IFUSP/P-112

# ON LINEAR EQUATIONS FOR THERMAL AVERAGES AND ON QUASI AVERAGES IN THE GENERALIZED DICKE MODEL.

by

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*Work supported by the Fundação de Amparo à Pesquisa do Estado de São Paulo.

## ABSTRACT

A rigorous justification of equations proposed by De Vries and Vertogen ( [1] ) is provided for mean field models and applied to a generalized Dicke model ( [3] , [4] , [5] ) with non zero counterrotating term.

Thermal expectation values of certain operators in the Dicke model is the "rotating-wave" approximation (i.e., with zero counterrotating term) may be obtained from the system of equations by a limiting process, which coincides with the method of "quasi-averages" ( [9] ). This point is illustrated by the calculation of the thermal expectation value of the same operator, considered in [1] . Finally, a discussion is made of quasi-averages in this model both from the mathematical (Proposition II-1) as well as from the physical point of view.

## I - INTRODUCTION AND SUMMARY

Let $H_N$ be a Hamiltonian for N two-level atoms in on mode of radiation field of the form

$$H_N = NP\left(\frac{S_N^3}{N}, \frac{S_N^+}{N}, \frac{S_N^-}{N}, \frac{a}{\sqrt{N}}, \frac{a^*}{\sqrt{N}}\right) \qquad \text{(I-1)}$$

defined on the Hilbert space $\mathcal{H}_N = \mathcal{F} \otimes \mathcal{H}_N^1$ where $\mathcal{F}$ F is Fock space for one Boson (photon) , $\mathcal{H}_N^1 \equiv \bigotimes_{i=1}^N \mathbb{C}^2(i)$ the Hilbert space of the N- atom system,

$$S_N^{3,\pm} \equiv \frac{1}{2} \sum_{i=1}^N \sigma_i^{3,\pm} \qquad \sigma_i^{\pm} = \sigma_i^1 \pm \sigma_i^2$$

$\sigma_i^{1,2,3}$ being Pauli matrices over $\mathbb{C}^2(i)$ , a and $a^*$ the photon annihilation and creation operators, and P a polynomial in the given operators. Some of the most general "mean-field" models in the literature may be so described : the Dicke maser model ([3] , [4] , [5] ), Hioe's model ([6]). (The BCS model in the strong-coupling limit ( [9] ) is even simpler and may also be tackled by the forthcoming methods).

Operators $\frac{S_N^{\pm,3}}{N}$ , $\frac{a}{\sqrt{N}}$ and $\frac{a^*}{\sqrt{N}}$ are called "intensive" ( [3] ). Thermal expectation values of intensive operators $O_N$ are defined by

$$O \equiv \lim_{N\to\infty} \langle O_N \rangle_{\beta,N} \equiv \lim_{N\to\infty} \rho_\beta^N(O_N) \equiv \lim_{N\to\infty} \frac{Tr_{\mathcal{H}_N}\left(e^{-\beta H_N} O_N\right)}{Z_N(\beta)} \qquad \text{(I-2)}$$

where we defined the "Gibbs state" $\rho_\beta^N(\cdot) = \langle \cdot \rangle_{\beta,N} =$ $= Tr_{\mathcal{H}_N}(e^{-\beta H_N} \cdot)/Z_N(\beta)$ to abbreviate notation, and

$$Z_N(\beta) = Tr_{\mathcal{H}_N} e^{-\beta H_N}$$

For the Dicke model ([3] , [4] , [5] ), Hioe's ( [6] ) and the BCS model ( [9] ) it was explicitly proved in the given references that the limits (I-2) exist for all polynomials in the intensive variables.

In ([1]) certain linear equations for thermal expectation values were proposed and used to compute the average value of $S_N^3/N$ , reproduciong the known result ( [3] ). Subsequently, Pimentel and Zimerman applied this method to several models (including the ones mentioned above), always reproducing the correct thermal averages already known from the literature ( [2] ). As no theoretical explanation was offered by the autohrs, and given the great attraction of the method due to its simplicity, we propose to remedy this flaw in sect. II, where we present a rigorous interpretation of their procedure for Hamiltonians of type (I-1) (which is easily adaptable to other mean-field Hamiltonians as the BCS model ( [9] )). For this purpose, it is necessary to present two formalisms : a) a formalism for Hamiltonians of a certain class (A) not exhibiting a certain kind of symmetry, under a certain set ($C_1$) of assumptions; b) a formalism allowing calculation of thermal averages of certain operators for Hamiltonians of the complementary class (B) by limiting processes ("quasi-averages", [9] ) from the equations deduced for Hamiltonians of class (A), also under an assumption ($C_2$) countained in Proposition II-1.

In Sect. III we illustrate this formalism, taking as class (A) Hamiltonian the generalized Dicke Hamiltonian $H^1$, that is, with nonzero counterrotating term ([4] ,[5] ,[2] ) and as class (B) Hamiltonian the Dicke Hamiltonian in the "rotating wave" approximation $H^2$, that is, without counterrotating term

([3]). In Sect. IV we discuss the meaning of "quasi-averages" in this model, in greater detail.

## II - A GENERAL FORMALISM

Let $H_N$ be of the form (I-1). $H_N$ belongs to class (B) if an operator $C_N$ over $\mathcal{H}_N$ exists such that

$$[C_N, H_N] = 0 \tag{II-1}$$

and such that (II-1) implies that certain intensive operators have zero thermal average. (A) is the complementary class. Let $H_N$ be of class (A). We have

$$\rho_\beta^N([H_N, O_N]) = 0 \qquad \forall N, \beta \tag{II-2}$$

where $O_N$ is any intensive operator, whence the system of equations

$$\lim_{N\to\infty} \rho_\beta^N([H_N, O_N^{(i)}]) = 0 \qquad i=1,2,\dots,5 \ ; \forall \beta \in I \tag{II-3}$$

follows, where $O_N^{(i)}$ are the operators $S_N^{\pm,3}/N$, $a/\sqrt{N}$, $a^*/\sqrt{N}$, if the limits in (II-3) exist, and I is a nonempty subset of $\mathbb{R}_+$.

The commutator $[H_N, O_N^{(i)}]$ is a polynomial in the intensive operators, but it in general involves products as, e.g., $\frac{S_N^+}{N}\frac{a}{\sqrt{N}}$. Hence, in order that the system (II-3) become a system in the thermal averages $O_\beta^{(i)} \equiv \lim_{N\to\infty} \langle O_N^{(i)} \rangle_{\beta,N}$ ( we note $S_\beta^3 \equiv \lim_{N\to\infty} \langle S_N^3/N \rangle_{\beta,N}$ and similarly for the other operators), it is necessary that one have

$$\text{(C-1a)} \qquad \lim_{N\to\infty} \langle O_N^{(i)} O_N^{(j)} \rangle_{\beta,N} = O_\beta^{(i)} O_\beta^{(j)}$$

$$\forall \beta \in I \ ; \ \forall i,j \in [1,5] \tag{II-4}$$

under assumption (C-1a) the limits in (II-3) exist and furnish a system of equations for the $O^{(i)}$. If, however, one or more of the $O_\beta^{(i)}$ are zero identically, one or more equations of (II-3) will consist of the identity $0 = 0$, which fact in general will not allow them to be solved (this occurs in the case of $H^2$, see sect. III). We impose therefore

$$(C\text{-}1b) \qquad O_\beta^{(i)} \neq 0 \qquad \forall i \in [1,5] \; ; \forall \beta \in I \tag{II-5}$$

Under assumptions C-1 we expect that some thermal averages can be determined (for $\beta \in I$) solving (II-3). This will be illustrated in sect. III for the Hamiltonian $H^1$. For Hamiltonians of class (B) in general no one of assumptions (C-1a) and (C-1b) holds. This is illustrated for $H^2$ in Sect.III and justifies our division into two classes. In Sect.III we also verify (C-1) for $H^1$ and use the equations thereby obtained to calculate $S_\beta^3$, which is shown to coincide with the explicitly calculated value.

Let now $H_N(\mu)$ be of class (A) $\forall \mu \neq 0$, such that $H_N(\mu) = H_N(0) + \mu A_N$ ; $A_N = N P_N$, $P_N$ polynomial in the intensive operators

$$\frac{a}{\sqrt{N}} \, , \; \frac{a^*}{\sqrt{N}} \, , \; \frac{S_N^+}{N} \, , \; \frac{S_N^-}{N} \, , \; \frac{S_N^3}{N} \tag{II-6}$$

and such that $H_N = H_N(0)$ be of class B (one such example is given in Sect. III). Let $O_N$ be an intensive operator and consider the sequence of "free energies"

$$f_N(\beta, \rho, \mu) \equiv -\frac{\beta^{-1}}{N} \log Z_N^1(\beta, \rho, \mu) \tag{II-7a}$$

where $$Z_N^1(\beta,\rho,\mu) \equiv Tr_{\mathcal{H}_N}\, e^{-\beta[H_N(\mu)+\rho N O_N]} \tag{II-7b}$$

Let also $$f_N(\beta,\rho) = f_N(\beta,\rho,0) \tag{II-7c}$$

and denote also $f(\beta,\rho,\mu) \equiv \lim_{N\to\infty} f_N(\beta,\rho,\mu)$, and $f(\beta,\rho) \equiv \lim_{N\to\infty} f_N(\beta,\rho)$ if these limits exist.

<u>Proposition II-1</u> If $f(\beta,\rho)$ is differentiable at $\rho=0$ (C-2) the quasi-average of $O_N$, defined by $\left(\langle O_N\rangle_{\beta,N,\mu} \equiv \frac{Tr_{\mathcal{H}_N}\, e^{-\beta H_N(\mu)} O_N}{Tr_{\mathcal{H}_N}\, e^{-\beta H_N(\mu)}}\right)$

$$\lim_{\mu\to 0_+} O_{\beta,\mu}\quad,\text{ where }\quad O_{\beta,\mu} \equiv \lim_{N\to\infty} \langle O_N\rangle_{\beta,N,\mu}$$

and the thermal average of $O_N$ in the system described by the Hamiltonian $H_N$ (0) coincide, i.e.,

$$\lim_{\mu\to 0_+} O_{\beta,\mu} = O_\beta \equiv \lim_{N\to\infty} \langle O_N\rangle_{\beta,N,\mu=0} \tag{II-8}$$

<u>Proof.</u> $\{f_N(\beta,\rho,\mu)\}$ is a sequence of concave functions of $\rho$ in $-\infty<\rho<\infty$ (this may be proved by using the results of [10] and the methods in the appendix of [4] ).Hence $f(\beta,\rho,\mu)$ will be, if it exists, a concave function of $\rho$ . The sequence $f(\beta,\rho,\mu)$ in $\mu$ (putting, e.g., $\mu=\frac{1}{n}$ and taking $n\to\infty$ ) is therefore a sequence of concave functions of $\rho$ and by Griffiths' lemma (see, e.e., [4] , appendix).

$$\frac{\partial}{\partial\rho}\lim_{\mu\to 0_+} f(\beta,\rho,\mu)\Big|_{\rho=0} = \lim_{\mu\to 0_+}\frac{\partial}{\partial\rho} f(\beta,\rho,\mu)\Big|_{\rho=0} \tag{II-9}$$

<u>if</u> the limit $\lim_{\mu\to 0_+} f(\beta,\rho,\mu)$ (which exists because $f(\beta,\rho,\mu)$ is a concave, hence continuous, function of $\mu$) is differentiable at $\rho=0$ . But

$$\lim_{\mu\to 0_+} f(\beta,\rho,\mu) = \lim_{\mu\to 0_+}\lim_{N\to\infty}\left[-\frac{\beta^{-1}}{N}\log Z_N^1(\beta,\rho,\mu)\right] =$$

$$= \lim_{N\to\infty}\lim_{\mu\to 0_+}\left[-\frac{\beta^{-1}}{N}\log Z_N^1(\beta,\rho,\mu)\right] = \lim_{N\to\infty} f_N(\beta,\rho) = f(\beta,\rho) \tag{II-10}$$

if the sequence $\{f_N(\beta,\rho,\mu)\}$ is uniformly continuous in $\mu$ for $\mu$ in some neighbourhood of the origin. This is true if $\left|\frac{\partial f_N(\beta,\rho,\mu)}{\partial\mu}\right|$ is uniformly bounded (in N) for $\mu$ in some neighbourhood of the origin, which itself holds if and only if

$$\langle A_N\rangle_{\beta,N,\rho,\mu} \equiv \frac{Tr_{\mathcal{H}_N}\left(A_N\ e^{-\beta[H_N(\mu)+\rho N O_N]}\right)}{Z_N^1(\beta,\rho,\mu)}$$

is uniformly (in N) bounded in absolute value for $\mu$ in some neighbourhood of the origin. For $A_N = N\ P_N$ (cf.(II-6)) this may be explicitly proved in all mean-field models. Differentiability of $\lim_{\mu\to 0_+} f(\beta,\rho,\mu)$ at $\rho=0$ is therefore equivalent to the differentiability at $\rho=0$ of the r.h.s. of (II-10). (II-8) follows by Griffiths' lemma. ∎

In ([4] , appendix) it is shown by examples that in general intensive operators $O_N$ not invariant by the simmetry transformation (i.e., such that $[C_N, O_N] \neq 0$ ) the derivative of $f(\beta,\rho)$ at $\rho=0$ does not exist; a discussion of the general reason for this is also given there. Meanwhile, it is explicitly verified in the models ( [4] , appendix) that the derivative <u>exists</u> in case of operators invariant by the symmetry transformation (which we shall call "gauge-invariant" operators).

In Sect. III we consider the thermal average of the gauge-invariant operator $S_N^3/N$ in $H^2$. The remarks above apply and by the previous proposition $S_\beta^3 = \lim_{\mu\to 0_+} S_{\beta,\mu}^3$ (II-11). This quasi-average is, on the other hand, calculable from the equations obtained for $H^1$ taking the limit $\mu\to 0_+$ , allowing for an explicit verification of (II-11) in this special case.

## III - APPLICATION

We take ( [3] , [4] , [5] )

$$H_N^1 = H_N(\mu) = H_N(0) + \mu(S_N^- a + S_N^+ a^*)/\sqrt{N} \qquad \text{(III-1)}$$

where

$$H_N^2 = H_N(0) = a^*a + \mathcal{E} S_N^3 + \frac{\lambda}{\sqrt{N}}(S_N^+ a + S_N^- a^*) \qquad \text{(III-2)}$$

$H_N^1$ is the "generalized" Dicke Hamiltonian, the term with coefficient $\mu$ being the "counterrotating" one and $H_N^2$ is the Dicke Hamiltonian in the rotating-wavw approximation, the term with coefficient $\lambda$ being the "rotating"one ( [7] ). $H_N^1$ exhibits a superradiant ( [7] ) phase transition at a critical temperature $T_c$ ($\mu$) defined by

$$\frac{\mathcal{E}}{(\lambda+\mu)^2} = \tanh\left[\frac{1}{2}\beta_c(\mu)\mathcal{E}\right] \;, \quad \beta_c(\mu) = \frac{1}{kT_c(\mu)} \qquad \text{(III-3)}$$

$H_N^2$ exhibits the same behaviour, where the critical temperature is given by (III-3) putting $\mu = 0$ , whence it follows that

$$T_c(\mu) \geqslant T_c(0) \qquad if \quad \mu \geqslant 0 \qquad \text{(III-4)}$$

Both $H_N^1$ and $H_N^2$ commute with $\underline{S}_N^2 = \sum_{j=1}^{3}\left(\sum_{i=1}^{N} S_i^{(j)}\right)^2$ ,but $H_N^2$ presents an additional symmetry:

$$[C_N, H_N^2] = 0 \qquad \text{(III-5)}$$

where

$$C_N = a^*a + S_N^3 \qquad \text{(III-6)}$$

while $[\underline{S}_N^2, H_N] = 0$ does not imply that any thermal averages are zero, $[C_N, H_N^2] = 0$ implies that for $H^2$

$$\left\langle \frac{a}{\sqrt{N}} \right\rangle_{\beta,N} = \left\langle \frac{a^*}{\sqrt{N}} \right\rangle_{\beta,N} = \left\langle \frac{S_N^+}{N} \right\rangle_{\beta,N} = \left\langle \frac{S_N^-}{N} \right\rangle_{\beta,N} = 0 \quad \text{(III-7)}$$

for instance, $[C_N, a] = -a$ and $\langle [C_N, a] \rangle_{\beta,N} = 0$ because $[C_N, H_N^2] = 0$ (III-7 shows that (C-1b) does not hold for $H^2$. Further, (C-1a) does not hold either, because of spontaneous symmetry breakdown ( [3] ). Hence $H^2$ is of class (B). It may be shown explicitly that $H^1$ is of class (A).

Letting $\alpha_{\beta,\mu} = \lim_{N\to\infty} \left\langle \frac{a}{\sqrt{N}} \right\rangle_{\beta,N,\mu}$ , $\alpha^*_{\beta,\mu} = \lim_{N\to\infty} \left\langle \frac{a^*}{\sqrt{N}} \right\rangle_{\beta,N,\mu}$

and similarly for $S^{\pm,3}_{\beta,\mu}$ , it may readily be verified that (II-3) yields, under assumption (C-1a):

$$\alpha^*_{\beta,\mu} + \lambda S^+_{\beta,\mu} + \mu S^-_{\beta,\mu} = 0 \quad \text{(III-8a)}$$

$$\alpha_{\beta,\mu} + \lambda S^-_{\beta,\mu} + \mu S^+_{\beta,\mu} = 0 \quad \text{(III-8b)}$$

$$\lambda \alpha_{\beta,\mu} S^+_{\beta,\mu} - \lambda \alpha^*_{\beta,\mu} S^-_{\beta,\mu} + \mu S^+_{\beta,\mu} \alpha^*_{\beta,\mu} - \mu S^-_{\beta,\mu} \alpha_{\beta,\mu} = 0 \quad \text{(III-8c)}$$

$$\varepsilon S^+_{\beta,\mu} - 2\lambda \alpha^*_{\beta,\mu} S^3_{\beta,\mu} - 2\mu \alpha_{\beta,\mu} S^3_{\beta,\mu} = 0 \quad \text{(III-8d)}$$

$$\varepsilon S^-_{\beta,\mu} - 2\lambda \alpha_{\beta,\mu} S^3_{\beta,\mu} - 2\mu \alpha^*_{\beta,\mu} S^3_{\beta,\mu} = 0 \quad \text{(III-8e)}$$

from (III-8a,b,d) we obtain under assumption (C-1b), $\alpha^*_{\beta,\mu} = \overline{\alpha_{\beta,\mu}}$ and $\lambda, \mu \geq 0$ ,

$$S^3_{\beta,\mu} = \frac{\varepsilon}{2(\lambda^2-\mu^2)} \left( \frac{\mu \alpha_{\beta,\mu} - \lambda \alpha^*_{\beta,\mu}}{\lambda \alpha^*_{\beta,\mu} + \mu \alpha_{\beta,\mu}} \right) . \quad \text{(III-9)}$$

by using the techinique of ( [4] , appendix) it may be shown ( [8] ) that, for $T \lesssim T_c(\mu)$,

$$\alpha_{\beta,\mu} = \alpha^*_{\beta,\mu} = -\sqrt{Y_0(\mu)} \qquad \text{(III-10)}$$

where $Y_0(\mu)$ is the solution of the equation

$$\tanh\left[\beta\varepsilon\left(1+\frac{4}{\varepsilon^2}(\lambda+\mu)^2 y\right)^{1/2}\right] = \frac{\varepsilon}{2(\lambda+\mu)^2}\left[1+\frac{4}{\varepsilon^2}(\lambda+\mu)^2 y\right]^{1/2} \qquad \text{(III-11)}$$

which is known ( [4] , [5] ) to satisfy

$$Y_0(\mu) > 0 \quad \text{for} \quad T < T_c(\mu) \qquad \text{(III-12)}$$

It may also be shown that ( [8] or [4] , appendix)

$$S^3_{\beta,\mu} = -\frac{\varepsilon}{2(\lambda+\mu)^2} \qquad \text{(III-13)}$$

Further, it was shown in [8] that for $T \leqslant T_c\ (\mu)$

$$\lim_{N\to\infty} \left\langle \frac{S^3_N}{N}\frac{a}{\sqrt{N}}\right\rangle_{\beta,N,\mu} = \lim_{N\to\infty} \left\langle \frac{S^3_N}{N}\frac{a^*}{\sqrt{N}}\right\rangle_{\beta,N,\mu} = \frac{\varepsilon}{2(\lambda+\mu)^2}\sqrt{Y_0(\mu)} \qquad \text{(III-14)}$$

hence by (III-10) and (III-13)

$$\lim_{N\to\infty} \left\langle \frac{S^3_N}{N}\frac{a}{\sqrt{N}}\right\rangle_{\beta,N,\mu} = \alpha_{\beta,\mu}\, S^3_{\beta,\mu} \qquad \text{(III-14)}$$

(III-14) was necessary to deduce (III-8d). Other relations similar to (III-14) necessary to prove (III-8c) can be verified analogously ( [8] ).

By ( [4] , appendix or [8] ) it may be shown that the free energy $f(\beta,\rho)$ corresponding to $O_N = S^3_N/N$ is differentiable at $\rho=0$ and hence by Griffiths' lemma

$$S^3_\beta = \left.\frac{\partial f(\beta,\rho)}{\partial\rho}\right|_{\rho=0} = -\frac{\varepsilon}{2\lambda^2} \qquad \text{(III-15)}$$

It follows from (III-10) and (III-4) that for $T < T_c(0)$

$$\lim_{\mu\to 0_+} \alpha_{\beta,\mu} = \lim_{\mu\to 0_+} \alpha_{\beta,\mu} = -\sqrt{Y_0(0)} \tag{III-16}$$

where $Y_0(0)$ is the solution of eq. (III-11) putting there $\mu=0$, which is known ( [3],[5] ) to satisfy

$$Y_0(0) > 0 \quad \text{for} \quad T < T_c(0) \tag{III-17}$$

From (III-9), (III-16) and (III-17) it follows that

$$\lim_{\mu\to 0_+} S^3_{\beta,\mu} = -\frac{\varepsilon}{2\lambda^2} \tag{III-18}$$

confirming numerically (II-8) in this special case. This corresponds precisely to the application made in [1] .

## IV - QUASI- AVERAGES

(III-16) allows a better clarification, in physical terms, of the role of quasi-averages in this model. (III-7) and (III-16) imply that

$$\lim_{\mu\to 0_+} \lim_{N\to\infty} \left\langle \frac{a^\#}{\sqrt{N}} \right\rangle_{\beta,N,\mu} \neq \lim_{N\to\infty} \lim_{\mu\to 0_+} \left\langle \frac{a^\#}{\sqrt{N}} \right\rangle_{\beta,N,\mu} \tag{IV-1}$$

which is another ( [10] ) illustration of the well-know fact that in general quasi-averages do not coincide with the averages (as in the case where there is a spontaneous magnetization in a ferromagnetic model). As in the ferromagnetic case, (IV-1) is due to the existence of a phase transition in the model, which is characterized by

$$\lim_{N\to\infty} \left\langle \frac{a^* a}{N} \right\rangle_{\beta,N,\mu} = \begin{cases} 0 & \text{if } T > T_c(\mu) \\ \gamma(\mu) > 0 & \text{if } T < T_c(\mu) \end{cases}$$

corresponding to spontaneous emission of photons below $T_c$. For the model with $\mu \neq 0$ (C-1a) holds and, besides, for

$$T < T_c(0) \quad , \quad \lim_{\mu\to 0_+} \gamma(\mu) \neq 0$$

.Equation (IV-1) is a corollary of these facts.

Acknowledgement: W.F.W. should like to thank B.M. Pimentel and Prof. A.H.Zimerman for stimulating discussions.

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