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Two level systems interacting with bosons: thermodynamic limit of thermodynamic functions.

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Abstract: For a two-level system coupled linearly to bosons, we reduce the existence of the thermodynamic limit of the thermodynamic functions to that of the corresponding limit for the free bosons. The case where the interaction is with the radiation-field is treated as a particularly relevant example.

1. Introduction

The Hamiltonian

$$H = \varepsilon S_3 + \sum_n \omega_n a_n a_n + S_2 \sum_n (\bar{\lambda}_n a_n + \lambda_n a_n^*) \qquad (1.1)$$

describing a two-level system - specified by:

$$S_3 = \begin{pmatrix} 1 , & 0 \\ 0 , & 1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 0 , & -i \\ i , & 0 \end{pmatrix}, \quad S_1 = \begin{pmatrix} 0 , & 1 \\ 1 , & 0 \end{pmatrix} \quad -$$

interacting with bosons - $[a_n, a_m] = \delta_{nm}$ - appears in quantum optics and solid-state physics [1)]. The ω_n's are the frequencies of the free bosons, ε is the level spacing, and the λ_n's are (complex) coupling constants. Replacing ε, and all λ_n's by their negative values, one obtains a Hamiltonian which is unitarily equivalent. We assume henceforth that $\varepsilon \geq 0$.

In semiclassical radiation theory, H is derived from "first principles" as follows. One starts with the Hamiltonian for a system of K particles of masses m_j and charges z_j $(j=1,2,...,K)$ coupled to the electromagnetic field described in the Coulomb-gauge and quantized transversally in the usual manner, say in a cube of side-length ℓ. One then selects two

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1) Relevant references to the literature up to 1980 are given in Pfeifer's thesis [1], where a thorough analysis of this Hamiltonian is given.

orthogonal eigenvectors Ψ_1, Ψ_2 of the <u>free</u> particle Hamiltonian having opposite parity, and projects the <u>full</u> Hamiltonian with these vectors. Upon <u>neglecting</u> terms which are quadratic in the field annihilation and creation operators, one obtains H up to a constant. The sums in (1.1) are then over $\underline{n}=(n_1,n_2,n_3)$ with each n_k running in $\mathbb{Z}\setminus\{0\}$, and over the polarization-index $\alpha\in\{1,2\}$. The frequencies are

$$\omega_{\underline{n}} = c|\underline{k}_{\underline{n}}| \quad \text{, with} \quad \underline{k}_{\underline{n}} = (2\pi/\ell)\underline{n} \ ,$$

and the coupling constants are ($\underline{e}_{\underline{n},\alpha}$ is the polarization vector orthogonal to $\underline{n}$)

$$\lambda_{\underline{n},\alpha} = (2\pi/\omega_{\underline{n}}\ell^3)^{1/2} \underline{e}_{\underline{n},\alpha} \cdot \sum_{j=1}^{K} (z_j/m_j) \langle \Psi_2, \cos(\underline{k}_n \cdot \underline{x}_j) \nabla_j \Psi_1 \rangle \ .$$

Pfeifer [1] shows that

$$\lim_{\ell\to\infty} \sum_{\underline{n},\alpha} |\lambda_{\underline{n},\alpha}|^2 \omega_{\underline{n}}^{-1} < \infty \qquad (1.2)$$

but,

$$\lim_{\ell\to\infty} \sum_{\underline{n},\alpha} |\lambda_{\underline{n},\alpha}|^2 \omega_{\underline{n}}^{-2} = \infty \ .$$

The convergence, resp. divergence of the above limits is essential for Pfeifer's arguments supporting the appearance of

a <u>ground-state degeneracy</u> for (1.1) in the bulk-limit .

Here we propose to begin the study of the thermodynamic-limit of the model, by proving existence of the limit of the mean thermodynamic functions. In section 2, we introduce notation, and collect results of a very general nature which will be of use in a forthcoming study of the limit of the Gibbs-states ([2]). In section 3, we prove that, under certain necessary and sufficent conditions on the coupling constants and frequencies, the thermodynamic-limit of the thermodynamic functions computed from H exists whenever the corresponding limit for the free bosons exist, and that the limits are equal up to certain ε-independent constants.

2. Some generalities

We adopt the standard Fock-space formalism and notation. Consider a Hilbert space $\mathcal{H}$ with scalar-product $\langle .,. \rangle$ [2)], and let $\mathcal{F}$ be the symmetric Fock-space built upon $\mathcal{H}$. We write a(f) for the annihilation operator smeared with f, and the Weyl-operators are given by

$$W(f)=\exp\{a^*(f)-a(f)\} \ , \ f\in\mathcal{H}; \qquad W(f)W(g)=e^{-i\,\mathrm{Im}\langle f,g\rangle}W(f+g) \ .$$

We write $d\Gamma(.)$ and $\Gamma(.)$ for the second-quantization maps, and for the normalized Fock-vacuum vector.

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2) This is our notation for all scalar products, which will not be distinguished, and are assumed linear in the second entry.

In this setting, the operator (1.1) corresponds, upon performing a unitary transformation on the two-level system which sends S_3 and S_2 into S_1 and S_3 respectively, to

$$H = \varepsilon S_1 \otimes 1 + 1 \otimes d\Gamma(h) + S_3 \otimes (a^*(\lambda) + a(\lambda)) \quad , \quad \text{on } \mathbb{C}^2 \otimes F. \qquad (2.1)$$

where we have also introduced tensor product notation which will be used throughout, and the one-particle Hamiltonian h is a positive, injective, selfadjoint operator acting on H. It is possible to make sense of

$$H^o = H - \varepsilon S_1 \otimes 1 = 1 \otimes d\Gamma(h) + S_3 \otimes (a^*(\lambda) + a(\lambda)) \quad , \qquad (2.2)$$

and thus of H, as a selfadjoint operator when $\|h^{-1/2}\lambda\|^2 < \infty$ holds true without assuming that $\lambda \in H$ [3]. If one assumes that $\lambda \in D(h^{-1/2})$ [4], then the inequality $|h^{-1/2}\lambda><h^{-1/2}\lambda| \leqslant \Lambda 1$, where

$$\Lambda = \|h^{-1/2}\lambda\|^2 \qquad \text{(this is (1.2))} \quad . \qquad (2.3)$$

entails $|\lambda><\lambda| \leqslant \Lambda h$, and thus $a^*(\lambda)a(\lambda) \leqslant \Lambda\, d\Gamma(h)$. One then proves that $S_3 \otimes (a^*(\lambda) + a(\lambda))$ is $(1 \otimes d\Gamma(h))$-bounded with relative bound zero, so (2.2) is selfadjoint by the Kato-

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3) This involves quadratic form techniques and the KLMN Theorem, see [3], Lemma 1.

4) D(.) denotes domain of.

Rellich Theorem. If, more restrictively $\lambda \in D(h^{-1})$ [5], then an application of the "quadratures formula" ([4]) shows that

$$W(\mp h^{-1}\lambda)\, d\Gamma(h)\, W(\pm h^{-1}\lambda) = d\Gamma(h) \pm (a^*(\lambda) + a(\lambda)) + \Lambda 1 \qquad (2.4)$$

All this leads to the following characterization of (2.1) as a selfadjoint operator; we omit the details of the proof.

Lemma: If $\lambda \in D(h^{-1/2})$ then H given by (2.2) is selfadjoint on $D(1 \otimes d\Gamma(h))$, bounded below by $-(\Lambda + \varepsilon)$, and commutes with the selfadjoint unitary $S_1 \otimes \Gamma(-1)$. If moreover $\lambda \in D(h^{-1})$, then

$$H = \varepsilon S_1 \otimes 1 + U^*(1 \otimes d\Gamma(h))U - \Lambda 1 \quad . \qquad (2.5)$$

where the unitary operator U is given by

$$U = P_+ \otimes W(h^{-1}\lambda) + P_- \otimes W(-h^{-1}\lambda) \quad , \qquad (2.6)$$

where $P_\pm$ are the spectral projections of S_3 to the eigenvalues ± 1.

The operator inequality $-1 \leqslant S_1 \leqslant 1$ entails (recall $\varepsilon \geqslant 0$)

$$H^o - \varepsilon 1 \leqslant H \leqslant H^o + \varepsilon 1 \quad . \qquad (2.7)$$

If $\lambda \in D(h^{-1})$, the operator H^o has the vectors $z_\pm \otimes W(\mp h^{-1}\lambda)$ with $P_\pm z_\pm = z_\pm$ as orthogonal ground-states with energy $-\Lambda$. If

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5) Recall that $D(h^{-1})$ is a core for $h^{-1/2}$.

also $h \geq c1$, with $c>0$, then regular perturbation theory shows that the degeneracy is lifted for $\varepsilon>0$ sufficently small, and one has two eigenvalues of opposite "parity" $(S_1 \otimes \Gamma(-1))$ at the bottom of the spectrum [6]. For a wealth of information on H when h acts on a finite-dimensional Hilbert space, see [1].

3. The thermodynamic limit of the mean thermodynamic functions

Let V be a subset of $\mathbb{R}^3$ of finite Lebesgue-measure (i.e. volume) $|V|$. To the positive, injective, selfadjoint operator h_V acting on $L^2(V)$, and $\lambda_V \in D(h_V^{-1/2})$, associate the selfadjoint operators (Lemma)

$$H_V^o = 1 \otimes d\Gamma(h_V) + S_3 \otimes (a^*(\lambda_V) + a(\lambda_V)) ,$$
$$H_V = H_V^o + \varepsilon S_1 \otimes 1 ,$$

acting on $\mathbb{C}^2 \otimes F_V$, where F_V is the Fock-space built upon $L^2(V)$. If the condition

$$\exp\{-\beta(h_V)\} \text{ is a trace-class operator for some (hence all) } 0 < \beta < \infty ; \tag{3.1}$$

holds true, then $\exp\{-\beta d\Gamma(h_V - \mu 1)\}$ is trace-class for every $\beta \in (0,\infty)$, and every $\mu \in (-\infty, 0]$. By the injectivity assumption,

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6) No general statements about ground state(s) are available whenever h is not discrete, and λ is not in $D(h^{-1})$, or the lower bound on h is zero.

h_V^{-1} is bounded; also, $(h_V - \mu 1)^{-1} \leq h_V^{-1}$. Let $N_V = d\Gamma(1)$ be the number operator on F_V. Formula (2.5) applied to the $h_V - \mu 1$, gives

$$H^o - \mu(1 \otimes N_V) = U_{V,\mu}(1 \otimes d\Gamma(h_V - \mu 1))U_{V,\mu} - \Lambda_{V,\mu} 1, \tag{3.2}$$

where

$$U_{V,\mu} = P_+ \otimes W([h_V - \mu 1]^{-1}\lambda_V) + P_- \otimes W(-[h_V - \mu 1]^{-1}\lambda_V) ,$$
$$\Lambda_{V,\mu} = \|[h_V - \mu 1]^{-1/2}\lambda_V\|^2 , \qquad \mu \in (-\infty, 0]. \tag{3.3}$$

Notice that $\Lambda_{V,\mu}$ is a convex and increasing function of μ. It follows that $\exp\{-\beta(H^o - \mu(1 \otimes N_V))\}$ and $\exp\{-\beta(H_V - \mu(1 \otimes N_V))\}$ are also trace-class for every $\beta \in (0,\infty)$, and $\mu \in (-\infty, 0]$. Consider the partition function and the mean free energy based on H_V:

$$Z_V(\beta,\mu;\varepsilon) = \mathrm{Tr}(\exp\{-\beta(H_V - \mu(1 \otimes N_V))\});$$

$$f_V(\beta,\mu;\varepsilon) = (-1/\beta|V|)^{-1}\log(Z_V(\beta,\mu;\varepsilon)) .$$

Denote the corresponding functions based on the free boson Hamiltonian $d\Gamma(h_V)$ by the same symbols with a superscript ^{o}, and of course no argument ε.

Due to (3.2), we have $Z_V(\beta,\mu;0) = 2\exp\{\beta\Lambda_{V,\mu}\}Z_V^o(\beta,\mu)$, and the inequality (2.7) implies

$$\begin{aligned} &-|V|^{-1}[\beta^{-1}\log(2) + \varepsilon + \Lambda_{V,\mu}] + f_V^o(\beta,\mu) \\ &\leq f_V(\beta,\mu;\varepsilon) \\ &\leq -|V|^{-1}[\beta^{-1}\log(2) - \varepsilon + \Lambda_{V,\mu}] + f_V^o(\beta,\mu) \end{aligned} \tag{3.4}$$

If $|V|^{-1}\Lambda_{V,\mu}$ has a limit as $|V| \to \infty$ [7], then the thermodynamic limit of the mean free energy is reduced to that of the mean free energy of the free bosons, and is independent of ε. This proves the following.

Theorem: Assume $\{(h_\ell, V_\ell) : \ell = 1,2,\dots\}$ is a sequence consisting of finite volume subsets V_ℓ of $\mathbb{R}^3$ with $\lim_{\ell\to\infty} |V_\ell| = \infty$, and positive, injective selfadjoint operators h_ℓ acting on $L^2(V_\ell)$, such that condition (3.1) is satisfied for every $\ell = 1,2,3,\dots$. Suppose further that (we replace the index V_ℓ by ℓ)

$$\lim_{\ell\to\infty} \Lambda_{\ell,\mu}/|V_\ell| = C_\Lambda(\mu) \tag{3.5}$$

$$\lim_{\ell\to\infty} f^o_\ell(\beta,\mu) = f^o(\beta,\mu) \tag{3.6}$$

exist for some $0 < \beta < \infty$, and some $\mu \leq 0$, then

$$\lim_{\ell\to\infty} f_\ell(\beta,\mu;\varepsilon) = f^o(\beta,\mu) - C_\Lambda(\mu) \quad . \tag{3.7}$$

Notice that by (3.4), existence of any two of the three limits (3.5),(3.6)&(3.7) will insure existence of the third one. Furthermore, the above result generalizes upon replacing the two-level system by an arbitrary system as follows. S_1 is replaceable by any bounded selfadjoint operator A ((2.7) still

7) The case $\varepsilon = \varepsilon(V)$ with $|\varepsilon(V)| \leq k|V|$, could also be handled.

holds with ε replaced by $\varepsilon\|A\|$), and S_3 is replaceable by a bounded selfadjoint operator B with purely discrete spectrum (formula (2.4) applied to each eigenspace of B shows that H^o is the direct-sum of operators which are unitarily equivalent to $d\Gamma(h-\mu 1)$ up to certain constants depending on μ and the eigenvalue of B in question); condition (3.5) is then replaced by the existence of the limit of $(\beta|V|)^{-1}\log(\sum \exp(\beta\Lambda_{V,\mu} b_n^2))$, where the sum is over the eigenvalues $\{b_n\}$ of B.

Under differentiability conditions on $f^o(\beta,\mu)$, an application of Griffiths' Lemma ([5],[6]) will prove existence of the thermodynamic limit of the mean internal energy $u_V(\beta,0;\varepsilon)$, and the mean entropy $s_V(\beta,0;\varepsilon)$, or the mean boson-number expectation $n_V(\beta,0;\varepsilon)$ at $\mu=0$. If the Theorem applies in a small neighbourhood of β, at $\mu=0$, and $f^o(\cdot,0)$ is differentiable at β, then:

$$\lim_{\ell\to\infty} u_\ell(\beta,0;\varepsilon) = u^o(\beta,0) - C_\Lambda(0)$$

$$\lim_{\ell\to\infty} s_\ell(\beta,0;\varepsilon) = s^o(\beta,0).$$

The derivative at $\mu=0$ of $\Lambda_{V,\mu}$ is readily computed by using, e.g. the Neumann series for $(h_V-\mu 1)^{-1}$, it equals $\|h_V^{-1}\lambda_V\|^2$. Thus, if the Theorem applies for some β, and small neighbourhood of $\mu=0$, if $f^o(\beta,\cdot)$ is differentiable at $\mu=0$, and if $\lim_{\ell\to\infty} |V_\ell|^{-1}\|h_\ell^{-1}\lambda_\ell\|^2 = C'_\Lambda$ exists, then

$$\lim_{\ell\to\infty} n_\ell(\beta,0;\varepsilon) = n^o(\beta,0) + C'_\Lambda \quad .$$

We return to the specific model considered in the introduction. The two polarizations do not interact; for each one of these, the one-particle hamiltonian is $h_\ell = c(-\Delta)^{1/2}$, where Δ is the Dirichlet-Lapalcian on $V_\ell = [-\ell/2, \ell/2]^3$. Disregarding the possibility of different "chemical potentials" for the polarizations, we obtain

$$\lim_{\ell\to\infty} f_\ell(\beta,\mu;\mathcal{E}) = 2f^0(\beta,\mu) \quad ,$$

since due to (1.2), $C_\Lambda(\mu)=0$ for all $\mu \leq 0$. The factor 2 comes from the two polarizations, and $f^0(\beta,\mu) = \lim_{\ell\to\infty} f^0_\ell(\beta,\mu)$, where

$$\begin{aligned} f^0_\ell(\beta,\mu) &= (-\beta\ell^3)^{-1}\log[\mathrm{Tr}(\exp\{-\beta d\Gamma(h_\ell - \mu 1)\})] \\ &= 3\beta^{-1}\ell^{-3} \sum_{\underline{n}\in Z^3\setminus\{0\}} \log(1-\exp\{-\beta(\omega_{\underline{n}}(\ell)-\mu)\}) . \end{aligned}$$

By standard arguments for Riemann approximation of integrals,

$$\begin{aligned} f^0(\beta,\mu) &= (3/2\pi^2)\beta^{-1} \int_0^\infty r^2 \log(1-\exp^{-\beta(cr-\mu)})\, dr \\ &= -(3/\pi^2)\, c^{-3}\beta^{-4} \sum_{n\geq 1} n^{-4}\, e^{\beta\mu n} \quad . \end{aligned}$$

Differentiating with respect to β (resp. μ) at $\mu=0$,

$$u^0(\beta,0) = -3\ f^0(\beta,0) \quad , \quad s^0(\beta,0) = -4k\ f^0(\beta,0) \quad ,$$

$$\begin{aligned} n^0(\beta,0) &= (3/2\pi^2) \int_0^\infty r^2 e^{-\beta cr}(1-e^{-\beta cr})^{-1}\, dr \\ &= (3/\pi^2)\, c^{-3}\beta^{-3} \sum_{n\geq 1} n^{-3} \quad . \end{aligned}$$

It follows that,

$$\lim_{\ell\to\infty} u_\ell(\beta,0;\mathcal{E}) = 2u^0(\beta,0) \quad , \quad \lim_{\ell\to\infty} s_\ell(\beta,0;\ ) = 2s^0(\beta,0) \quad .$$

It remains to discuss the limit of $|V_\ell|^{-1}\, \| h_\ell^{-1}\lambda_\ell \|^2$. Pfeifer ([1]), shows that $\lim_{\ell\to\infty} \|\lambda_\ell\|^2$ exists. We have $\|h_\ell^{-1}\| = (\min\{\omega_{\underline{n}}(\ell) : \underline{n} \in Z^3\setminus\{0\}\})^{-1} = (2\sqrt{3}\,\pi c)^{-1}\ell$; thus $\|h_\ell^{-1}\lambda_\ell\|^2 \leq K\ \ell^2\ \|\lambda_\ell\|^2$, with K independent of ℓ. We conclude that $C'_\Lambda = 0$, and thus

$$\lim_{\ell\to\infty} n_\ell(\beta,0;\mathcal{E}) = 2n^0(\beta,0) \quad .$$

In the canonical formalism, the interacting two-level system is thermodynamically fully equivalent to the free radiation field.

References

[1] P. Pfeifer, Chiral molecules - a Superselection Rule Induced by the Radiation Field. Diss ETH No. 6551, ok Gotthard S+D AG, Zurich 1980.

[2] G.A. Raggio, in preparation.

[3] E.B. Davies, Ann. Inst. H. Poincare A35, 149 (1981).

[4] J.M. Cook, J. Math. Phys. 2, 33 (1961).

[5] R.B. Griffiths, J. Math. Phys. 5, 1215 (1964).

[6] J.T. Lewis, and J.V. Pule, *The equivalence of ensembles in statistical mechanics*. In: *Stochastic Analysis and Applications*, Proceedings, Swansea 1983; Lecture Notes in Mathematics 1095, Springer, Berlin 1984.