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Are super-radiant phase transitions possible?

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An argument is given which rules out super-radiant phase transitions in which the atomic states involved are connected by electric-dipole matrix elements. The argument is based on gauge invariance, and is valid even in the presence of direct interatomic interactions. Its relevance is demonstrated by presenting a number of two-level models exhibiting super-radiant phase transitions which are not forbidden by previous sum-rule arguments. As a preliminary to the argument, the nature of the super-radiant phase transition is discussed, and a simple model is given which reproduces its main features. It is argued, finally, that in at least one case in which our argument fails a super-radiant phase transition is possible in principle.

I. INTRODUCTION

The possibility of a phase transition involving resonant interaction of a collection of atoms with the electromagnetic field in a cavity is a very attractive one. The order parameter for such a transition, being the field itself, would be accessible to refined measurements, possibly giving a new method of studying interacting atomic systems. A super-radiant phase transition of the kind described was shown by Hepp and Lieb[1] to follow rigorously from a thermodynamic treatment of the Dicke model,[2] used previously to discuss radiation phenomena far from thermal equilibrium. Later, Rzążewski, Wódkiewicz, and Żakowicz[3] showed that this result is a consequence of the neglect of the A^2 and counter-rotating terms in the Dicke Hamiltonian, and that the Thomas-Reiche-Kuhn sum rule places a constraint on the coefficients of these terms which rules out the phase transition.[4]

Underlying this result is the fact that gauge invariance requires the presence of the A^2 and counter-rotating terms, as has recently been reemphasized by Wooley.[5] In fact, the sum rule can be derived from charge-current conservation,[6] an immediate consequence of gauge invariance. When these terms are dropped, the remaining part of the kinetic energy term in the fundamental Hamiltonian can become negative, allowing false conclusions concerning the energies and thermal properties of the system.

The work cited above does not make clear, however, the impossibility of some kind of phase transition involving an electromagnetic field which becomes large due to interactions with an atomic system. Indeed, phase transitions are exhibited by a number of extended versions of the Dicke model which have been treated in the literature.[7-10] We have constructed additional examples which show that phase transitions can occur in two-level systems which satisfy all the constraints imposed by the sum rule. These models have direct interatomic interactions in addition to the proper A^2 and counter-rotating terms.

In the present paper, we seek a criterion which will enable us to assess the validity of these models and to determine whether a phase transition of super-radiant type can occur in principle in a physical system. We find an argument, based on the gauge invariance of the fundamental Hamiltonian, which is stronger than previous arguments, and which can be applied more generally. One of the consequences of the argument is that no two-level model where the atoms make electric-dipole transitions can validly exhibit a super-radiant phase transition. We then show that there still exist physical systems for which such a phase transition is not ruled out.

We begin by describing some preliminary notions concerning the nature of the phase transition which have motivated our work. In the model introduced by Dicke, a single mode of the electromagnetic field interacts with a collection of N two-level atoms via a term proportional to AD, where A is a component of the vector potential and D the corresponding component of the total electric-dipole moment of the atoms. If this system is brought to thermal equilibrium below a critical temperature T_c, it is found to be in a state which differs from the normal equilibrium state above T_c in several respects, provided the strength of the atom-field interaction is large enough to satisfy a certain condition given by Hepp and Lieb. The photon number n is macroscopic and of the order of the number N of atoms, rather than being of order unity as given by the Planck formula. Furthermore, A and D become large—A of order $\sqrt{N}$ and D of order N—and have a well-defined relative phase.

When the temperature is decreased to zero, the system retains these properties as it continuously

approaches the ground state. The normal ground state with $n=0$ and $A=D=0$ is thus unstable with respect to a state having a large dipole moment and large expectation value of the vector potential. This instability is essential for the existence of a phase transition of the kind discussed here. As T increases to T_c, the large entropy of the normal state makes itself felt, and the phase transition takes place.

A simple model, which illustrates the mechanism for this phase transition in its most basic form, consists of a large number of harmonic oscillators, one of which makes a negative[11] rather than a positive contribution to the energy. This oscillator, which we refer to subsequently as the negative-frequency oscillator, tends to become highly excited, and indeed the system would be unstable without the inclusion in the Hamiltonian of a term which limits these excitations. If this term is collective in nature, restricting the total number of excitations of both positive- and negative-frequency oscillators, then there is a phase transition in which the negative-frequency oscillator is highly excited below T_c, and essentially unexcited above T_c. The two principal features of this many-oscillator model, the negative-frequency oscillator and the mechanism limiting its excitations, can be identified in the Dicke Hamiltonian when a transformation to new variables is made. The negative-frequency oscillator occurs precisely when the parameters of the model satisfy the condition for the existence of a phase transition given in Ref. 1. The presence of a mechanism limiting its excitations stems from the fact that the amount of excitation energy that can be accommodated by the atoms is limited. The many-oscillator model and its connection with the Dicke model are discussed fully in Sec. II.

With the addition of the A^2 and counter-rotating terms to the Dicke Hamiltonian, the phase transition does not occur. Let us consider, however, the addition of terms describing direct interatomic interactions. If the interactions tend toward the formation of a dipole moment in the atomic system, it might still be energetically favorable for the field to become large in the ground state of the system. We have constructed two types of models for which this is the case. In the first type, the interaction is formally the same as the exchange interaction between spin-$\frac{1}{2}$ atoms, while in the second type, it has the form of a dipole-dipole interaction. For suitably chosen interactions of both types, the normal state does not have the lowest energy and is unstable with respect to the super-radiant state. A phase transition is therefore indicated. Due to the interatomic interaction, a simple exact treatment of the thermodynamics along the lines of Wang and Hioe[12] is not possible. We therefore treat these models in the mean-field approximation, finding a second-order phase transition for those models with super-radiant ground states. The details of these models and a discussion of their thermal behavior are given in Sec. III.

Although these extensions of the Dicke model provide interesting mathematical examples of second-order phase transitions, we must be cautious in asserting that they correspond with reality in their thermal behavior or in the nature of their ground states. The arguments of Rzążewski, Wódkiewicz, and Żakowicz show that when the atoms do not interact directly, the atomic parameters of the model are restricted in such a way that a phase transition is not possible. The same arguments are not sufficient, as we will show, to exclude a phase transition in the models including interatomic interactions. We formulate in this paper, however, a new argument which is capable of ruling out phase transitions both in the Dicke model and in the models presented in Sec. III. The starting point for this argument is the one-mode approximation to the full-gauge-invariant Hamiltonian describing atoms interacting with the field. This argument applies when the dipole approximation is valid. It fails when the atomic transitions occur via magnetic-dipole interactions with the electron spin or via higher-order terms which enter when the dipole approximation is not made. We argue that phase transitions are possible in principle in at least some of these cases. Whether or not the conditions necessary for their observation can be brought about is a practical question which we leave for later investigation.

II. MANY-OSCILLATOR MODEL

We present here a simple model which exhibits a phase transition analogous to the one that occurs in the Dicke model. Our Hamiltonian, characterized by positive constants ω, Ω, and γ, is taken to be

$$H=\sum_{j=1}^{N-1}\omega b_j^\dagger b_j-\Omega b_0^\dagger b_0+\frac{\gamma}{2N}\left(b_0^\dagger b_0+\sum_{j=1}^{N-1}b_j^\dagger b_j\right)^2, \quad (1)$$

where the operators b_j satisfy boson commutation rules $[b_j b_k^\dagger]=\delta_{jk}$, and where the quadratic contribution of one of the operators b_0 is negative rather than positive. This is the Hamiltonian of a system of N harmonic oscillators, one of which has a negative frequency. The final term, proportional to γ/N, insures that the Hamiltonian is bounded from below, and is thus capable of representing a stable physical system.

The thermal behavior of the system is easily treated in terms of two dimensionless variables,

$$x=\frac{1}{N}\sum_{j=1}^{N-1} b_j^\dagger b_j$$

representing the number of phonons shared by the positive-frequency oscillators, and

$$y=(1/N)b_0^\dagger b_0$$

representing the number of quanta in the negative-frequency oscillator. The entropy is calculated from the number of ways of assigning Nx excitations to $N-1$ equivalent oscillators. This leads to the following expression for the intensive free energy $f\equiv F/N$ of the system:

$$f=\omega x-\Omega y+\tfrac{1}{2}\gamma(x+y)^2 - kT[(1+x)\ln(1+x)-x\ln x]\,. \tag{2}$$

This expression has a minimum at values of x and y given by the equations

$$x+y=\Omega/\gamma\,, \tag{3}$$

$$x=(e^{(\omega+\Omega)/kT}-1)^{-1}\,. \tag{4}$$

At absolute zero, $x=0$ and y has the value Ω/γ characteristic of the ground state. As T increases, x increases because of the much greater entropy of the positive-energy oscillators. The rate of increase of x is continuous until x reaches the value Ω/γ at which $y=0$, as indicated by Eq. (3). This occurs at the critical temperature

$$kT_c=(\omega+\Omega)/\ln(1+\gamma/\Omega)\,. \tag{5}$$

Since y is inherently positive, the position of the minimum, Eqs. (3) and (4), will pass out of the physical region $x, y\geq 0$ for temperatures greater than T_c. The state of the system is then determined by minimizing Eq. (2) on the boundary $y=0$ of the physical region. This leads to the transcendental equation

$$\omega+\gamma x=kT\ln[(1+x)/x]\,, \tag{6}$$

which determines the value of x for $T>T_c$. Note that the values of x and y are continuous at T_c, but that dx/dT and dy/dT suffer discontinuities. The energy of our system,

$$E=N[\omega x-\Omega y+\tfrac{1}{2}\gamma(x+y)^2]\,,$$

will therefore be continuous at $T=T_c$, while the specific heat dE/dT will have discontinuity properties characterizing a second-order phase transition.

It is interesting to observe that if the last term in Eq. (1) had the form $(2N)^{-1}\gamma(b_0^\dagger b_0)^2$, involving only the negative-frequency oscillator, then the system would still be stable but no phase transition would take place. The quantities x and y would be independent of one another and continuous over the whole range of temperatures. An element of competition between the negative-frequency mode and the collection of positive-frequency modes is essential for a phase transition.

The form of the last term in Eq. (1) is not unique. As long as it allows for competition between the modes, a phase transition is possible. We can even construct a simpler model, though one less physical in its behavior, by omitting the last term in (1) and placing instead a cutoff on the *total* number of excitations, i.e., by requiring $N(x+y)\leq N_0=\text{const}$.

In order to establish the connection between this model and the Dicke model, we introduce a set of collective atomic coordinates, defined by the relations

$$b_r^\dagger=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}\sigma_j^\dagger\exp\left(2\pi i\frac{jr}{N}\right),\quad r=0,1,\ldots,N-1 \tag{7}$$

and express the Dicke Hamiltonian[13] in terms of them,

$$H=\epsilon\sum_r b_r^\dagger b_r+\omega a^\dagger a+\lambda(b_0 a^\dagger+b_0^\dagger a)\,. \tag{8}$$

Noting that the field a interacts only with the atomic coordinate b_0, we make a linear transformation which eliminates the coupling term by introducing the operators[14]

$$A=a\cos\theta-b_0\sin\theta\,,\quad B=a\sin\theta+b_0\cos\theta\,, \tag{9}$$

with

$$\tan 2\theta=2\lambda/(\epsilon-\omega)\,. \tag{10}$$

The new form of the Hamiltonian is

$$H=\sum_{r=1}^{N-1}\epsilon b_r^\dagger b_r+\{[\tfrac{1}{2}(\epsilon+\omega)+\tfrac{1}{2}[(\epsilon-\omega)^2+4\lambda^2]^{1/2}\}B^\dagger B + \{[\tfrac{1}{2}(\epsilon+\omega)-\tfrac{1}{2}[(\epsilon-\omega)^2+4\lambda^2]^{1/2}\}A^\dagger A\,. \tag{11}$$

If, for the moment, we regard A, B, and b_r as the annihilation operators of independent harmonic oscillators, the connection with the previous model begins to appear. The condition that the $A^\dagger A$ term have a negative coefficient is precisely the condition $\lambda^2>\epsilon\omega$ given by Hepp and Lieb for the existence of a phase transition. When this condition is satisfied, the negative-frequency mode tends to become highly excited in the ground state of the system, and many photons and atomic excitations are present. However, A, B, and b_r are not independent oscillator annihilation operators, since the original atomic coordinates b_r satisfy commutation relations

$$[b_r,b_s^\dagger]=\delta_{rs}-\frac{1}{N}\sum_j(1+\sigma_j^3)\exp\left(\frac{2\pi i(r-s)j}{N}\right), \tag{12}$$

which deviate from boson commutation relations because of the second term on the right. We cannot therefore conclude that $A^\dagger A$ becomes infinite in the ground state even though its coefficient in Eq. (11) is negative. There is, in fact, a limiting mechanism present which performs the same function as the last term in the many-oscillator Hamiltonian of Eq. (1). This mechanism is most readily seen with reference to Eqs. (9) and (11). When the condition $\lambda^2 > \epsilon\omega$ is satisfied so that the last term in Eq. (11) is negative, the ground state of the system will be that state in which the value of A is the largest possible, and the values of B and b_r are the smallest possible. Equation (9) shows that this occurs when

$$b_0 \approx -a\tan\theta\,, \quad b_r \approx 0 \quad \text{for } r \neq 0\,. \tag{13}$$

From Eq. (7), however, it is seen that b_0, which is a measure of the total number of atoms excited, can be at most of order $\sqrt{N}$. Thus, if a is greater than $O(\sqrt{N})$ the equality (13) cannot be satisfied since θ is independent of N. A and B then both become large and of the same order as a. Summarizing the argument, we can say that, beginning with the normal state, the energy decreases as we increase the number of photons and the number of excited atoms as long as a is less than or of the order of $\sqrt{N}$, and increases again for larger a. We therefore have a stable minimum for some value of $\sim\sqrt{N}$. Thus, $A^\dagger A$ does not become infinitely large. The competitive nature of the limiting mechanism is established by noting that if b_0 is of the order $\sqrt{N}$ as required for large A, then Eq. (7) shows that σ_j^+ must be of the order unity for every atom. This implies that b_r for $r \neq 0$ must be small due to the oscillating factor in the summation in Eq. (7). Thus $A^\dagger A$ can become large only when $b_r^\dagger b_r$ becomes small. We have now demonstrated a complete analogy between the many-oscillator model and the Dicke model.

III. MODELS WITH INTERACTIONS

In this section we discuss a number of extensions[15] of the Dicke model which include interatomic interaction potentials V. We present three cases in which the ground state is super-radiant and a second-order phase transition occurs. The models considered all have Hamiltonians of the general form

$$H = H_1 + V\,, \tag{14}$$

$$H_1 = \frac{\epsilon}{2}\sum_{j=1}^{N}(1+\sigma_j^3) + \omega a^\dagger a + \frac{\lambda}{\sqrt{N}}(a^\dagger + a)\sum_{j=1}^{N}\sigma_j^1 + \kappa(a+a^\dagger)^2 - \kappa\,. \tag{15}$$

H_1 is seen to be the Hamiltonian of the Dicke model extended to include the A^2 term as well as the counter-rotating terms. The atomic states have energies 0 and ϵ, and are described with the aid of the Pauli matrices, while $a^\dagger$ is the creation operator for photons in the single mode of energy ω which is retained in the model. The parameters λ and κ describing the atom-field interaction are given by

$$\lambda = (\epsilon^2 N \mathcal{P}^2/2\omega\mathcal{V})^{1/2}\,, \quad \kappa = e^2\hbar^2 N/2\omega\mathcal{V}\,, \tag{16}$$

where $\mathcal{P}$ is the matrix element of the electric-dipole-moment operator between the two atomic states, $\mathcal{V}$ is the volume in which the field mode is confined, and m is the mass of the electron. Rzążewski, Wódkiewicz and Żakowicz have pointed out that the dipole sum rule implies the inequality

$$\lambda^2 \leq \kappa\epsilon\,. \tag{17}$$

We begin by testing the stability of the normal ground state for the Hamiltonian (14) with $V = 0$. This state has all atoms in the ground state and no photons present, and will be denoted by $|0\rangle$. The term $-\kappa$ included in the Hamiltonian (15) implies that $\langle 0|H|0\rangle = 0$, so that energies are measured relative to the state $|0\rangle$. We make use of the variational method with the four-parameter trial wave function

$$|\psi\rangle = \prod_j (\cos\theta + e^{i\phi}\sin\theta\sigma_j^+)\,|\alpha\rangle\,, \tag{18}$$

which is the product of a simple uncorrelated state for the atoms and a coherent state with complex parameter α for the field. We find that

$$\frac{\langle\psi|H|\psi\rangle}{N\epsilon} = \sin^2\theta + \frac{\omega}{\epsilon}y^2 + \frac{4\lambda y}{\epsilon}\sin\theta\cos\theta\cos\chi\cos\phi + (4\kappa y^2/\epsilon)\cos^2\chi\,, \tag{19}$$

in which we have introduced the notation

$$\alpha = \sqrt{N}y e^{i\chi}\,. \tag{20}$$

The minimum value of this expression with respect to ϕ, χ, and y in the domain

$$0 \leq \phi, \chi \leq 2\pi\,, \quad 0 \leq \theta \leq \tfrac{1}{2}\pi\,, \quad 0 \leq y \leq \infty\,, \tag{21}$$

occurs for the parameter values

$$\cos\phi = -\cos\chi = \pm 1\,, \qquad y = 2\lambda\sin\theta\cos\theta/(4\kappa+\omega)\,. \tag{22}$$

If we substitute these values into (4), we obtain

$$\langle\psi|H|\psi\rangle/N\epsilon = \sin^2\theta - \xi\sin^2\theta(1-\sin^2\theta)\,, \tag{23}$$

in which the parameter ξ is defined

$$\xi = 4\lambda^2/(4\kappa\epsilon + \omega\epsilon) \geq 0\,. \tag{24}$$

If $\xi \geq 1$, the value of θ which yields the minimum

value of (21), $\sin^2\theta=(\xi-1)/2\xi$, lies within the physical range $0\leq\sin^2\theta\leq 1$. If $\xi<1$ however, it lies outside this range, so that the physical minimum occurs for $\sin^2\theta=0$. Reference to Eqs. (18), (20), and (22) shows that this is the normal ground state. The parameter ξ therefore plays the role of determining whether the normal ground state is unstable with respect to a super-radiant state of the form (18). In the present case with $V=0$, condition (17) guarantees that $\xi<1$ via the definition (24), so that the normal ground state is stable. Our conclusion is therefore compatible with the result of Ref. 3.

The variational method used here cannot rigorously establish the stability of the ground state, since there could be a state which is not expressible in the form (18) which has lower energy than the normal state.[16] We can, however, use this method to establish the existence of a state of lower energy than the normal ground state. Although the trial state (18) is of simple form, it yields the exact ground-state energy of the original Dicke Hamiltonian without the A^2 and counter-rotating terms. As we now demonstrate, it is also capable of proving the normal ground state to be unstable in a number of cases with $V\neq 0$.

The contribution of V to the expectation value (19) can depend only on the atomic parameters θ and ϕ, and, in fact, depends only on θ in our examples. Indeed, (6) remains valid with a modified value of ξ. In the following three models, ξ can become greater than unity, allowing a super-radiant ground state and a second-order phase transition.

(i) *A linear chain of atoms in which neighboring atoms can exchange excitations directly.* Here, the potential is

$$V=-g\sum_{j=1}^{N-1}(\sigma_j^-\sigma_{j+1}^+ + \sigma_j^+\sigma_{j+1}^-)\,. \tag{25}$$

This potential is the atomic analog of an anisotropic exchange model (x-y model) of ferromagnetism. Minimization of the energy H_1+V gives Eq. (23), with

$$\xi=4\lambda^2/(4\kappa\epsilon+\omega\epsilon)+2g/\epsilon\,. \tag{26}$$

If g can be regarded as an independent parameter, then ξ may take on values greater than unity. We show in Appendix B that g is restricted by the dipole rule, but that the restriction does not prevent ξ in Eq. (26) from becoming larger than unity. This model then has a super-radiant ground state.

(ii) *Atoms separated by a distance r, arranged in a linear chain aligned with the polarization vector of the field, and interacting via dipole-dipole interactions.* The potential is

$$V=-\frac{2\mathcal{P}^2}{r^3}\sum_{j<k}\frac{\sigma_j^{(1)}\sigma_j^{(1)}}{|j-k|^3}\,. \tag{27}$$

The x component of the dipole-moment operator is given by $\mathcal{P}\sigma^{(1)}$, and the y and z components of the dipole-moment operator are suppressed in the model (they do *not* correspond to $\mathcal{P}\sigma^{(2)}$ and $\mathcal{P}\sigma^{(3)}$). This leads to some error in calculating the energy, since these components contribute to the dipole-dipole interaction, but the error is minimal in the super-radiant ground state where there is a strong tendency toward alignment along the x axis. The error becomes larger for excited states where this alignment breaks down. With the potential (27) ξ takes on the value

$$\xi=\frac{4\lambda^2}{4\kappa\epsilon+\omega\epsilon}+\frac{8\mathcal{P}^2}{\epsilon r^3 N}\sum_{j<k}|j-k|^{-3}\,. \tag{28}$$

The independent parameter r can be varied to make $\xi>1$, yielding a super-radiant ground state.

(iii) *Atoms in a thin slab in an orientation perpendicular to the propagation vector of the field, and interacting via their dipole moments.* In this improved version of model (ii), the thickness h_1 of the slab is taken much smaller than the wavelength, and a continuous distribution of atoms is assumed in calculating the dipole-dipole interaction. The integrals are extended to infinity in the transverse direction, and cut off at a lower limit equal to r. The result is the same as for model (ii), except that the sum is replaced by $\pi N h_1/16r$.

We note also one interesting case in which direct interatomic interactions do not lead to a phase transition. This is the analog of the isotropic Heisenberg ferromagnet, which differs from model (i) by the addition of a term $-(g/2)\sum_j\sigma_j^{(3)}\sigma_{j+1}^{(3)}$ to the Hamiltonian. Here, ξ is found to have the same value (24) that it has for noninteracting atoms. This Hamiltonian, being isotropic in the equivalent spin space of the two-level atoms, makes it favorable for adjacent atoms to be in the same state, but immaterial whether that state has a dipole moment, i.e., a nonvanishing value of $\sigma^{(1)}$.

In the Introduction, we argued that if the ground state is super-radiant, then a second-order phase transition will occur at high enough temperatures. To show this rigorously, we would have all the difficulties of treating a fully interacting spin system. The simple method of Wang and Hioe,[12] for example, is not readily applicable. We therefore give an approximate treatment of the thermodynamic behavior by means of an effective field method. We deal only with model (i), since the other models can be handled in the same fashion. The components of the effective field are defined

to be proportional to the thermal averages of $\sigma^{(1)}$ and $\sigma^{(2)}$:

$$B^{(1)} \equiv g\langle\sigma^{(1)}\rangle, \quad B^{(2)} \equiv g\langle\sigma^{(2)}\rangle, \quad B^{(3)} \equiv 0. \tag{29}$$

Replacing the spin variables by these averages, we then determine the optimum values of the field variables y and χ by minimizing the coherent-state expectation value of the resulting Hamiltonian. We obtain

$$\cos\chi = \pm 1 \tag{30}$$

and

$$y = \lambda |B^{(1)}|/g(4\kappa + \omega). \tag{31}$$

The effective Hamiltonian for a single atom then becomes

$$H_{\text{eff}} = -\tfrac{1}{2}\epsilon(\xi B^{(1)}/g)\sigma^{(1)} - B^2\sigma^{(2)} + \tfrac{1}{2}\epsilon\sigma^{(3)}, \tag{32}$$

where ξ has the value given in Eq. (26). We now require the thermal average of $\vec{\sigma}$ calculated from Eq. (32) to be in agreement with Eqs. (29). This demands that $B^2 = 0$, and that $B^{(1)}$ satisfies the equation

$$R = \xi \tanh\tfrac{1}{2}\beta\epsilon R, \tag{33}$$

where

$$R = [1 + (\xi B^{(1)}/g)^2]^{1/2}. \tag{34}$$

A graphical analysis, Fig. 1, shows that there is a nonzero solution provided (a) that $\xi > 1$, and (b) that β is larger than a critical value determined by

$$\xi \tanh\tfrac{1}{2}\beta_c\epsilon = 1. \tag{35}$$

At this value of β, a second-order phase transition occurs. Thus the same condition, $\xi > 1$, implies

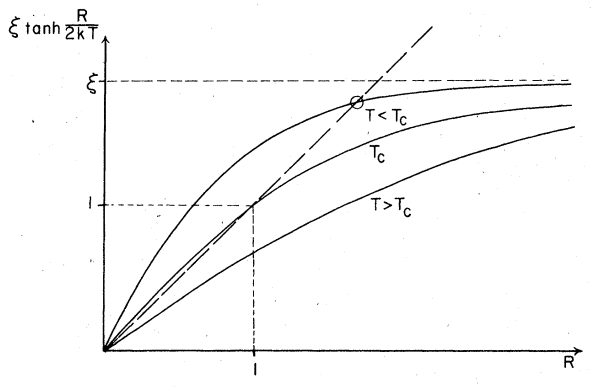

FIG. 1. $\xi\tanh(R/2kT)$ vs R for three values of T. Intersections of these curves with the dashed 45° line determine the mean-field parameter R for given T. R must not be less than unity. The intersection occurs at the point (1,1) for $T = T_C$, and there is no intersection for $T > T_C$, implying $R = 1$. If $\xi < 1$, there is no intersection for any value of T.

that the ground state is super-radiant and that a second-order phase transition takes place.

IV. GAUGE INVARIANCE

In this final section, we present a new argument which bears on the question of the existence of phase transitions which are super-radiant in the sense that the field has a macroscopic expectation value below the transition temperature. The previous sum-rule arguments are traceable to the requirement of gauge invariance, since this requirement implies charge-current conservation from which the sum rule can be derived. We include such a derivation in Appendix A, since it is not the most familiar one. The argument given here also stems from gauge invariance, since it begins with the one-mode approximation to the fundamental gauge-invariant Hamiltonian:

$$H_1 = \sum_j \frac{[p_j - \gamma(a + a^\dagger)]^2}{2m} + V(\vec{r}_j) + \omega a^\dagger a. \tag{36}$$

This Hamiltonian differs from that of the Dicke model not only in the presence of the A^2 and counter-rotating terms, but also in that it does not make the two-level approximation. It retains the full infinite-dimensional Hilbert space necessary to support the position and momentum operators of the atomic electron. We have suppressed the components of the momentum which are not parallel to the polarization vector of the field, since they do not affect the argument.

If Eq. (36) is regarded as describing a classical system with a well-defined minimum of the potential V, then the minimum value of H_1 is obtained by choosing $\vec{r}_j$ to minimize V, p_j to make the velocity $v_j = P_j - \gamma(a + a^\dagger)$ equal to zero, and $a = 0$ to minimize the free field energy. The classical minimum energy is therefore obtained when $a = 0$, indicating that the normal state is stable for all V. If there is a super-radiant phase transition, it must be a purely quantum phenomenon.

Let us now consider a quantum-mechanical system described by the Hamiltonian H_1. We begin by showing that the expectation value of the photon annihilation operator a cannot have a nonvanishing expectation value in the ground state of this system. This is demonstrated with the aid of the unitary operator

$$U = \exp\left(-iK\sum_j x_j - a\chi^* + a^\dagger\chi\right), \tag{37}$$

which imparts a momentum K to each particle and adds χ to the photon annihilation operator:

$$Up_jU^\dagger = P_j + K, \quad UaU^\dagger = a + \chi. \tag{38}$$

Now, if ψ_0 is some presumed ground state of the system for which $\langle\psi_0|a|\psi_0\rangle \neq 0$, we choose the values of the parameters K and χ to be

$$K = 2\gamma \operatorname{Re}\chi\,, \quad \chi = -\langle\psi_0|a|\psi_0\rangle\,. \tag{39}$$

It is then readily seen that the state

$$|\psi\rangle = U^\dagger|\psi_0\rangle \tag{40}$$

has the properties

$$\langle\psi|a|\psi\rangle = 0 \tag{41}$$

and

$$\langle\psi|H_1|\psi\rangle = \langle\psi_0|H_1|\psi_0\rangle - \omega|\langle\psi_0|a|\psi_0\rangle|^2\,. \tag{42}$$

Thus $|\psi_0\rangle$ cannot be the ground state if $\langle\psi_0|a|\psi_0\rangle \neq 0$. We conclude the argument by observing that a system that undergoes a super-radiant phase transition must have a ground state with $\langle\psi_0|a|\psi_0\rangle \neq 0$, since this state can be reached by cooling the system to absolute zero.

The latter remark requires some clarification, since the symmetry of the Hamiltonians considered here seems to imply that $\langle\psi_0|a|\psi_0\rangle = 0$ in the ground state, even for those Hamiltonians which give rise to phase transitions. This is indeed true for the Dicke Hamiltonian, as can be seen from the work of Tavis and Cummings,[17] and for the oscillator model of Sec. II, as can be verified explicitly from the formulas in that section. However, when the number N of atoms becomes large there are states ψ_1 which differ in energy from the ground state by quantities of the order of N^{-1}, and for which $\langle\psi_0|a|\psi_1\rangle$ is nonvanishing. In that case, the state $|\psi_0\rangle + e^{i\phi}|\psi_1\rangle$ yields a nonzero expectation value of a, with phase dependent on ϕ. These states are degenerate with the ground state in the thermodynamic limit $N \to \infty$. States of this form lead to the lack of dependence of the energy, or free energy, of the system on the phase of $\langle a\rangle$, which is evident in the variational calculations of Sec. III, and in other treatments, such as the coupled order-parameter treatment of Gilmore and Bowden.[18] Even for N finite, we can safely conclude that the lowering of energy calculated in Eq. (42) is not a result of delocalizing $\langle a\rangle$ by going to a symmetric ground state. Apart from having a different and much stronger N dependence, the negative term in Eq. (42) receives a large contribution from the free field energy which does not play a role in the delocalization.

To explore the range of validity of the foregoing argument, let us introduce terms describing the electron spin into the Hamiltonian. (Here, in contrast to the previous sections, $\vec{\sigma}$ is the true spin operator of the electron rather than a formal operator connecting two electronic states.) Including the spin-orbit term and a term representing the interaction of the spin magnetic moment with the magnetic field of the mode, we write

$$H_2 = H_1 + \sum_j V_{(\mathrm{SO})}(r_j^2)\vec{\sigma}_j\cdot\vec{r}_j x[\vec{p}_j - \hat{x}\gamma(a+a^\dagger)] + i\xi(a-a^\dagger)\sum_j \sigma_j^{(y)}\,. \tag{43}$$

We have assumed here that the field propagates along the z axis, and that $\vec{A}$ has the direction of the unit vector $\hat{x}$ along the x axis. The parameter ζ has the value

$$\zeta = (e\hbar/2mc)(h\omega/2\mathcal{V})^{1/2}\,. \tag{44}$$

The operator U of Eq. (37) leaves the spin-orbit term invariant, since it commutes with all of its factors by virtue of Eq. (38). Our argument remains valid, therefore, in the presence of spin-orbit coupling. The magnetic coupling of the spin, on the other hand, is modified by the transformation (37) so that in place of Eq. (42), we find

$$\langle\psi|H_2|\psi\rangle = \langle\psi_0|H_2|\psi_0\rangle - \omega|\langle\psi_0|a|\psi_0\rangle|^2 + i\xi(\chi-\chi^*)\langle\psi_0\Big|\sum_j \sigma_j^{(y)}\Big|\psi_0\rangle\,. \tag{45}$$

The only way we can guarantee that the energy is lowered by the transformation is to show that the last term is negative or zero. It is clear, however, in view of Eq. (39) for χ, that this term will be positive in just the case we are attempting to rule out, namely, the case where super-radiant correlations between the field and the spin magnetic moment make the last term in Eq. (43) large and negative. If we wish to lower the energy by means of the transformation of Eq. (37), we must choose χ in order to make the last term in Eq. (45) vanish. But then we can only conclude that the real part of $\langle\psi|a|\psi\rangle$ is zero, which allows the expectation value of the magnetic field to be large in the ground state.

It appears, therefore, that we cannot rule out phase transitions based on magnetic-dipole interactions. A realization of this possibility might consist of a cavity with a constant magnetic field in the z direction. The magnitude of the field would be chosen so that the Larmor frequency is resonant with a mode of the cavity having its magnetic field in the y direction. This system would be well described by the Hamiltonian[19]

$$H = \hbar\omega_L\Big(\sum_j \sigma_j^{(z)} + a^\dagger a\Big) + i\xi(a-a^\dagger)\sum_j \sigma_j^{(y)}\,, \tag{46}$$

which is of the Dicke form, and which is obtained from the fundamental Hamiltonian without making any approximations which violate gauge invari-

ance. The sum-rule argument would not restrict its parameters. A super-radiant phase transition would be possible in principle for this system, but further analysis is needed to determine whether the conditions necessary for its observation could be brought about in practice.

Our argument fails to rule out phase transitions when the Hamiltonian includes terms in the vector potential which go beyond the dipole approximation. It is possible in this case that some extension of our argument or of the sum-rule argument might rule them out, however, and we leave this question open.

APPENDIX A: SUM RULE AND CHARGE-CURRENT CONSERVATION

In this appendix, we give a proof, adapted from Ref. 5, that the sum rule follows from charge-current conservation. If we transfer an infinitesimal momentum $\hat{x}\hbar K$ to the system when it is in its ground state, the current will be changed from $\vec{j}_0$ to

$$\vec{j} = \vec{j}_0 - \hat{x}(\hbar K/m)\rho_0 . \tag{A1}$$

Assuming that $\nabla\cdot\vec{j}_0 = 0$, we have

$$\dot{\rho} = -\nabla\cdot\vec{j} = \frac{\hbar K}{m}\frac{\partial\rho_0}{\partial x} . \tag{A2}$$

This relation allows us to evaluate the moment of $\dot{\rho}$ as follows:

$$\int x\dot{\rho}\, d^3r = \frac{\hbar K}{m}\int x\frac{\partial\rho_0}{\partial x}\, d^3r = -\frac{e\hbar K}{m} . \tag{A3}$$

If, on the other hand, we write $\rho = e\psi^*\psi$, and use the Schrödinger equation, we find that

$$\int x\dot{\rho}\, d^3r = e\int x(\dot{\psi}^*\psi + \psi^*\dot{\psi})d^3r$$

$$= \frac{e}{\hbar}\int x[i(H\psi)^*\psi - i\psi^*H\psi]d^3r . \tag{A4}$$

An evaluation of this integral with

$$\psi = (1 - iKx)\psi_0 \tag{A5}$$

leads, after some calculations in which only the Hermiticity of H is assumed, to the equation

$$\sum_n (E_n - E_0)\left|\int \psi_0^* x\psi_n d^3r\right|^2 = \frac{\hbar^2}{2m} , \tag{A6}$$

by comparison with Eq. (A3).

APPENDIX B: SUM-RULE RESTRICTION ON AN INTERACTING SYSTEM

Here we use the two-atom form of the sum rule to derive a restriction on the parameter g which measures the strength of the interatomic interaction in the first model of Sec. III. Then we show that this restriction does not prevent the parameter ξ of the section from exceeding unity, and therefore permits a super-radiant phase transition. The argument is in the same spirit as that of Ref. 3, and shows that this type of argument does not rule out phase transitions in the more general systems considered in Sec. III.

A pair of interacting atoms is subject to the dipole sum rule in the form

$$\sum_n |\langle\psi_0|(x_1+x_2)|\psi_n\rangle|^2(E_n - E_0) = \frac{\hbar^2}{m} . \tag{B1}$$

The eigenstates and energies are those of the two-atom system, and x_1 and x_2 are the x coordinates of the atomic electrons. In model (i) of Sec. III, this pair of atoms is described in the two-level approximation by the Hamiltonian

$$H_p = \frac{\epsilon}{2}\sum_{j=1}^{2}(1+\sigma_j^{(3)}) - g(\sigma_1^-\sigma_2^+ + \sigma_1^+\sigma_2^-) . \tag{B2}$$

H_p can easily be diagonalized to yield the eigenstates and energy eigenvalues 2ϵ, $\epsilon+g$, $\epsilon-g$, and 0. We can also express $\langle\psi_0|(x_1+x_2|\psi_n\rangle$ in terms of the matrix element $\mathcal{P}/e$ of x between the two levels of a single atom. Using these results in conjunction with Eq. (B1) yields an inequality, since only four states can be included in the summation. The inequality takes on different forms according to whether $g<\epsilon$ or $g>\epsilon$.

For $g<\epsilon$, we obtain

$$\epsilon - g \le e^2\hbar^2/2m\mathcal{P}^2 , \tag{B3}$$

and for $g>\epsilon$,

$$g \le e^2h^2/4m\mathcal{P}^2 . \tag{B4}$$

The consequences of these inequalities are best expressed in terms of the dimensionless parameters $x = g/\epsilon$, $y = \lambda^2/k\epsilon$, and $z = \omega/4\kappa$. The value

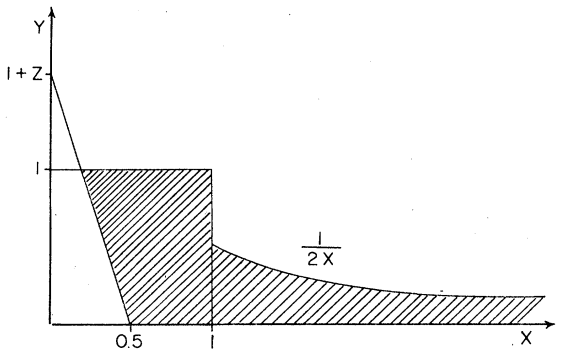

FIG. 2. Region of x-y plane where $\xi>1$ and $x \ge 1-y^{-1}$ for $x<1$ and $x \le (2y)^{-1}$ for $x>1$.

of y must remain less than unity by virtue of Eq. (17), and all three parameters are positive. The inequalities in Eqs. (B3) and (B4) become

$$x \geq 1 - y^{-1} \quad \text{if } x \leq 1 \tag{B3'}$$

and

$$x \leq (2y)^{-1} \quad \text{if } x \geq 1 . \tag{B4'}$$

The condition $\xi > 1$ for the existence of a phase transition can be written with the aid of Eq. (26):

$$y(1+z)^{-1} + 2x > 1 . \tag{B5}$$

The fact that the condition (B5) is compatible with the sum-rule results, Eqs. (B3') and (B4'), is shown in Fig. 2, where values in the shaded region satisfy both restrictions. The sum-rule argument does not, therefore, rule out a phase transition in this case.

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