IS THE WANG–HIOE METHOD UNRESTRICTEDLY APPLICABLE
TO THE SUPERRADIANCE PHASE TRANSITION PROBLEM?

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When applying the Wang–Hioe procedure and the Power–Zinau–Babiker canonical transformation to determine the thermodynamical properties of systems, the latter has to be applied prior to the former.

Since Hepp and Lieb [1] (see also ref. [2]) in 1973 proved the existence of the superradiance phase transition (SPhT) for Dicke's model, much attention has been given to the equilibrium thermodynamics of systems in interaction with a radiation field. The problem is of fundamental significance: to what extent is Hepp and Lieb's result attributable to the considerable simplifications of Dicke's hamiltonian, and to what extent is it a general property of systems interacting with radiation? When dealing with the problem, use is generally made of the highly efficient method of Wang and Hioe [3]. In brief, the latter consists in replacing the products of field operators occurring in the expression for the partition function by normal products of the operators. The field thus becomes classical: the field operators go over into c-numbers. This replacement is correct in the thermodynamical limit only. Now from statistical physics it is well known that the transition to the thermodynamical limit has to be performed at the end of the calculations — subsequent to all canonical transformations — since otherwise one is in danger of obtaining results that are unphysical. The situation should be similar in the Wang–Hioe case. Our communication is intended to show that the sequence in which a canonical transformation and the Wang–Hioe procedure are performed is not irrelevant, because the Wang–Hioe procedure involves a camouflaged transition to the thermodynamical limit.

We consider a dynamical system of N identical hydrogen-like atoms in interaction with radiation. To the aims of this paper, it suffices to conceive of the atom as a single Dirac electron in the potential of the immobile nucleus ion. The positions of the nuclei are denoted as r_n ($n = 1, 2, ..., N$). The hamiltonian of the system is now of the form

$$\mathcal{H}^A = \sum_{n=1}^{N} [\boldsymbol{\alpha}_n \cdot (\boldsymbol{p}_n - eA(r_n + x_n)) + \beta_n m]$$
$$+ \Phi(x_1, ..., x_N) ,$$

with x_n and $\boldsymbol{p}_n$ the position and momentum operators of the electron in atom n fulfilling the commutation rules

$$[x_{n\nu}, p_{m\mu}] = \mathrm{i}\delta_{nm}\delta_{\nu\mu} .$$

Φ is the total Coulomb potential, comprising the potentials of the nuclei and the direct Coulomb interactions of the electrons. A is the vector potential of the radiation field. We assume the Coulomb gauge div $A = 0$. The hamiltonian describing the radiation field is given by

$$\mathcal{H}^F = 2^{-1} \int (E_\perp^2 + B^2) \, \mathrm{d}^3 r ,$$

where $E_\perp = -\dot{A}$, $B = \mathrm{curl}\, A$. Dealing with the field as quantized, the following commutation rules are fulfilled for the Coulomb gauge:

$$[A_\mu(r, t), \dot{A}_\nu(r', t)] = \mathrm{i}\delta_{\mu\nu}^\perp(r - r') ,$$

$$[A_\mu(r, t), A_\nu(r', t)] = 0 = [\dot{A}_\mu(r, t), \dot{A}_\nu(r', t)] .$$

The total hamiltonian is expressed as:

$$\mathcal{H} = \mathcal{H}^A + \mathcal{H}^F . \tag{1}$$

The charge density and current density operators of the system are:

$$\rho(r) = e \sum_{n=1}^{N} \delta(r - r_n - x_n) ,$$

$$J(r) = e \sum_{n=1}^{N} \alpha_n \delta(r - r_n - x_n) .$$

Accordingly, we define the electric and magnetic polarisation operators as:

$$P(r) = e \sum_{n=1}^{N} \int_0^1 d\lambda \, x_n \delta(r - r_n - \lambda x_n) ,$$

$$M(r) = e \sum_{n=1}^{N} \int_0^1 \lambda \, d\lambda \, x_n \times \alpha_n \delta(r - r_n - \lambda x_n) .$$

The above are compact expressions of the series of electric and magnetic multipoles, respectively [5–7].

The thermodynamical properties of the system are given by the partition function:

$$Z[\mathcal{H}] = \text{Tr}_A \, \text{Tr}_F \, [\exp(-\beta \mathcal{H})] ,$$

where $\text{Tr}_A(\ )$ and $\text{Tr}_F(\ )$ are traces, in the Hilbert space, of the atomic system and the field, respectively. The essential feature of the Wang–Hioe procedure consists of the replacement of $\text{Tr}_F [\exp(-\beta \mathcal{H})]$ by the expression $\text{Tr}_F [:\exp(-\beta \mathcal{H}):]$, equivalent to $\text{Tr}_F [\exp(-\beta \mathcal{H})]$ in the thermodynamical limit. The colons denote normal ordering of the field operators. It is convenient to apply the coherent state representation. For an M-mode field, described by the vector potential:

$$A(r) = \sum_{\kappa=1}^{M} (u_\kappa(r)a_\kappa + u_\kappa^*(r)a_\kappa^+) ,$$

we now have [8]

$$\text{Tr}_F(...) = \pi^{-M} \int dz^M \langle z^M | ... | z^M \rangle ,$$

where

$$dz^M = \prod_{\kappa=1}^{M} d \, \text{Re} \, z_\kappa \, d \, \text{Im} \, z_\kappa ,$$

$$|z^M\rangle = |z_1, z_2, ..., z_M\rangle .$$

We thus arrive at the following expression for the partition function:

$$Z[\mathcal{H}] = \pi^{-M} \int dz^M \, \text{Tr}_A \, [\exp(-\beta \mathcal{H}')] , \tag{2}$$

where

$$\mathcal{H}' = \sum_{n=1}^{N} [\alpha_n \cdot (p_n - eA_{cl}(r_n + x_n))] \left[+ \beta m \right]$$

$$+ \Phi(x_1, ..., x_N) + 2^{-1} \int (E_{\perp cl}^2 + B_{cl}^2) \, d^3r .$$

The classical field occurring above is defined by a vector potential of the form

$$A_{cl}(r) = \sum_{\kappa=1}^{M} (u_\kappa(r)z_\kappa + u_\kappa^*(r)z_\kappa^*) .$$

In Tr_A of eq. (2), we perform the canonical Power–Zienau–Babiker [7] transformation

$$\mathcal{H}' \to \bar{\mathcal{H}} = U_{cl} \mathcal{H}' U_{cl}^+ , \tag{3}$$

where

$$U_{cl} = \exp\left(-i \int P \cdot A_{cl} \, d^3r\right).$$

We thus obtain the following expression:

$$\bar{\mathcal{H}} = \sum_{n=1}^{N} (\alpha_n \cdot p_n + \beta_n m) + \Phi(x_1, ..., x_N)$$

$$+ 2^{-1} \int (E_{\perp cl}^2 + B_{cl}^2) \, d^3r - \int M \cdot B_{cl} \, d^3r ,$$

wherein no coupling occurs between the field and the atomic system provided that the magnetisation, related to the orbital angular momentum and the spin magnetisation is neglected ($M = 0$). As a result, no SPhT can appear in this case, since the partition function

$$Z[\mathcal{H}] = \pi^{-M} \int dz^M \, \text{Tr}_A \, [\exp(-\beta \bar{\mathcal{H}})] \tag{4}$$

factorizes obviously into parts dependent on the variables of the medium and those of the field, respectively. The same result is obtained on applying the Wang–Hioe procedure to the hamiltonian

$$\mathcal{H}_0 = \sum_{n=1}^{N} (\alpha_n \cdot p_n + \beta_n m) + \Phi(x_1, ..., x_N)$$

$$+ 2^{-1} \int (E_\perp^2 + B^2) \, d^3r ,$$

where, ab initio, no coupling exists between the field and the medium.

The result derived above is startling since it shows that, in the thermodynamical limit, all quantities involving field—medium coupling vanish. The circumstance that, in the hamiltonian $\mathcal{H}'$, the field is a classical one appears to be irrelevant since Takatsuji [9] has proved the existence of a SPhT in systems of two-level atoms in a classical field.

Now, the sequence of the whole procedure can be inverted. We shall apply the canonical Power—Zienau—Babiker transformation directly to the hamiltonian $\mathcal{H}$ (1) by having recourse to the unitary operator U with quantized vector potential:

$$U = \exp\left(-\mathrm{i} \int P \cdot A \, \mathrm{d}^3 r\right). \tag{5}$$

On transformation, the hamiltonian takes the form:

$$\mathcal{H} \equiv U \mathcal{H} U^+ = \sum_{n=1}^{N} (\alpha_n \cdot p_n + \beta_n m) + \Phi(x_1, ..., x_N)$$

$$+ 2^{-1} \int (E_\perp^2 + B^2) \, \mathrm{d}^3 r$$

$$- \int (P \cdot E_\perp + M \cdot B) \, \mathrm{d}^3 r + 2^{-1} \int |P_\perp|^2 \, \mathrm{d}^3 r .$$

It is only at this stage that we apply the Wang—Hioe approach, obtaining in place of (4) the following expression for the partition function:

$$Z[\mathcal{H}] = \pi^{-M} \int \mathrm{d}z^M \, \mathrm{Tr}_A \left[\exp(-\beta \overline{\mathcal{H}})\right] , \tag{6}$$

where

$$\overline{\mathcal{H}} = \sum_{n=1}^{N} (\alpha_n \cdot p_n + \beta_n m) + \Phi(x_1, ..., x_N)$$

$$+ 2^{-1} \int (E_{\perp\mathrm{cl}}^2 + B_{\mathrm{cl}}^2) \, \mathrm{d}^3 r$$

$$- \int (P \cdot E_{\perp\mathrm{cl}} + M \cdot B_{\mathrm{cl}}) \, \mathrm{d}^3 r + 2^{-1} \int |P_\perp|^2 \, \mathrm{d}^3 r .$$

In the present case we do not succeed in separating the atomic and the field variables even in the zero magnetisation ($M = 0$) approximation.

At this point we face the following, essential question: are the procedures leading to (4) and to (6)

equivalent and, if not, which of them should be used when calculating the partition function? The decision is achieved easily on having recourse to the following simple hamiltonian:

$$h = \sin[V^{-1/2}\mu\mathrm{i}(a - a^+)]S_y + \cos[V^{-1/2}\mu\mathrm{i}(a-a^+)]S_z$$

$$- V^{-1}\mu^2 S_x^2 + a^+ a ,$$

where

$$S_{x,y,z} = \sum_{n=1}^{N} \sigma_{nx,y,z} .$$

The σ_n are spin $1/2$ operators. Their components fulfil the well-known commutation rules:

$$[\sigma_{n\mu}, \sigma_{m\nu}] = \mathrm{i}\delta_{nm}\epsilon_{\mu\nu\lambda}\sigma_{n\lambda} , \quad \mu, \nu, \lambda = x, y, z .$$

Above, a^+ and a are boson creation and annihilation operators. The model, though quite simple, presents the same difficulties as the one considered hitherto. The canonical transformation to be applied now consists in using the unitary operator u (the counterpart of U, eq. (5)), defined as:

$$u = \exp[V^{-1/2}\mu(a - a^+)S_x] .$$

We obtain the relations:

$$uS_x u^+ = S_x ,$$

$$uS_y u^+ = \cos[V^{-1/2}\mu\mathrm{i}(a - a^+)]S_y$$

$$+ \sin[V^{-1/2}\mu\mathrm{i}(a - a^+)]S_z ,$$

$$uS_z u^+ = -\sin[V^{-1/2}\mu\mathrm{i}(a - a^+)]S_y$$

$$+ \cos[V^{-1/2}\mu\mathrm{i}(a - a^+)]S_z , \quad$$

$$uau^+ = a + V^{-1/2}\mu S_x , \quad ua^+u^+ = a^+ + V^{-1/2}\mu S_x ,$$

leading to the following expression in which we recognize the Dicke hamiltonian:

$$k = uhu^+ = S_z + a^+ a + V^{-1/2}\mu(a^+ + a)S_x . \tag{7}$$

As proved strictly by various authors, the system described by (7) exhibits a second order SPhT. However, on applying the Wang—Hioe procedure first, we obtain for the partition function

$$Z[h] = \pi^{-1} \int \mathrm{d}z \, \mathrm{Tr}_A \left[\exp(-\beta h')\right] ,$$

where

$$h' = \sin[V^{-1/2}\mu i(z - z^*)]S_y$$

$$+ \cos[V^{-1/2}\mu i(z - z^*)]S_z - V^{-1}\mu^2 S_x^2 + |z|^2 .$$

On performing in Tr_A a canonical transformation with the following operator u_{cl} (the counterpart of (3)):

$$u_{cl} = \exp[V^{-1/2}\mu(z - z^*)S_x] ,$$

we obtain the partition function in the following form:

$$Z[h] = \pi^{-1} \int dz \, \mathrm{Tr}_A [\exp(-\beta \bar{h})] ,$$

where

$$\bar{h} = S_z - V^{-1}\lambda^2 S_x^2 + |z|^2 .$$

As seen, this partition function factorizes into two — one for the system of spins, and one for the boson field, leading to the fallacious conclusion that no SPhT is present.

The preceding example proves that the canonical transformations have to be performed first and the Wang—Hioe procedure afterwards. Otherwise, the canonical transformation is in fact performed in the thermodynamical limit, whereas numerous examples show that the transition to that limit has to be carried out at the end of the calculations.

The conclusion to be drawn is that calculations applying an incorrect sequence of transformations fail to prove or disprove the presence of a SPhT irrespective of whether the approximation $M = 0$ is used or not.

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