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Coulomb interactions, gauge invariance, and phase transitions of the Dicke model

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Abstract

Phase transitions of a generalized Dicke model in the Coulomb gauge—including A^2 terms in the matter–radiation coupling, as well as direct dipole–dipole interaction terms—are studied. After a brief review of previous work on the 'no-go theorem' for phase transitions in the Dicke model, it is shown that a consistent truncation of the radiation modes and of the direct interactions leads to a model that does have a phase transition. When transformed to the electric dipole gauge, such a system takes exactly the form of the original Dicke Hamiltonian, which displays the expected phase transition.

1. Introduction

The Dicke model [1] has been long studied as a model of collective behaviour of radiation coupled to matter. In its original form, it describes a set of two-level systems with constant energy, coupled to a single photon mode, i.e. a bosonic field. At low temperatures, the Dicke model has a phase transition, below which the two-level systems become polarized, and there is an expectation for the bosonic field [2–4]. This transition occurs even in the canonical ensemble, and so would describe the instability of the vacuum of the interacting light–matter system to spontaneous generation of a photon field. However, if the Dicke model is understood as an approximation of the interaction of light and matter in the Coulomb ($\mathbf{A} \cdot \mathbf{p}$) gauge, then the Dicke model neglects terms like A^2. As shown by Rzążewski *et al* [5, 6], including such terms prevents the phase transition occurring.

Generalizations of the Dicke model have been studied in many contexts, including polariton condensation [7–9], quantum computing [10–12], and the dynamics of strongly interacting fermionic atomic gases near a Feshbach resonance [13, 14]. In several of these examples, phase transitions are studied, but in the grand canonical ensemble, i.e. with constrained density, in which case the A^2 terms do not destroy the phase transition [8]. One reason for its wide use is that, in the rotating wave approximation, the generalization of the Dicke model with varying two-level system energies, but constant couplings to the photon field,

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corresponds to an integrable classical system [14]. This is because the Dicke Hamiltonian, like the closely related BCS Hamiltonian is in the class of Gaudin–Richardson models [15].

Since the two-level systems in the original Dicke model couple to the radiation field, they are electric dipoles, and as such one should also consider direct electrostatic interactions between them. The phase transition of an ensemble of two-level systems—describing dipoles with direct electrostatic interactions—to a state with macroscopic polarization has been considered by Emeljanov and Klimontovich [16]. The transition due to such direct interactions has also been considered in the presence of an interaction via coupling to a common bosonic mode [17]. However, the Coulomb interaction between dipoles, and the coupling of dipoles to the quantized electromagnetic field are not independent, both describe the coupling of matter to the electromagnetic field, and the atomic matrix elements for both interactions are related. Further, in the Coulomb gauge, the inclusion of both direct and photon mediated interactions is necessary to find an overall retarded interaction [18, 19]; and the division of the interaction between direct and photon mediated terms is gauge dependent. The importance of how the sum over photon modes is to be truncated in deriving the Dicke model was also discussed in part in [20].

In this paper, we discuss how the Dicke model can be realized as a consistent (as defined below) truncation of the full Hamiltonian of dipoles interacting with the electromagnetic field, if described in the electric dipole gauge. Since the presence or absence of a phase transition is of course gauge independent, the same transition must be present in the Coulomb gauge. In that case, the same truncation describes a generalized Dicke model, including both A^2 terms and a direct Coulomb interaction. This model shows a phase transition under identical conditions to those in the electric dipole gauge. The bosonic field that appears in the two gauges has a different meaning, and so whether it acquires a macroscopic expectation below the transition does depend on the gauge. However, the transverse electric field is a gauge independent quantity, and does not acquire a macroscopic value in either gauge, so the results here are not in contradiction with other more general no-go theorems [21, 22].

It is worth highlighting here certain differences between the Dicke model discussed in this paper (and studied by Hepp and Lieb [2, 4] and Wang and Hioe [3]), and the related models applied to microcavity polaritons [7–9]. The model studied in this paper can be seen as a truncation of the microscopic model of dipoles interacting with radiation; the Dicke models studied in microcavities are more phenomenological, for example including effects of disorder by the choice of energies and coupling strengths of the two-level systems [9]. The most important difference is that in microcavities, light is confined by the dielectric mirrors, and so the relevant photon modes start at a non-zero energy, however the Coulomb interactions between different two-level systems are not significantly affected by the mirrors. Thus, in the microcavity system, the spatial modes relevant to the photon mediated and direct interactions are quite different; in the microscopic model discussed here, the spatial modes relevant to both interactions are the same. Secondly, in microcavities, significant Coulomb interaction due to exchange terms may exist [23], which lead to a repulsive interaction; the treatment here assumes isolated dipoles, interacting via dipole–dipole coupling. Finally, as mentioned above, phase transitions in microcavities are normally discussed in the Grand Canonical ensemble, with a certain density of particles; the discussion here is for the instability of the vacuum, calculated in the canonical ensemble.

The remainder of this paper is organized as follows. In section 2 the full Hamiltonian in the Coulomb gauge is considered, and the considerations important in truncating the sum are discussed. A truncated version of this Coulomb gauge Hamiltonian, that gives a generalized Dicke model, is then given in section 3, and is shown to support a phase transition. These calculations are then repeated in the electric dipole gauge in section 4. Finally, section 5 contains conclusions, and some general comments about the importance of including direct Coulomb interactions when discussing choice of gauge for matter–radiation interactions.

2. The full Hamiltonian, truncation of sums

To begin, consider a system of atoms, interacting via the electromagnetic field, described in the Coulomb gauge. This interaction includes both a direct Coulomb term, and interaction via quantized radiation modes, which are described by operators $\psi_j^\dagger$ that create photons of wavevector $\mathbf{k}_j$, and polarization $\hat{\mathbf{e}}_j$. Writing $\mathbf{d}_i = \mathbf{r}_{e,i} - \mathbf{r}_{h,i}$ for the relative electron displacement, and $\mathbf{R}_i$ for the centre of mass of atom i, the full Hamiltonian may be written as:

$$H = \sum_i H_0(i) + \sum_j \hbar\omega_{k_j}\psi_j^\dagger\psi_j + \sum_{i,j}\left\{-\mathrm{i}\frac{e}{\hbar}[H_0(i),\mathbf{d}_i]\cdot\sqrt{\frac{\hbar}{2\omega_{k_j}\varepsilon_0 V}}\hat{\mathbf{e}}_j(\psi_j \mathrm{e}^{\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i} + \mathrm{h.c.})\right\}$$
$$+ \frac{e^2\hbar}{4m_\mathrm{r}\varepsilon_0 V}\sum_i\left[\sum_j\left(\frac{\psi_j \mathrm{e}^{\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i} + \psi_j^\dagger \mathrm{e}^{-\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i}}{\sqrt{\omega_{k_j}}}\right)\right]^2$$
$$- \frac{e^2}{2\varepsilon_0}\sum_{i\neq j}(\mathbf{d_i})_\alpha\delta^\parallel_{\alpha\beta}(\mathbf{R}_i-\mathbf{R}_j)(\mathbf{d_j})_\beta. \quad (1)$$

Here, H_0 is the bare Hamiltonian for a single atom, V the quantization volume, m_r the reduced mass, and $(\mathbf{d}_i)_\alpha$ is the α component of the displacement $\mathbf{d}_i$ of atom i. In this expression, both the coupling to transverse radiation, and the direct Coulomb term (the last term) have been written in the dipole approximation (i.e. assuming $d_i \ll |\mathbf{R}_i - \mathbf{R}_j|$). The coupling to transverse radiation, $\mathbf{A}\cdot\mathbf{p}$ has been rewritten using $\mathbf{p}_i = m\dot{\mathbf{r}}_i = m \times i[H_0, \mathbf{r}_i]/\hbar$. The direct dipole–dipole interaction can be written in terms of the longitudinal delta function, which is given explicitly by:

$$\delta^\parallel_{\alpha\beta}(\mathbf{r}) = \frac{1}{4\pi r^3}\left(\frac{3r_\alpha r_\beta}{r^2} - \delta_{\alpha\beta}\right) = \frac{\partial^2}{\partial r_\alpha\partial r_\beta}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}}{k^2}. \quad (2)$$

Let us now consider how to truncate this Hamiltonian in order to provide a simpler model. As discussed in section II.C.5 of [18], in the Coulomb gauge there is a non-retarded Coulomb potential between different dipoles. This is not physical; when combined with the photon mediated interaction only retarded interactions survive. In order for such a cancellation between instantaneous terms to hold in a truncated Hamiltonian, one must truncate both the sum over radiation modes, and the spatial harmonics involved in the direct Coulomb interaction. It is therefore helpful to write the Coulomb interaction as a sum over the same set of modes as the radiation term, thus:

$$\delta^\parallel_{\alpha\beta}(\mathbf{r}) = \frac{1}{V}\sum_k\left[\left(\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2}\right) - \delta_{\alpha\beta}\right]\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \quad (3)$$
$$= \left[\frac{1}{V}\sum_j(\hat{\mathbf{e}}_j)_\alpha(\hat{\mathbf{e}}_j)_\beta \mathrm{e}^{\mathrm{i}\mathbf{k}_j\cdot\mathbf{r}}\right] - \delta_{\alpha\beta}\delta(\mathbf{r}), \quad (4)$$

where equation (4), makes use of the set of polarization vectors $\hat{\mathbf{e}}_j$ which are perpendicular to $\mathbf{k}_j$. This description leaves a purely local term, $\delta(\mathbf{r})$ which should not contribute when considering the interaction between different dipoles.

Performing a truncation to include only the lowest radiation mode, and projecting the matter part into a two-level basis leads to a variant of the Dicke model:

$$H = \epsilon \sum_i S_i^z + \hbar\omega_0 \psi^\dagger \psi + \frac{g}{\sqrt{V}} \sum_i \mathrm{i}(S_i^+ - S_i^-)(\psi + \psi^\dagger) + \kappa(\psi + \psi^\dagger)^2 - \eta \sum_{i \neq j} (S_i^+ + S_i^-)(S_j^+ + S_j^-), \quad (5)$$

where S_i is a spin $1/2$ operator representing the two-level system (TLS) for atom i, and the interaction strengths are given by the parameters:

$$g = \frac{2\epsilon e d_{ab}}{\sqrt{2\hbar\omega_0\varepsilon_0}}, \qquad \kappa = \frac{N}{V}\frac{e^2\hbar}{4m_r\varepsilon_0\omega_0}, \qquad \eta = \frac{e^2 d_{ab}^2}{2\varepsilon_0 V}. \quad (6)$$

Note in equation (5) that the coupling of the TLS to radiation depends on the component S_j^y, while the dipole–dipole interaction depends on the component S_j^x. This difference can be understood by recalling that $\mathbf{p}_i = m \times i[H_0, \mathbf{r}_i]/\hbar$, and since $H_0 = \epsilon S_i^z$, the $\mathbf{p}$ and $\mathbf{r}$ matrix elements of a TLS must correspond to spin components rotated by $\pi/2$ about the z axis. Note also that although the dipole interaction including all $\mathbf{k}_j$ modes as given in equation (2) averages to zero after angular integration, the truncation to the lowest k mode gave a non-zero value, which favours dipole alignment. This is in part a result of truncation to the two-level basis. That this interaction is correct is confirmed by the discussion in section 4, where it is seen that this form is required so that Coulomb terms are cancelled in the electric dipole gauge, as should be the case [18].

3. Generalized Dicke model in the Coulomb gauge

Having derived the generalized Dicke model of equation (5), one may next consider phase transitions of this model. It is convenient to consider the partition function, written as a trace over coherent states. Introducing a real scalar field ϕ to decouple the dipole interactions, and writing $\psi = \psi' + \mathrm{i}\psi''$, the partition function is:

$$\mathcal{Z} = \int \mathrm{d}\psi' \int \mathrm{d}\psi'' \int \mathrm{d}\phi \exp\left[-\beta\left(\hbar\omega_0|\psi|^2 + 4\kappa\psi'^2 + \frac{\phi^2}{4\eta}\right)\right] \times \prod_{i=1}^{N}\left(\sum_{\mathbf{S}_i} \exp\left[-\beta\left(\phi S_i^x + 2\frac{g}{\sqrt{V}}\psi' S_i^y + \epsilon S_i^z\right)\right]\right). \quad (7)$$

Then, integrating over the TLS gives an effective action for the fields ψ and ϕ:

$$S_{\text{eff}} = \hbar\omega_0|\psi|^2 + 4\kappa\psi'^2 + \frac{\phi^2}{4\eta} - \frac{N}{\beta}\ln[\cosh(\beta E)], \qquad E^2 = \epsilon^2 + \frac{4g^2\psi'^2}{V} + \phi^2. \quad (8)$$

Since the model considered does not include spatial variation, one only need study mean-field properties, so a phase transition is signalled when a non-zero value of ϕ or ψ minimizes S_{eff}. It can immediately be seen that minimizing with respect to ψ'' yields the condition $\psi'' = 0$. Considering next ψ':

$$\left.\frac{1}{2}\frac{\partial S_{\text{eff}}}{\partial \psi'}\right|_{\psi''=0} = \hbar\omega_0\psi' + 4\kappa\psi' - \frac{N}{V}\frac{4g^2\psi'}{2E}\tanh(\beta E), \quad (9)$$

then since $\tanh(\beta E) \leqslant 1$, a solution with $\psi' \neq 0$ is possible only if:

$$\epsilon\frac{(\hbar\omega_0 + 4\kappa)}{2g^2 N/V} < 1. \quad (10)$$

However the Thomas–Reiche–Kuhn (TRK) sum rule (see e.g. [24]) implies $2\kappa\epsilon \geqslant g^2 N/V$. Since both terms in the numerator are positive, the TRK inequality prevents equation (10)

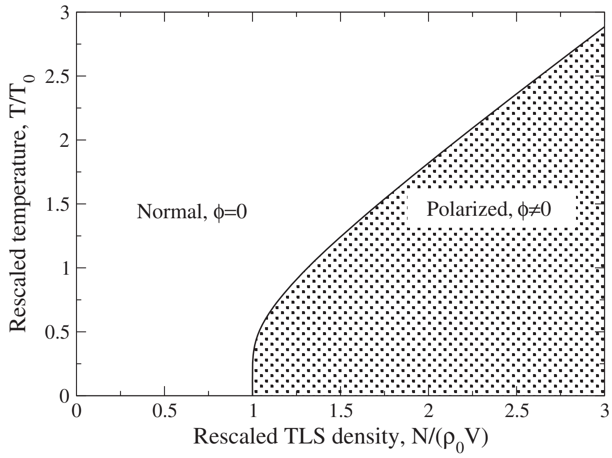

Figure 1. Critical conditions for a polarized phase, as given by equation (11); written in terms of density scale $\rho_0 = \epsilon/(2V\eta) = \epsilon\varepsilon_0/(e^2 d_{ab}^2)$, and temperature scale $T_0 = \epsilon$. It is clear that a transition can occur at low enough temperature as long as $N/V \geqslant \rho_0$.

from ever being satisfied. This is the result of Rzążewski *et al* [5, 6]. Considering now ϕ, minimization of S_{eff} yields:

$$\frac{1}{2}\frac{\partial S_{\text{eff}}}{\partial\phi}\bigg|_{\psi=0} = \frac{\phi}{4\eta} - N\frac{\phi}{2E}\tanh(\beta E), \tag{11}$$

i.e. the critical temperature (at which a solution with $\phi \neq 0$ first exists) is controlled by the equation $N\tanh(\beta\epsilon) = \epsilon/2\eta$; this is shown in figure 1. There exists a temperature at which a solution exists as long as:

$$\epsilon < 2\eta N = \frac{e^2 d_{ab}^2}{\varepsilon_0}\frac{N}{V}. \tag{12}$$

This requirement does not violate the TRK sum rule, and so at large enough densities of TLS, their mean-field Coulomb interaction causes a spontaneous polarization; i.e. the model is ferroelectric.

4. The electric dipole gauge

The previous analysis can be repeated in the electric dipole gauge, in which the truncated Hamiltonian will be shown to have a simpler (i.e. Dicke) form. To change gauge, one may introduce the unitary transformation:

$$U = \exp\left(\sum_j \lambda_j^*\psi_j - \lambda_j\psi_j^\dagger\right), \qquad \lambda_j = \frac{\mathrm{i}e}{\sqrt{2\varepsilon_0\hbar\omega_{k_j}V}}\sum_i \hat{\mathbf{e}}_j\cdot\mathbf{d}_i\mathrm{e}^{\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i}. \tag{13}$$

This is a transformation of the full Hamiltonian, equation (1), not the Hamiltonian in the TLS representation. This is important, since the bare TLS Hamiltonian, $H_0(i)$, differs between gauges, so the operations of gauge transformation and projecting onto a two-level basis do not commute. As shown in [18] (complements A_{IV} and C_{IV}), such a unitary transformation modifies two terms in equation (1). Firstly, the minimal coupling interaction disappears,

$(\mathbf{p} - e\mathbf{A})^2 \rightarrow \mathbf{p}^2$, if one makes the dipole approximation, as discussed earlier. Secondly, the transformation modifies the radiation Hamiltonian:

$$\sum_j \hbar\omega_{k_j} \psi_j^\dagger \psi_j \rightarrow \sum_j \hbar\omega_{k_j} \left(\psi_j^\dagger + \lambda_j^*\right)\left(\psi_j + \lambda_j\right). \tag{14}$$

The cross terms, $\lambda_j \psi^\dagger$ +h.c. describe a new matter–radiation interaction, which is in effect $\mathbf{D}\cdot\mathbf{r}$, where $\mathbf{D}$ is electric displacement. From the form of $\delta^{\parallel}_{\alpha\beta}(\mathbf{r})$ in equation (4), it is apparent that the term $\hbar\omega_{k_j}|\lambda_j|^2$ (arising from equation (14)) cancels the direct dipole–dipole interaction in equation (1). This cancellation requires that any truncation matches for the sums over the radiation modes in equation (1), the delta function (4), and in the transformation (13). Applying such a transformation, the full Hamiltonian of equation (1) in the electric dipole gauge becomes:

$$H = \sum_i H_0'(i) + \sum_j \hbar\omega_{k_j}\psi_j^\dagger\psi_j + \sum_i e\mathbf{d}_i \cdot \mathbf{D}_i, \tag{15}$$

$$\mathbf{D}_i = \sum_j \mathrm{i}\sqrt{\frac{\hbar\omega_{k_j}}{2\varepsilon_0 V}}\hat{\mathbf{e}}_j \left(\psi_j \mathrm{e}^{\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i} - \psi_j^\dagger \mathrm{e}^{-\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i}\right). \tag{16}$$

Note that if, in the Coulomb gauge, dipole interactions had been ignored, there would now be a non-physical interaction in the electric dipole gauge. This non-physical interaction would have the opposite sign to the physical interaction that should exist in the Coulomb gauge. Therefore, such a non-physical interaction can prevent the transition. This latter point was noted by Bialynicki-Birula and Rzążewski [25]. Such a non-physical interaction in the dipole gauge is a result of neglecting the physical interaction in the Coulomb gauge, and describes a model with instantaneous interactions.

Projected onto TLS, this yields the Dicke model:

$$H = \epsilon \sum_i S_i^z + \hbar\omega_0 \psi^\dagger\psi + \frac{g'}{\sqrt{V}} \sum_i \mathrm{i}(S_i^+ + S_i^-)(\psi - \psi^\dagger) \tag{17}$$

where the new coupling strength can be related to that in equation (6) by $g' = (\hbar\omega_0/2\epsilon)g$. Integrating over the TLS in the same way as before gives an effective action:

$$S_{\text{eff}} = \hbar\omega_0|\psi|^2 - \frac{N}{\beta}\ln\left[\cosh\left(\beta E\right)\right], \qquad E^2 = \epsilon^2 + \frac{4g^2\psi'^2}{V}\left(\frac{\hbar\omega_0}{2\epsilon}\right)^2. \tag{18}$$

Repeating the previous analysis, minimization gives:

$$\frac{1}{2}\frac{\partial S_{\text{eff}}}{\partial\psi'}\bigg|_{\psi''=0} = \hbar\omega_0\psi' - \frac{N}{V}\frac{4g^2\psi'}{2E}\left(\frac{\hbar\omega_0}{2\epsilon}\right)^2\tanh(\beta E), \tag{19}$$

and so a solution exists if:

$$\epsilon\frac{\hbar\omega_0}{2g^2N/V}\left(\frac{2\epsilon}{\hbar\omega_0}\right)^2 = \frac{\epsilon\varepsilon_0}{e^2 d_{ab}^2}\frac{V}{N} < 1. \tag{20}$$

This is identical to the condition in equation (12), and describes the same transition. Therefore, if the Dicke model is considered as light–matter interaction in the electric dipole gauge, the Hepp and Lieb transition is not an artefact of neglecting terms. Note that, since the bosonic modes in this gauge represent electric displacement (see equation (16)), then the transition to a state $\psi \neq 0$ just means spontaneous polarization, as $\psi \neq 0$ did in the Coulomb gauge; the transverse electric field is gauge invariant as expected.

5. Conclusion

As well as atoms confined in a cavity, the model of two-level systems interacting with radiation modes can also apply to localized electronic excitations, such as excitons, in a semiconductor. In a semiconductor one must however consider how other electrical excitations modify the electromagnetic field—i.e. screening of the Coulomb interaction, and of the photon field [19]. Such screening includes contributions due to optical phonons (in a dipolar material), free electrons, plasmons etc [26]. In practice, this means replacing the bare dielectric constant ε_0 by $\varepsilon_0\varepsilon_k$ in both the Coulomb interaction term, and the coupling to radiation modes. (However, if the dynamics of the system of interest are close to a resonance of some other excitation, it may be necessary to include the dynamics of such a response, which in a Hamiltonian formalism requires the explicit inclusion of those modes that lead to the resonance [19].) It is clear that to avoid introducing instantaneous interactions, it is again important to match the wavevector dependence of the screening of Coulomb interaction and the coupling of matter to radiation.

Such considerations are important, as it is common to write down models of such excitations in semiconductors in which the matter–radiation interaction is written in the electric dipole gauge, while a direct Coulomb term is also retained [26]. However, in the context of microcavity polaritons, such an approach can be reasonable, since the important radiation modes are those confined by the cavity, and thus having a large wavevector, while the important Coulomb terms may be more slowly varying. It is thus possible to perform a partial gauge transform, restricting the sum in equation (13) to radiation modes with large wavevector k thus leaving the small k part of the interaction in the Coulomb gauge, but transforming the high k part to the dipole gauge. This then allows the correct description of the light–matter coupling, in contexts where experimentally measured eigenstates and dipole matrix elements are used [27, 28].

In conclusion, including the effect of direct Coulomb interactions, a phase transition occurs in a Dicke-like model, leading to a spontaneous polarization of the two-level systems. In the electric dipole gauge, the system is described by the original Dicke Hamiltonian. The phase transition does not however lead to a spontaneous transverse electric field. In the Coulomb gauge, where the bosonic mode represents the transverse electric field there will therefore be no macroscopic occupation of the bosonic mode. The boson field in the electric dipole gauge represents electric displacement, and so the phase transition does lead to an expectation of the bosonic field. Since the system is neutral, $\mathbf{D}_\parallel = 0 = \varepsilon_0\mathbf{E}_\parallel + \mathbf{P}_\parallel$, and so a spontaneous polarization leads to a longitudinal electric field. Note that although the total polarization of a two-level system vanishes outside the system, the transverse and longitudinal parts of the polarization need not vanish.

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