$$H' = \sum_i \sum_k g_k a_k^\dagger C_{1,i}^\dagger C_{2,i} + \mathrm{HC} \tag{2.2}$$

where $a_k^\dagger (a_k)$ and $C_n^\dagger (C_n)$ are the creation (annihilation) operators of a photon and an atomic level occupation, with unperturbed energies ω_k and ϵ_n respectively. The coupling constant $g_k = -\mathrm{i}(\hbar\omega_k/2V)^{1/2}\boldsymbol{\epsilon}_k \cdot \boldsymbol{D}$, where $\boldsymbol{\epsilon}_k$ and $\boldsymbol{D}$ are the polarisation vector and the matrix element for the dipole moment between levels 1 and 2 (Loudon 1973). We also use units such that $\hbar = c = 1$. The equation of motion for a_k is

$$\mathrm{i}(\partial/\partial t)a_k^\dagger + \omega_k a_k^\dagger = -g_k^* \sum_i C_{2,i}^\dagger C_{1,i} \tag{2.3}$$

and the solution is given by

$$\begin{aligned} a_k^\dagger &= \mathrm{i}g_k \sum_i \lim_{\delta\to 0} \int_{-\infty}^{t} \mathrm{d}t'\ C_{2,i}^\dagger(t')C_{1,i}(t') \exp[\mathrm{i}\omega_k(t-t') + \delta t'] \\ &= -\lim_{\delta\to 0} \sum_i C_{2,i}^\dagger(t)C_{1,i}(t) g_k^*/[\omega_k - (\epsilon_2 - \epsilon_1) + \mathrm{i}\delta] \end{aligned} \tag{2.4}$$

where we have used $C_2^\dagger(t) = C_2^\dagger(t')\exp[\mathrm{i}\epsilon_2(t-t')]$. We obtain, by substitution of equation (2.4) into equation (2.2) and

$$\sum_k = V \int \mathrm{d}^3k/(2\pi)^3$$

the result

$$H' = -\bar{g}(1/N) \sum_{i\neq j} C_{2,i}^\dagger C_{1,j}^\dagger C_{2,j} C_{1,i} \tag{2.5}$$

where

$$\bar{g} = NV \lim_{\delta\to 0} \int [\mathrm{d}^3k/(2\pi)^3] |g_k|^2 \{[\omega_k - (\epsilon_2 - \epsilon_1) + \mathrm{i}\delta]^{-1} + \mathrm{cc}\}. \tag{2.6}$$

The terms $i = j$ can be considered as now included in H_0 with the effect of leading to frequency renormalisation.

The atomic interaction between two atoms i and j, as expressed in equation (2.5), is very similar to the interaction of a pair of localised spins caused by the virtual exchange of conducting electrons (RKKY interaction: Kittel 1963). It is also formally the same term which appears as the retarded dipole–dipole interaction in the analysis of the dynamical evolution of super-radiant emission of radiation (Bonifacio and Lugiato 1975, Narducci and Bowden 1976). However, equation (2.6) cannot be evaluated quantitatively because of the assumption in the Dicke model $V_g^{1/3} < \lambda = 2\pi/k$ which restricts the domain of the integration. Furthermore, since the factor $\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i)$ is neglected in equation (2.1), the spatial dependence of the atomic interaction cannot be discussed. In order to derive a correct expression for the atomic interaction, one has to start from the exact Hamiltonian for the radiation–atoms system, and the Dicke Hamiltonian is not adequate. Equation (2.5) serves to demonstrate in the spirit of the Dicke model how it originates from a system of atomic interaction induced by the virtual exchange of photons.

In previous works, equation (2.4) appears in the form

$$\langle a_k^\dagger \rangle = -(g_k^*/\omega_k) \sum_i \langle C_{2,i}^\dagger(t) C_{1,i}(t) \rangle \tag{2.7}$$

where $\langle\ \rangle$ denotes the ensemble average. The comparison of equations (2.7) and the results of equation (2.4), which is the exact equation of motion, indicates the effect of the choice of the variational states in the calculations (Hepp and Lieb 1973a, b, Rzażewski *et al* 1975, Wang and Hioe 1973, Gilmore and Bowden 1976a, b).

We will make two more comments on the difference between equations (2.7) and (2.4). First, we can also obtain equation (2.7) directly from equation (2.4) by taking the ensemble average of $a_k^\dagger$ and $C_2^\dagger C_1$. Then the previous results can be obtained by replacing $a_k^\dagger$ in equation (2.2) by the $\langle a_k^\dagger\rangle$ in equation (2.7). Second, in the previous work (Hepp and Lieb 1973b, Rzażewski and Wódkiewicz 1976) the integral like $\int \mathrm{d}^3k/\omega_k$ has been taken very seriously and even the cut-off of k is discussed. We wish to point out here that, because of the assumption $\lambda^3 \gg V_g$, the integral cannot be calculated. For the multimode case, any realistic consideration must include the factors $\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i)$ in equation (2.2) and obtain the spatial dependence of g in equation (2.6).

We can, however, write $\bar{g}$ in the form

$$\bar{g} \simeq (ND^2/\lambda_r^3)\left\{\lambda_r^3 \int \mathrm{d}\omega\, \omega S(\omega)/[\omega-(\epsilon_2-\epsilon_1)+\mathrm{i}\delta]+\mathrm{cc}\right\} \tag{2.8}$$

where $S(\omega)$, the density of states, is introduced through $\int \mathrm{d}^3k/(2\pi)^3 \to \int \mathrm{d}\omega\, S(\omega)$. If the main contribution to the integral comes from $\omega=\epsilon_2-\epsilon_1$, then the number in the braces is of the order of one. Hence, we take

$$\bar{g} = N\bar{D}^2/\lambda_r^3 \tag{2.9}$$

where $\bar{D} \propto D$, whose magnitude depends on the value of the integral in equation (2.8).

In the following section, we obtain the thermodynamics of the Dicke Hamiltonian by using H_0+H_{int}, where $H_{\mathrm{int}} \equiv H'$ in equation (2.5). This step, however, is not necessary in the Green's function method; we can start from equation (2.2) and perform the decoupling approximation $\langle a_k^\dagger C_2^\dagger C_1\rangle = \langle a_k^\dagger\rangle\langle C_2^\dagger C_1\rangle$ and substitute $\langle a_k\rangle$ from equation (2.7) to obtain identical results. It should be emphasised that the difference between this work and the previous one stems from equations (2.4)–(2.6) against equation (2.7). If one starts from H_0+H_{int}, then all the methods will give us the same results as those which we expect from the example provided by the BCS model (Fetter and Walecka 1971).

3. Two-level atoms

The two-time Green's function is defined by (Zubarev 1960)

$$G_{n,i}(t-t') = -\mathrm{i}\eta(t-t')\langle[C_{n,i}(t), C_{n,i}^\dagger(t')]\rangle \tag{3.1}$$

where η is the step function and $\langle 0\rangle$ (the ensemble average) is $\operatorname{Tr}\exp(-\beta H)0$, $H=H_0+H_{\mathrm{int}}$, $1=\Sigma_n |n\rangle\langle n|$ and $|n\rangle$ is defined as

$$|n\rangle = |N-n, n\rangle \tag{3.2}$$

where $N-n$ and n are the numbers of atoms in the ground state level one and excited state level two respectively. The term in square brackets in equation (3.1) is a commutator since $C_n (C_n^\dagger)$ is assumed to be a boson operator, but our calculations and the results are equally applicable to fermions.

The anomalous Green's functions $F_n (n=1, 2)$ are defined by

$$F_{1,i} = -\mathrm{i}\eta(t-t')\langle[C_{2,i}(t), C_{1,i}^{\dagger}(t')]\rangle \tag{3.3}$$

$$F_{2,i} = -\mathrm{i}\eta(t-t')\langle[C_{1,i}(t), C_{2,i}^{\dagger}(t')]\rangle. \tag{3.4}$$

The following calculations and approximations follow closely Gorkov's classical paper on superconductivity (Gorkov 1958).

The time-independent autocorrelation functions $\hat{F}_1$ and $\hat{F}_2$ are defined as

$$\hat{F}_1 = \langle C_1^{\dagger}(t)C_2(t)\rangle \tag{3.5}$$

$$\hat{F}_2 = \langle C_2^{\dagger}(t)C_1(t)\rangle. \tag{3.6}$$

We also introduce the Fourier transform

$$G_n(t-t') = \int_{-\infty}^{\infty} \exp[-\mathrm{i}(t-t')\omega]G_n(\omega)\,\mathrm{d}\omega \tag{3.7}$$

$$F_n(t-t') = \int_{-\infty}^{\infty} \exp[-\mathrm{i}(t-t')\omega]F_n(\omega)\,\mathrm{d}\omega. \tag{3.8}$$

The equation of motion for G_1 is

$$(\mathrm{i}\,\partial/\partial t - \epsilon_1)G_1(t-t') + \bar{g}\hat{F}_2F_1(t-t') = \delta(t-t') \tag{3.9}$$

where the decoupling approximation

$$\langle[C_2^{\dagger}C_1C_2(t), C_1^{\dagger}(t')]\rangle = \hat{F}_2F_1(t-t') \tag{3.10}$$

has been used and we have also dropped the index i in all G and F, because of the lack of spatial dependence in the Dicke model and the equivalence of all G_i and F_i for all i. We do not include the terms $\hat{G}_2G_1(t-t')$ in equation (3.10), since the effect is only to cause a shift in ϵ_1 and ϵ_2.

The Fourier transform of equation (3.9) is given by

$$(\omega-\epsilon_1)G_1(\omega) + \bar{g}\hat{F}_2F_1(\omega) = 1/2\pi. \tag{3.11}$$

Similarly

$$(\omega-\epsilon_2)F_1(\omega) + \bar{g}\hat{F}_1G_1(\omega) = 0 \tag{3.12}$$

and the solution of equations (3.11) and (3.12) is

$$(\omega-\bar{\epsilon}_1)(\omega-\bar{\epsilon}_2)G_1 = (\omega-\epsilon_2)/2\pi \tag{3.13}$$

$$(\omega-\bar{\epsilon}_1)(\omega-\bar{\epsilon}_2)F_1 = -\bar{g}\hat{F}_1/2\pi \tag{3.14}$$

where $\bar{\epsilon}_1$ and $\bar{\epsilon}_2$ are defined as the roots of

$$\omega^2 = (\epsilon_1+\epsilon_2)\omega - (-\epsilon_1\epsilon_2 + \bar{g}^2\hat{F}_1\hat{F}_2) = 0. \tag{3.15}$$

Notice that $\hat{F}_1$ is the complex conjugate of $\hat{F}_2$ and we write $\hat{F}_1 = \hat{F}_2^* = \hat{F}$ which is taken to be real. We also choose $\epsilon_1 + \epsilon_2 = 0$:

$$\bar{\epsilon}_{1,2} = \pm(\epsilon^2 + \Delta^2)^{1/2} \tag{3.16}$$

where $\Delta^2 = g^2|\hat{F}|^2$ may be called the gap or order parameter and ϵ is the unperturbed atomic level separation.

The solutions for G_2 and F_2 are similar to equations (3.13) and (3.14):

$$(\omega-\bar{\epsilon}_1)(\omega-\bar{\epsilon}_2)G_2=(\omega-\epsilon_1)/2\pi \tag{3.17}$$

$$(\omega-\bar{\epsilon}_1)(\omega-\bar{\epsilon}_2)F_2=-\bar{g}\hat{F}_2/2\pi. \tag{3.18}$$

In order to bring our calculation from quantum statistical mechanics to classical statistics, as in previous works, the density is normalised by assuming that there is one atom per lattice site, i.e.

$$\hat{G}_1+\hat{G}_2=1 \tag{3.19}$$

where $\hat{G}_n=\langle C_n^{\dagger}C_n\rangle$. $\hat{G}_n$ is related to G_n by (Zubarev 1960)

$$\begin{aligned}\hat{G}_n&=\mathrm{i}\lim_{\delta\to 0}\int_{-\infty}^{\infty}[\![[G_n(\omega+\mathrm{i}\delta)-G_n(\omega-\mathrm{i}\delta)]/\{\exp[(\omega-\mu)\beta]-1\}]\!]\,\mathrm{d}\omega\\&\equiv\hat{P}G_n(\omega)\end{aligned} \tag{3.20}$$

where μ is the chemical potential. Equation (3.19) then becomes

$$\sum_{i=1,2}\{\exp[\beta(\bar{\epsilon}_i-\mu)]-1\}^{-1}=1. \tag{3.21}$$

In the limit of classical statistics $\exp(-\beta\mu)\to\infty$, we obtain

$$\exp(\beta\mu)\approx[\exp(-\beta\bar{\epsilon}_1)+\exp(-\beta\bar{\epsilon}_2)]^{-1}. \tag{3.22}$$

Then the order parameter Δ is determined by using the operator $\hat{P}$, defined by equation (3.20), on both sides of equation (3.14) and solving for $\hat{F}_1$. The resultant expression is

$$\hat{F}_1=\bar{g}\hat{F}_1\tanh(\beta\bar{\epsilon})/2\bar{\epsilon} \tag{3.23}$$

where we have used equation (3.22) for $\exp(\beta\mu)$. There are two conditions which satisfy equation (3.23):

$$\hat{F}_1=0 \tag{3.24}$$

or

$$2\bar{\epsilon}/\bar{g}=\tanh(\beta\bar{\epsilon}) \tag{3.25}$$

whose solution for $\Delta\neq 0$ exists only if

$$2\epsilon/\bar{g}\leqslant 1 \tag{3.26}$$

which has also been derived earlier (Hepp and Lieb 1973a, b, Rzażewski *et al* 1975, Wang and Hioe 1973, Gilmore and Bowden 1976a, b). The critical temperature $T_c=\beta_c^{-1}/k$ is given by

$$2\epsilon/\bar{g}=\tanh\beta_c\epsilon \tag{3.27}$$

and solutions for Δ in the neighbourhood of β_c and $T\to 0$ can be easily obtained:

$$\begin{aligned}&\Delta^2=\epsilon^2(1-\beta_c/\beta)[(\sinh 2\beta_c\epsilon)/2\epsilon\beta_c-1] &&\beta\to\beta_c^+\\&\Delta^2=0 &&\beta\to\beta_c^-\end{aligned} \tag{3.28}$$

$$\Delta^2=(\bar{g}^2-4\epsilon^2)^{1/2} \qquad \beta\to\infty \tag{3.29}$$

respectively.

The free energy of the system is denoted by $\Omega(g)$ for the coupling constant g (Fetter and Walecka 1971):

$$\Omega(g)-\Omega(0)=\int_0^{\bar{g}}(\mathrm{d}\bar{g}/\bar{g})\langle H_{\mathrm{int}}\rangle \tag{3.30}$$

and $\langle H_{\mathrm{int}}\rangle=-\bar{g}|F|^2=-\Delta^2/\bar{g}$. $\Omega(g)$, then, can be obtained by integration by parts and using equation (3.25):

$$\Omega(g)-\Omega(0)=\Delta^2/\bar{g}-\beta^{-1}\ln(\cosh\beta\bar{\epsilon}). \tag{3.31}$$

Notice that equation (3.31) is an even function of Δ^2, and $\partial\Omega(\bar{g})/\partial\Delta^2=0$ because of equation (3.25). As a result, the discontinuity in the thermodynamic properties at $\beta=\beta_{\mathrm{c}}$ is contained in $\Delta\Omega$:

$$\Delta\Omega=(\partial^2\Omega/\partial\Delta^2)\Delta^4 \qquad \beta\approx\beta_{\mathrm{c}}. \tag{3.32}$$

Since Δ^4 changes from zero to $(1-\beta_{\mathrm{c}}/\beta)^2$ from equation (3.28), the second-order derivative (the specific heat) is discontinuous as β passes through β_{c}.

Our results for the phase transition in the two-level Dicke model without spatial dependence, and in the absence of the A^2 term (3.26), seem identical to the results of Hepp and Lieb (1973a, b), Rzażewski *et al* (1975), Wang and Hioe (1973) and Gilmore and Bowden (1976a, b). The essential difference is that in equation (3.26) $\bar{\rho}$ appears instead of $\bar{\rho}_0$. This difference is due to the fact that we have consistently taken the 'point model' assumption, equation (1.4), into the calculation.

4. Three-level atoms

In the three-level model, the summation over n in equation (2.1) extends from 1 to 3 and H' becomes

$$H'=\sum_k g_k a_k^\dagger(C_{2,i}^\dagger+C_{3,i}^\dagger C_{2,i}+C_{3,i}^\dagger C_{1,i})+\mathrm{HC} \tag{4.1}$$

and $a_k^\dagger$ from equation (2.4) now consists of three terms:

$$a_k^\dagger=-\lim_{\delta\to 0}\sum_{i=1}^{N}\{g_k^* C_{1,i}^\dagger C_{2,i}/[\omega_k-(\epsilon_2-\epsilon_1)+\mathrm{i}\delta]+(2\to 3)+(1\to 2)\} \tag{4.2}$$

where $(2\to 3)$ is a term obtained by changing the index from 2 to 3 in the previous term.

Substitution of equation (4.2) in equation (4.1) leads to nine terms, of which three terms are given by

$$H_1'=-g_{12}\sum_{i\neq j}C_{2,i}^\dagger C_{1,j}^\dagger C_{2,j}C_{1,j}-g_{23}\sum_{i\neq j}C_{3,i}^\dagger C_{2,j}^\dagger C_{3,j}C_{2,i}-g_{31}\sum_{i\neq j}C_{3,i}^\dagger C_{1,j}^\dagger C_{3,j}C_{1,i}. \tag{4.3}$$

The rest of the terms denoted by $H_2'=H'-H_1'$ are not important, as shown later. The coupling constant g_{ij} is defined similar to $\bar{g}$ in equation (2.6), and will not be repeated here. We also introduce the notation

$$F_{n,n'}(t-t')=-\mathrm{i}\eta(t-t')\langle[C_{n,i}(t),\,C_{n'}^\dagger(t')]\rangle. \tag{4.4}$$

The ensemble average in G_m is defined earlier (equation (3.1)), and $F_{n,n'}$ is taken over all states

$$\sum_{nn'n''}\langle n,n',n''|\,|n,n',n''\rangle$$

where n, n', n'' are the numbers of atoms in the levels 1, 2 and 3, respectively, and $n+n'+n''=N$.

A similar decoupling approximation to that in equation (3.10) is to be used to write down the equations of motion. H_2', however, gives rise to terms like

$$\sum_{n,n_2,n_3} \langle n_1, n_2, n_3 | [C_{1,j} C^{\dagger}_{3,i} C_{2,i} C^{\dagger}_{2,j}] | n_1 n_2 n_3 \rangle,$$

which is zero in our approximation. Consequently, unless we introduce a higher-order hierarchy of Green's functions, H_2' does not contribute to the equation of motion for G or F. We have

$$(\omega-\epsilon_1)G_1 + g_{21}\hat{F}_{12}F_{21} + g_{31}\hat{F}_{13}F_{31} = 1/2\pi \tag{4.5}$$

$$(\omega-\epsilon_2)F_{21} + g_{21}\hat{F}_{21}G_1 + g_{32}\hat{F}_{23}F_{31} = 0 \tag{4.6}$$

$$(\omega-\epsilon_3)F_{31} + g_{32}\hat{F}_{32}F_{21} + g_{31}\hat{F}_{31}G_1 = 0. \tag{4.7}$$

The solutions are given by

$$F_{21} = [-g_{21}\hat{F}_{21}(\omega-\omega_3) + g_{23}\hat{F}_{23}g_{31}\hat{F}_{31}]/D \tag{4.8}$$

$$F_{31} = [-g_{31}\hat{F}_{31}(\omega-\epsilon_2) + g_{21}\hat{F}_{21}g_{32}\hat{F}_{32}]/D \tag{4.9}$$

$$G_1 = [(\omega-\epsilon_2)(\omega-\epsilon_3) - g_{23}|F_{23}|^2]/D \tag{4.10}$$

and

$$D = 2\pi[(\omega-\epsilon_1)(\omega-\epsilon_2)(\omega-\epsilon_3) - \Delta_{12}^2(\omega-\epsilon_3) - \Delta_{23}^2(\omega-\epsilon_1) - \Delta_{13}^2(\omega-\epsilon_2) + 2\Delta_{12}\Delta_{23}\Delta_{31}] \tag{4.11}$$

where $\Delta_{ij}^2 = |g_{ij}F_{ij}|^2$.

All other terms $F_{m,n}$, G_n can be obtained similarly. For example,

$$F_{32} = [-g_{32}\hat{F}_{32}(\omega-\epsilon_1) + g_{31}\hat{F}_{31}g_{12}\hat{F}_{12}]/D. \tag{4.12}$$

We follow the same kind of normalisation condition given by equation (3.19):

$$\sum_i \hat{G}_i = 1 \tag{4.13}$$

which, in the limit of classical statistics, is equivalent to

$$\exp(\beta\mu)\sum_i \exp(-\beta\epsilon_i) = 1. \tag{4.14}$$

Next, we solve equations (4.8)–(4.12) and their complex conjugates simultaneously. It is useful to rewrite them in a more compact form by application of the operator $\hat{P}$ defined in equation (3.20):

$$g_{21}\hat{F}_{21}[g_{21}^{-1} + \hat{P}D_3^{-1}] = g_{23}\hat{F}_{23}g_{31}\hat{F}_{31}\hat{P}D^{-1} \tag{4.15}$$

$$g_{31}\hat{F}_{31}[g_{31}^{-1} + \hat{P}D_2^{-1}] = g_{21}\hat{F}_{21}g_{32}\hat{F}_{32}\hat{P}D^{-1} \tag{4.16}$$

$$g_{32}\hat{F}_{32}[g_{32}^{-1} + \hat{P}D_1^{-1}] = g_{31}\hat{F}_{31}g_{12}\hat{F}_{12}\hat{P}D^{-1}. \tag{4.17}$$

Here $D_i^{-1} \equiv (\omega-\epsilon_i)/D$.

All these functions $\hat{P}D_i^{-1}$ and $\hat{P}D^{-1}$ are explicitly given in the Appendix. Although the details of the functions are not important, it should be pointed out that Δ_{ij}^2 for all i and j are the lowest order in Δ_{ij} that appears in these functions, as well as $\bar{\epsilon}_i$, which are the three roots of D.

Next, we look for a solution of equations (4.15)–(4.17) as β becomes larger (or the temperature becomes smaller), and ask the question: can they be simultaneously satisfied at $\beta = \beta_c$ such that Δ_{ij} behaves as $(\beta - \beta_c)^\alpha$, $(\alpha \neq 0)$ when $\beta \to \beta_c^+$ and $\Delta_{ij} = 0$ as $\beta \to \beta_c^-$?

This can be seen to be impossible by taking the product of equations (4.15) and (4.17). The RHS of the resultant expression at $\beta = \beta_c$ is proportional to $(\Delta_{13}\Delta_{23}\Delta_{12})^2$, whereas the LHS is proportional to $\Delta_{13}\Delta_{23}\Delta_{12}$. This contradiction can only be resolved if one of the functions, say $g_{21}^{-1} + \hat{P}D_3^{-1}$, is equal to zero at $\beta = \beta_c$. If this is indeed the case, then at $\beta = \beta_c^+$, the LHS of equation (4.15) is $\propto (\beta - \beta_c)^{3\alpha}$, which is the product of Δ_{12} and the correction to $g_{21}^{-1} + \hat{P}D_3^{-1}$ at $\beta = \beta_c^+$, whereas the RHS of equation (4.15) $\approx (\beta - \beta_c)^{2\alpha}$. The solution $\alpha = 0$ implies that Δ_{ij} cannot have a discontinuity at β_c, since for each β all Δ_{ij} can be solved from equations (4.15)–(4.17) and they are continuous functions of β.

Excluding this possibility, we can find the solutions as follows: first we examine the solution of three equations

$$g_{ij}^{-1} + \hat{P}D_k^{-1} = 0 \qquad (i \neq j \neq k) \tag{4.18}$$

and find the smallest β_c (say $k = 3$) of the three; then the solution of equations (4.15)–(4.17) at $\beta = \beta_c$ is given by

$$\begin{aligned} \Delta_{12}^2 &= c(\beta - \beta_c) && \beta \to \beta_c^+ \\ \Delta_{12}^2 &= 0 && \beta \to \beta_c^- \end{aligned} \tag{4.19}$$

$$\Delta_{23} = \Delta_{31} = 0 \tag{4.20}$$

where the proportionality constant c is defined in equation (3.28). Since the third level is not involved in the phase transition, the existence of the solution, equation (4.19), is subject to the same condition given in equation (3.26), and the nature of this phase transition is similar to that given in the previous section.

As β becomes larger, both equation (4.16) and (4.17) may admit a nonvanishing solution for F_{13} and F_{23} at $\beta = \beta_c'$, which is the solution of the resultant equation of the product of equations (4.16) and (4.17):

$$(g_{31}^{-1} + \hat{P}D_2^{-1})(g_{32}^{-1} + \hat{P}D_1^{-1}) = \Delta_{12}^2(\beta_c')(\hat{P}D^{-1})^2. \tag{4.21}$$

This equation is similar to the two-band BCS model (Sung and Shen 1965) and its solution β_c' cannot be expressed analytically in terms of g_{ij}, but the condition for the existence of the solution to (4.21) can be found by the observation that the LHS is greater than the RHS at $\beta \approx \beta_c$. Consequently, if equation (4.21) has a solution β_c' where $\beta_c < \beta_c' < \infty$, then the LHS must be less than the RHS as $\beta \to \infty$. This condition can be explicitly written down by substitution of all the functions in equation (4.21) from the Appendix. We obtain

$$[(\bar{\epsilon}_1 - \bar{\epsilon}_2)(\bar{\epsilon}_1 - \bar{\epsilon}_3)g_{32}^{-1} + (\bar{\epsilon}_1 - \bar{\epsilon}_1)][(\bar{\epsilon}_1 - \bar{\epsilon}_2)(\bar{\epsilon}_1 - \bar{\epsilon}_3)g_{32}^{-1} + 2\bar{\epsilon}_2 - \epsilon_1 - \epsilon_2] \leqslant \Delta_{12}^2 \tag{4.22}$$

where all quantities are given at $\beta \to \infty$.

Next, we examine the property of the solution at $\beta = \beta_c'$, and solve for q, q' and q'' in equations (4.23)–(4.27) consistently:

$$\Delta_{32} = q\Delta_{31} \tag{4.23}$$

$$\Delta_{31} = 0, \qquad \beta = \beta_c'^- \tag{4.24}$$

$$\Delta_{31}=q'(\beta-\beta'_{\mathrm{c}})^{1/2}, \qquad \beta=\beta_{\mathrm{c}}'^{+} \tag{4.25}$$

$$\Delta_{12}=\Delta_{12}^{0}(\beta=\beta_{\mathrm{c}}'^{-}), \qquad \beta=\beta_{\mathrm{c}}'^{-} \tag{4.26}$$

$$\Delta_{12}=\Delta_{12}^{0}(\beta=\beta_{\mathrm{c}}'^{+})+q''(\beta-\beta'_{\mathrm{c}}), \qquad \beta=\beta_{\mathrm{c}}'^{+} \tag{4.27}$$

where, at $\beta=\beta_{\mathrm{c}}'^{-}$, both $\Delta_{32}=\Delta_{31}=0$ and Δ_{12}^{0} are the solutions of equation (4.15). q can be easily obtained by taking the ratio of equations (4.16) and (4.17):

$$q=(g_{31}^{-1}+\hat{P}D_{2}^{-1})/(g_{32}^{-1}+\hat{P}D_{1}^{-1})|_{\beta=\beta_{\mathrm{c}}^{1-}} \tag{4.28}$$

where the $|_{\beta=\beta_{\mathrm{c}}^{1-}}$ implies that all the quantities in equation (4.28) are the values at $\beta=\beta_{\mathrm{c}}'^{-}$. The correction to Δ_{12}, $q''(\beta-\beta'_{\mathrm{c}})$, is related to Δ_{13} and Δ_{23} from equation (4.15), where the RHS of equation (4.15) jumps from 0 to $qq'(\beta-\beta'_{\mathrm{c}})(PD^{-1})$, which is equal to $q''(\beta-\beta_{\mathrm{c}})$ from the LHS of equation (4.15):

$$q''[g_{21}^{-1}+\hat{P}D_{3}^{-1}]|_{\beta=\beta'_{\mathrm{c}}}=qq'(\hat{P}D^{-1})|_{\beta=\beta'_{\mathrm{c}}}. \tag{4.29}$$

Another expression relating q' and q'' is obtained by expanding equation (4.21) around $\beta=\beta'_{\mathrm{c}}$. As remarked earlier, all terms in equation (4.21) are functions of Δ_{12}^{2}, Δ_{23}^{2} and Δ_{13}^{2}, and since it is exactly satisfied at $\beta=\beta'_{\mathrm{c}}$, the terms proportional to $(\beta-\beta'_{\mathrm{c}})$ in the Taylor series expansion at $\beta=\beta_{\mathrm{c}}'^{+}$ form another equation

$$(\partial/\partial\beta)(g_{31}^{-1}+\hat{P}D_{2}^{-1})(g_{32}^{-1}+\hat{P}D_{1}^{-1})|_{\beta=\beta_{\mathrm{c}}'^{-}}=(\partial/\partial\beta)[\Delta_{12}^{2}(\hat{P}D^{-1})^{2}]|_{\beta=\beta'_{\mathrm{c}}}. \tag{4.30}$$

The qualitative features of equations (4.28)–(4.30) and Δ_{ij} are shown in figure 1.

We compute the free energy using equation (3.30):

$$\begin{aligned}\Omega(g)-\Omega(0)&=-\left[\int^{g_{12}}(\Delta_{12}/g_{12}^{2})\,\mathrm{d}g_{12}+(2\to3)+(1\to2)\right]\\&=[\Delta_{12}^{2}/g_{12}+(2\to3)+(1\to2)]-2\left[\int^{g_{12}}(\Delta_{12}/g_{12})\,\mathrm{d}\Delta_{12}+(2\to3)+(1\to2)\right].\end{aligned} \tag{4.31}$$

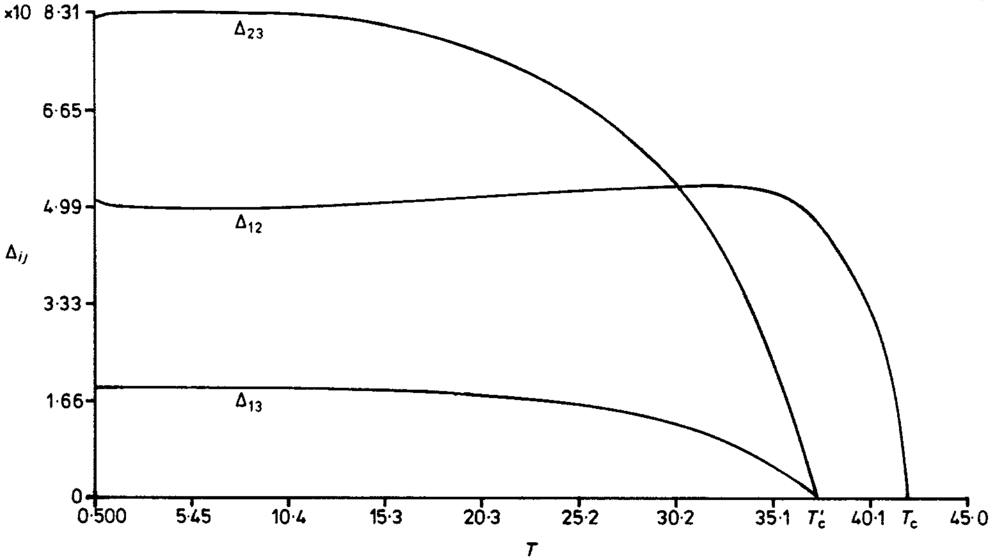

Figure 1. Schematic plot of Δ_{ij} as a function of temperature for the three-level Dicke model for the explicit values of the parameters $g_{12}=2{\cdot}0$, $g_{13}=0{\cdot}8$, $g_{23}=1{\cdot}8$ and $\bullet=0{\cdot}2$'(courtesy of Central Florida Regional Data Center).

The integrals in equation (4.31) can be computed by expressing $\Delta_{12} = g_{21}F_{21}$ in equation (4.8). The sum of the three integrals in the square brackets is given by

$$[\ ] = \tfrac{1}{2}P \ln D + \text{const.} \tag{4.32}$$

Notice that the order of integration and the operator $\hat{P}$ has been exchanged, which is justified since $\hat{P}$ is essentially an integration operator. However, $\hat{P}$ is not meaningful unless the function to which it applies is the ratio of two polynomials. Thus we write

$$D = \prod_{i=1}^{3} (\omega - \bar{\epsilon}_i),$$

and use

$$\ln(\omega - \bar{\epsilon}) = -\int^{1} \bar{\epsilon}\, \mathrm{d}\lambda/(\omega - \lambda\bar{\epsilon});$$

then

$$\hat{P} \ln D = \sum_{i=1}^{3} \hat{P} \ln(\omega - \bar{\epsilon}_i) = (1/\beta) \sum_{i=1}^{3} \ln\{1 - \exp[-\beta(\bar{\epsilon}_i - \mu)]\}. \tag{4.33}$$

The free energy given in equation (4.31) is simply that of a system of non-interacting three-level atoms with normalised $\bar{\epsilon}_i$ minus the interaction energy Δ_{12}^2/g_{12}, which is a well known result in the mean field approximation. Instead of proving $\partial\Omega/\partial\Delta_{ij} = 0$ explicitly as we did earlier, we would simply point out that Luttinger and Ward (1960) have shown that calculations based on equation (3.30) always satisfy the variational principle if it is consistently carried out.

Results for the three-level Dicke model and for r-level systems have been obtained earlier by Gilmore (1977) using a different method.

5. Summary

We have applied the Green's function method to the study of the phase transition in the continuous multimode Dicke model of two-level and three-level atoms. In both cases, we have demonstrated that the interaction explicitly in the form of atomic pair interactions via their mutual radiation field, equations (2.5) and (4.3), leads to the phase transitions: equations (3.27), (4.18) and (4.21). Our results for the conditions for the existence of the phase transition in the two-level case is identical in form to that obtained in previous works for the one-mode Dicke model (Hepp and Lieb 1973a, b, Wang and Hioe 1973, Gilmore and Bowden 1976a, b, c). The difference is in the appearance in our results of $\bar{\rho}$ (equation (1.2)) rather than $\bar{\rho}_0$ (equation (1.3)). This difference is due entirely to the consistent consideration of the assumption of the 'point model' (equation (1.4)) in our calculations. We wish to emphasise that the condition of the point model, when explicitly imposed in a calculation, must be taken seriously. Failure to do so can lead to erroneous requirements such as equation (1.5), and has led to strange results in the literature (Rzażewski and Wódkiewicz 1976).

The explicit form for the interaction, equation (2.5), for the two-level case indicates the formal equivalence of this model to BCS theory (Fetter and Walecka 1971), whereas the explicit interaction, equation (4.3), indicates the similarity of the three-level model to the two-band BCS model (Sung and Shen 1965). The interaction, equation (2.5), is also formally equivalent to the retarded dipole–dipole interaction which is responsible for the collective renormalisations in the dynamic evolution of superfluorescence (Bonifacio and Lugiato 1975, Narducci and Bowden 1976). This demonstrates the formal equivalence of the interactions which lead to the phase transition and to collective spontaneous relaxation, and their relation to BCS theory (Fetter and Walecka 1971). In the case of the thermodynamic equilibrium phase transition for two-level atoms, the correspondence with the BCS model is direct. In fact, we use the very same method for calculation of the phase transition that Gorkov used in his classic paper to obtain the results of the BCS theory (Gorkov 1958).

The application of the Green's function method in dealing with more complicated systems is demonstrated in the treatment of the Dicke model for three-level atoms in thermodynamic equilibrium. We have shown that there may be two second-order phase transitions. If so, the behaviour of the order parameters is as shown in figure 1.

Acknowledgments

The authors wish to acknowledge useful and stimulating discussions with Dr R Gilmore and Dr J D Stettler.

Appendix

$\hat{P}(2\pi D)^{-1}$ can be evaluated by using $D = \Pi_{i=1}^{3}(\omega - \bar{\epsilon}_i)$:

$$\hat{P}(2\pi D)^{-1} = \sum_{\substack{i=1,2,3\\ i\neq j\neq k}} \exp[\beta(\bar{\epsilon}_i - \mu)](\bar{\epsilon}_i - \bar{\epsilon}_j)^{-1}(\bar{\epsilon}_i - \bar{\epsilon}_k)^{-1}. \tag{A.1}$$

In equation (A.1), we have implicitly used the classical statistical approximation $\exp(-\beta\mu) \to \infty$. Similarly,

$$\hat{P}D_3^{-1} = \exp(\beta\mu)(\exp(-\beta\bar{\epsilon}_1) - \exp(-\beta\bar{\epsilon}_2))/(\bar{\epsilon}_1 - \bar{\epsilon}_2) + (\bar{\epsilon}_3 - \epsilon_3)P(2\pi D)^{-1}. \tag{A.2}$$

Combining equations (A.1), (A.2) and

$$\left.\begin{aligned} \exp[-\beta(\mu - \bar{\epsilon}_1)] &= 1 \\ \exp[-\beta(\mu - \bar{\epsilon}_2)] &= 0 \\ \exp[-\beta(\mu - \bar{\epsilon}_3)] &= 0 \end{aligned}\right. \qquad \text{as } \beta \to \infty$$

we obtain the zero-temperature limit of

$$\hat{P}D_1^{-1} = (\bar{\epsilon}_1 - \epsilon_1)(\bar{\epsilon}_1 - \bar{\epsilon}_2)^{-1}(\bar{\epsilon}_1 - \bar{\epsilon}_3)^{-1} \tag{A.3}$$

$$\hat{P}D_2^{-1} = 1/(\bar{\epsilon}_3 - \bar{\epsilon}_1) + (\bar{\epsilon}_2 - \epsilon_2)(\bar{\epsilon}_1 - \bar{\epsilon}_2)^{-1}(\bar{\epsilon}_1 - \bar{\epsilon}_3)^{-1}. \tag{A.4}$$

References

Bonifacio R, Haake F and Schwendimann P 1971a *Phys. Rev.* A **4** 302
—— 1971b *Phys. Rev.* A **4** 854
Bonifacio R and Lugiato L A 1975 *Phys. Rev.* A **11** 1507
Bowden C M and Sung C C 1978 *J. Phys. A: Math. Gen.* **11** 151
Dicke R H 1954 *Phys. Rev.* **93** 99

Fetter A L and Walecka J D 1971 *Quantum Theory of Many-Body Systems* (New York: McGraw-Hill)
Gilmore R 1977 *J. Phys. A: Math. Gen.* **10** L131
Gilmore R and Bowden C M 1976a *Phys. Rev.* A **13** 1898
—— 1976b *J. Math. Phys.* **17** 1617
—— 1976c *Cooperative Effects in Matter and Radiation* ed C M Bowden, D W Howgate and H R Robl (New York: Plenum)
—— 1978 *Proc. 4th Rochester Conf. on Coherence and Quantum Optics* ed L Mandel and E Wolf (New York: Plenum)
Gorkov L P 1958 *Sov. Phys.-JETP* **34** 505
Hepp K and Lieb E H 1973a *Ann. Phys., NY* **76** 360
—— 1973b *Phys. Rev.* **8** 2517
Hioe F T 1973 *Phys. Rev.* A **8** 1440
Kittel C 1963 *Quantum Theory of Solids* (New York: Wiley)
Knight J M, Aharonov Y and Hsieh G T C 1978 *Phys. Rev.* A **17** 1454
Lee B S 1976 *J. Phys. A: Math. Gen.* **9** 573
Loudon R 1973 *The Quantum Theory of Light* (Oxford: Clarendon)
Luttinger J M and Ward J C 1960 *Phys. Rev.* **118** 1417
McGillivray J C and Feld M S 1976 *Phys. Rev.* A **14**
Merzbacher E 1963 *Quantum Mechanics* (New York: Wiley)
Mihalache D 1977 *Phys. Rev. Lett.* **63** A241
Narducci L M and Bowden C M 1976 *J. Phys. A: Math. Gen.* **9** L75
Provost J P, Rocca F, Vallee G and Sirugue 1976 *Physica* **85** A 202
Rzażewski K and Wódkiewicz K 1976 *Phys. Rev.* **13** A 1967
Rzażewski K, Wódkiewicz K and Zakowicz W 1975 *Phys. Rev. Lett.* **35** 432
Sung C C and Bowden C M 1979 *J. Phys. A: Math. Gen.* **12**
Sung C C and Shen Y L 1965 *Phys. Lett.* **19** 101
Wang Y K and Hioe F T 1973 *Phys. Rev.* A **7** 831
Zubarev D N 1960 *Usp. Fiz. Nauk* **71** 71