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The Equilibrium Thermodynamics of a Spin-Boson Model

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We consider the equilibrium thermodynamics of a Dicke-type model for N identical spins of arbitrary magnitude interacting linearly and homogeneously with a boson field in a volume V_N, in the limit $N \to \infty$, $V_N \to \infty$, with $N/V_N = \text{const}$. The system exhibits a second-order phase transition; complete information on the spin polarizations and their correlations is obtained. The proofs use a general result on the free energy of quantum spin systems based on the large deviation principle and the Berezin–Lieb inequalities.

KEY WORDS: Spins coupled to a boson field; Dicke maser model; second-order phase transition; large deviations.

1. INTRODUCTION

In 1954, Dicke[1] introduced the Hamiltonian

$$H_n = \omega a^* a + \varepsilon \sum_{k=1}^{n} S^z_{(k)} + n^{-1/2}\lambda \sum_{k=1}^{n} [a S^+_{(k)} + a^* S^-_{(k)}]$$

as a caricature for a system of n identical atoms, described in a two-level approximation by spin-1/2 operators $\mathbf{S}_{(k)}$, interacting with one mode of the quantized electromagnetic field of frequency ω in the dipole and rotating-wave approximations. The dynamics of the Dicke maser model has since been studied extensively.[2,3]

In 1973 interest in the *thermodynamics* of the Dicke maser model was boosted when Hepp and Lieb[4] gave a rigorous and complete discussion of the thermodynamics of the model and discovered its second-order phase

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transition. Subsequently these authors[5] considered many-mode versions, removing also the rotating-wave approximation:

$$H_n = \sum_{\nu=1}^{M} \omega_n(\nu)\, a_\nu^* a_\nu + \varepsilon \sum_{k=1}^{n} S_{(k)}^z + n^{-1/2} \sum_{\nu=1}^{M} \sum_{k=1}^{n} [\lambda_n(\nu)\, a_\nu^* + \overline{\lambda_n(\nu)}\, a_\nu]\, S_{(k)}^x$$

The approximating Hamiltonian method has been used to study the model and its variations. These studies include models with infinitely many modes,[6,7] arbitrary spins (i.e., not restricted to be of magnitude 1/2), and also models where the coupling constants λ depend on the spin index.[8] Reviews of these results are given in Refs. 9 and 10. The thermodynamic equilibrium states have also been analyzed,[11,12] using the methods of algebraic quantum statistical mechanics.

Here, we consider the equilibrium thermodynamics of the infinitely many-mode model specified by the Hamiltonian

$$H_n = \sum_{\nu\geqslant 1} \omega_n(\nu)\, a_\nu^* a_\nu + \varepsilon \sum_{k=1}^{n} S_{(k)}^z + V_n^{-1/2} \sum_{\nu\geqslant 1} \sum_{k=1}^{n} [\lambda_n(\nu)\, a_\nu^* + \overline{\lambda_n(\nu)}\, a_\nu]\, S_{(k)}^x$$

where the spin operators $\mathbf{S}_{(k)}$ are copies of a spin operator $\mathbf{S}$ of arbitrary magnitude $j = 1/2, 1, 3/2, 2,\ldots$. The quantity V_n is the quantization volume of the boson field, and we will consider the thermodynamic limit where $n \to \infty$, $V_n \to \infty$, but the density of spins $\rho = n/V_n$ remains constant. We assume that the strictly positive frequencies $\{\omega_n(\nu)\colon \nu \geqslant 1\}$ satisfy

$$\sum_{\nu\geqslant 1} e^{-\beta\omega_n(\nu)} < \infty$$

and the complex coupling constants $\{\lambda_n(\nu)\colon \nu \geqslant 1\}$ satisfy

$$\sum_{\nu\geqslant 1} |\lambda_n(\nu)|^2 < \infty$$

These conditions guarantee the self-adjointness of H_n and the finiteness of the associated partition function. The equilibrium thermodynamics of the model is obtained as an application of a general result for quantum spin system,[13] obtained by a combination of large deviation methods and Berezin–Lieb inequalities. Only two conditions are required, namely: the existence of the thermodynamic limit $f^0(\beta) = \lim_{n\to\infty} f_n^0(\beta)$ of the free-energy density $f_n^0(\beta)$ of the free boson field, where

$$\begin{aligned} f_n^0(\beta) &= (-1/\beta V_n) \log \operatorname{trace}_{\text{bosons}} \exp\left[-\beta \sum_{\nu\geqslant 1} \omega_n(\nu)\, a_\nu^* a_\nu\right] \\ &= (1/\beta V_n) \sum_{\nu\geqslant 1} \log\{1 - \exp[-\beta\omega_n(\nu)]\} \end{aligned}$$

and the existence of the limit

$$\Lambda = \lim_{n \to \infty} \sum_{\nu \geqslant 1} \omega_n(\nu)^{-1} |\lambda_n(\nu)|^2$$

Previous results[6] on the infinitely many-mode case were derived under stronger assumptions. The generalization to spins of arbitrary magnitude is of interest because the Hamiltonian H_n describes a system of quantum spins interacting with the quantized electromagnetic field and with an external magnetic field $\mathbf{B} = (0, 0, -\varepsilon)$; in atomic physics, models with two-level atoms are of greatest interest.

Briefly and qualitatively, our results are the following:

Let $\eta = |\varepsilon|/2j\rho\Lambda$; for $\eta \geqslant 1$, the thermodynamic properties of the system are identical with those of the noninteracting system [obtained by setting $\lambda_n(\nu) = 0$, for all n and $\nu \geqslant 1$]; for $\eta < 1$ we recover the second-order phase transition discovered by Hepp and Lieb[4]: there exists a nonzero finite critical temperature T_c depending on $j\,|\varepsilon|$ and η, at which the second derivative of the specific free energy with respect to the temperature is discontinuous.

The following rigorous results appear to be new:

1. The mean spin polarization in the z direction is always dispersion-free; below T_c this polarization is given by $-\varepsilon/2\rho\Lambda$ and is thus independent of the temperature and of the magnitude j of the spins (see Fig. 1).
2. The mean spin polarization in the x direction has nonzero dispersion below T_c (see Fig. 2).
3. There is a spontaneous polarization in the x direction below T_c: perturbing the Hamiltonian H_n by $\alpha \sum S^x_{(k)}$, the mean spin polarization in the x direction is an odd function of α, which does not go to zero as $\alpha \to 0$ for $T < T_c$ when $\eta < 1$ (see Fig. 4).
4. The boson density, as a function of frequency, is equal to the free boson density for $\eta \geqslant 1$, and for $\eta < 1$ when $T \geqslant T_c$; for $\eta < 1$ and $T < T_c$ the difference between the boson density and the free boson density is positive and increases with increasing frequency.

2. THE RESULTS

Let $\mathbf{S} = (S^x, S^y, S^z)$ be spin operators of magnitude $j \in \{1/2, 1, 3/2,...\}$, acting on the $(2j+1)$-dimensional Hilbert space $\mathfrak{D}(j)$, and satisfying the usual commutation relations $[S^x, S^y] = iS^z$ (and cyclic permutations). We let $\mathfrak{K}_n$ be the n-fold $(n = 1, 2, 3,...)$ tensor product of $\mathfrak{D}(j)$, and let

$\mathbf{S}_{(k)}$ $(k=1, 2,..., n)$ be a copy of $\mathbf{S}$ acting on the kth component of $\mathfrak{K}_n$. We set

$$\mathbf{S}_n = \sum_{k=1}^{n} \mathbf{S}_{(k)} \qquad \text{on} \quad \mathfrak{K}_n$$

For each $n=1, 2,...,$ the boson field is specified by the one-particle Hamiltonian $\mathfrak{h}_n$ acting on the Hilbert space $L^2(\mathscr{A}_n)$ where $\mathscr{A}_n$ is a bounded subset of $\mathbb{R}^d$ $(d=1, 2, 3,...)$ of volume (i.e., Lebesgue measure) V_n. The Hamiltonian $\mathfrak{h}_n$ is assumed to be a positive, injective self-adjoint operator such that $\exp(-\beta\mathfrak{h}_n)$ is a trace-class operator for each $\beta > 0$. This implies that $\mathfrak{h}_n$ has a bounded inverse.

The Hamiltonian for the composite system of n spins (of magnitude j) interacting with the boson field is[2]

$$H_n = d\Gamma(\mathfrak{h}_n) \otimes 1 + \varepsilon 1 \otimes S_n^z + V_n^{-1/2}[a^*(\lambda_n) + a(\lambda_n)] \otimes S_n^x \tag{1}$$

on the Hilbert space $\mathfrak{F} \otimes \mathfrak{K}_n$, where $\mathfrak{F}$ is the symmetric Fock space built upon $L^2(\mathscr{A}_n)$, ε is real, and $\lambda_n \in L^2(\mathscr{A}_n)$. Here, $a(\cdot)$ denotes the usual annihilation operator on $\mathfrak{F}$, and $d\Gamma(\cdot)$ is the second-quantization map. It can be easily verified (see Appendix A) that (1) does indeed define a self-adjoint operator with domain equal to that of $d\Gamma(\mathfrak{h}_n) \otimes 1$, and that

$$Z_n(\beta) = \operatorname*{trace}_{\mathfrak{F} \otimes \mathfrak{K}_n} \exp(-\beta H_n)$$

is finite for all $\beta > 0$. We use the notation

$$\langle X \rangle_n = Z_n(\beta)^{-1} \operatorname*{trace}_{\mathfrak{F} \otimes \mathfrak{K}_n} [\exp(-\beta H_n)\, X]$$

The Hamiltonian H_n has a symmetry which we will exploit: Let U be the unique unitary operator on $\mathfrak{D}(j)$ such that

$$U^* S^x U = -S^x, \qquad U^* S^y U = -S^y, \qquad U^* S^z U = S^z$$

Let $U_{(k)}$ denote a copy of U acting on the kth component of $\mathfrak{K}_n$; then the unitary operator on $\mathfrak{F} \otimes \mathfrak{K}_n$ given by

$$U_n = \Gamma(-1) \otimes \left(\prod_{k=1}^{n} U_{(k)} \right)$$

[2] Since $\mathfrak{h}_n$ has a spectrum consisting entirely of eigenvalues $\{\omega_n(v): v \geqslant 1\}$ of finite multiplicity, this is a rewriting of the infinite-mode Hamiltonian of Section 1; $\{\lambda_n(v): v \geqslant 1\}$ are the expansion coefficients of λ_n in an eigenbasis of $\mathfrak{h}_n$.

satisfies

$$U_n^*(1\otimes S_n^x)\,U_n=-1\otimes S_n^x,\qquad U_n^*(1\otimes S_n^y)\,U_n=-1\otimes S_n^y$$
$$U_n^*(1\otimes S_n^z)\,U_n=1\otimes S_n^z,\qquad U_n^*(d\Gamma(\cdot)\otimes 1)\,U_n=d\Gamma(\cdot)\otimes 1 \tag{2}$$
$$U_n^*(a(\cdot)\otimes 1)\,U_n=-a(\cdot)\otimes 1$$

Hence, we have $[H_n, U_n]=0$.

To obtain information on the spin polarizations and their fluctuations, we consider the family of Hamiltonians $\{K_n(\alpha, \mathbf{t})\colon \alpha\in\mathbb{R}, \mathbf{t}=(t_x, t_y, t_z)\in\mathbb{R}^3\}$ defined by

$$K_n(\alpha, \mathbf{t})=H_n+\alpha 1\otimes S_n^x+n^{-1}1\otimes[t_x(S_n^x)^2+t_y(S_n^y)^2+t_z(S_n^z)^2]$$

We set

$$f_n(\beta, \alpha, \mathbf{t})=(-\beta V_n)^{-1}\log \operatorname*{trace}_{\mathfrak{F}\otimes\mathfrak{K}_n}\exp[-\beta K_n(\alpha, \mathbf{t})]$$

To apply Theorem 3 of Ref. 13,[3] we first notice that, in the terminology of Section 2 of Ref. 13, $K_n(\alpha, \mathbf{t})$ is homogeneously decomposable [see (I2.8)], with

$$K_n(\alpha, \mathbf{t}; J)=d\Gamma(\mathfrak{h}_n)\otimes 1+\varepsilon 1\otimes {}^JS^z+V_n^{-1/2}[a^*(\lambda_n)+a(\lambda_n)]\otimes {}^JS^x$$
$$+\alpha 1\otimes {}^JS^x+n^{-1}1\otimes[t_x({}^JS^x)^2+t_y({}^JS^y)^2+t_z({}^JS^z)^2]$$

where J is an integer (resp. half-integer) less than or equal to the integer (resp. half-integer) nj. The lower and upper symbols of $K_n(\alpha, \mathbf{t}; J)$ are the operators on $\mathfrak{F}$ given (see table on p. 330 of Ref. 14, or Appendix 3 of Ref. 13), respectively, by [$\mathbf{e}=(x, y, z)$, $x^2+y^2+z^2=1$, is in the unit sphere $S^2\subset\mathbb{R}^3$]:

$$K_n^l(\alpha, \mathbf{t}; J, \mathbf{e})=d\Gamma(\mathfrak{h}_n)+\varepsilon Jz1+V_n^{-1/2}Jx[a^*(\lambda_n)+a(\lambda_n)]$$
$$+\alpha Jx1+n^{-1}J(J-\tfrac{1}{2})(t_xx^2+t_yy^2+t_zz^2)\,1$$
$$+(J/2n)(t_x+t_y+t_z)\,1$$
$$K_n^u(\alpha, \mathbf{t}; J, \mathbf{e})=d\Gamma(\mathfrak{h}_n)+\varepsilon(J+1)\,z1+V_n^{-1/2}(J+1)\,x[a^*(\lambda_n)+a(\lambda_n)]$$
$$+\alpha(J+1)\,x1+n^{-1}(J+1)(J+\tfrac{3}{2})(t_xx^2+t_yy^2+t_zz^2)\,1$$
$$-[(J+1)/2n](t_x+t_y+t_z)\,1$$

[3] The equation $(x\cdot y)$ of Ref. 13 will be referred to as $(Ix\cdot y)$.

The corresponding "lower", and "upper" semiclassical free energies defined by (I4.8) and (I4.9) are easily computed to be

$$\underset{\sim}{f}{}_n^j(\beta, \alpha, \mathbf{t}; J/nj, \mathbf{e})$$
$$\equiv (-\beta n)^{-1} \log \underset{\mathfrak{F}}{\operatorname{trace}} \exp[-\beta K_n^l(\beta, \alpha, \mathbf{t}; J, \mathbf{e})]$$
$$= \rho^{-1} f_n^0(\beta) - \rho A_n (J/n)^2 x^2 + \varepsilon(J/n) z + \alpha(J/n) x$$
$$+ n^{-2} J(J - \tfrac{1}{2})(t_x x^2 + t_y y^2 + t_z z^2) + (J/2n^2)(t_x + t_y + t_z) \tag{3a}$$
$$\tilde{f}{}_n^j(\beta, \alpha, \mathbf{t}; J/nj, \mathbf{e})$$
$$\equiv (-\beta n)^{-1} \log \underset{\mathfrak{F}}{\operatorname{trace}} \exp[-\beta K_n^u(\alpha, \mathbf{t}; J, \mathbf{e})]$$
$$= \rho^{-1} f_n^0(\beta) - \rho A_n[(J+1)/n]^2 x^2 + \varepsilon[(J+1)/n] z + \alpha[(J+1)/n] x$$
$$+ n^{-2}(J+1)(J+\tfrac{3}{2})(t_x x^2 + t_y y^2 + t_z z^2)$$
$$- [(J+1)/2n^2](t_x + t_y + t_z) \tag{3b}$$

where

$$f_n^0(\beta) = (-\beta V_n) \log \underset{\mathfrak{F}}{\operatorname{trace}} \exp[-\beta d\Gamma(\mathfrak{h}_n)]$$

is the free energy density of the free boson field, and

$$A_n = \|\mathfrak{h}_n^{-1/2} \lambda_n\|^2 = \langle \lambda_n, \mathfrak{h}_n^{-1} \lambda_n \rangle$$

For $u \in [0, 1]$, let

$$\underset{\sim}{f}{}_n^j(\beta, \alpha, \mathbf{t}; u, \mathbf{e})$$
$$= \rho^{-1} f_n^0(\beta) - \rho A_n j^2 u^2 x^2 + \varepsilon j u z + \alpha j u x$$
$$+ j^2 u^2 (t_x x^2 + t_y y^2 + t_z z^2)$$
$$+ (j/2n)\, u[t_x(1 - x^2) + t_y(1 - y^2) + t_z(1 - z^2)]$$
$$\tilde{f}{}_n^j(\beta, \alpha, \mathbf{t}; u, \mathbf{e})$$
$$= \rho^{-1} f_n^0(\beta) - \rho A_n j^2 u^2 x^2 + \varepsilon j u z + \alpha j u x$$
$$+ j^2 u^2 (t_x x^2 + t_y y^2 + t_z z^2)$$
$$- \rho A_n[(2unj + 1)/n^2]\, x^2 + \varepsilon(z/n) + \alpha(x/n)$$
$$+ [(5nju + 3)/2n^2](t_x x^2 + t_y y^2 + t_z z^2)$$
$$- [(nju + 1)/2n^2](t_x + t_y + t_z)$$

Then, $\underset{\sim}{f}{}_n^j(\beta, \alpha, \mathbf{t}; \cdot)$ and $\tilde{f}_n^j(\beta, \alpha, \mathbf{t}; \cdot)$ are continuous functions on $[0, 1] \times S^2$, coinciding with (3a) and (3b), respectively, for all $u = J/nj$, and converging uniformly to

$$f^j(\beta, \alpha, \mathbf{t}; u, \mathbf{e}) = \rho^{-1} f^0(\beta) - \rho \Lambda j^2 u^2 x^2 + \varepsilon j u z + \alpha j u x \\ + j^2 u^2 (t_x x^2 + t_y y^2 + t_z z^2)$$

if

$$f^0(\beta) = \lim_{V_n \to \infty} f_n^0(\beta) \qquad \text{and} \qquad \Lambda = \lim_{n \to \infty} \Lambda_n \tag{4}$$

both exist.

This verifies the conditions of Theorem 3 of Ref. 13, and proves the following result:

Theorem. If condition (4) is met for some $\beta > 0$, then

$$\lim_{\substack{n \to \infty \\ \rho = \text{const}}} f_n(\beta, \alpha, \mathbf{t}) = f(\beta, \alpha, \mathbf{t})$$

exists and is given by

$$f(\beta, \alpha, \mathbf{t}) = f^0(\beta) + \rho \inf_{u \in [0,1]} \inf_{\mathbf{e} \in S^2} [\varphi^j(\varepsilon, \alpha, \mathbf{t}; u, \mathbf{e}) - \beta^{-1} I^j(u)]$$

where

$$\varphi^j(\varepsilon, \alpha, \mathbf{t}; u, \mathbf{e}) = j\varepsilon u z + j\alpha u x + j^2 u^2 [(t_x - \rho\Lambda)\, x^2 + t_y y^2 + t_z z^2]$$

and[4]

$$I^j(u) = \inf_{a \geq 0} \left\{ \log \frac{\sinh[a(2j+1)/2j]}{\sinh(a/2j)} - au \right\}, \qquad u \in [0, 1] \tag{5}$$

We define the mean free energy f_n by[5]

$$f_n(\beta) = (-\beta V_n)^{-1} \log Z_n(\beta)$$

the mean spin-polarization vector $\mathbf{P}_n$ by

$$\mathbf{P}_n(\beta) = n^{-1} \langle 1 \otimes \mathbf{S}_n \rangle_n$$

[4] This function is denoted by I_0^j in Ref. 13.

[5] All the following quantities depend on the density ρ and on j, but we avoid overloading the notation.

and the (Hermitian, 3×3) two-correlation matrix $\mathfrak{D}_n$ by

$$\mathfrak{D}_n^{a,b}(\beta) = n^{-2}(\langle 1 \otimes S_n^a S_n^b \rangle_n - \langle 1 \otimes S_n^a \rangle_n \langle 1 \otimes S_n^b \rangle_n), \qquad a, b \in \{x, y, z\}$$

By (2), the x and y components of $\mathbf{P}_n$ are both zero. Moreover,

$$f_n(\beta) = f_n(\beta, 0, \mathbf{0}) \tag{6}$$

$$P_n^z(\beta) = \rho^{-1}(\partial f_n/\partial \varepsilon)(\beta) \tag{7}$$

$$\mathfrak{D}_n^{aa}(\beta) = \rho^{-1}(\partial f_n/\partial t_a)(\beta, 0; \mathbf{0}) - P_n^a(\beta)^2, \qquad a \in \{x, y, z\} \tag{8}$$

To proceed, we assume that condition (4) is met for every $\beta > 0$, and that $\Lambda > 0$.[6] The solution of the variational problem obtained in the theorem when at most one of the four real parameters α, $\mathbf{t}$ is not zero is quite straightforward; we comment on this in Appendix B. The essential ingredient is the strict concavity of the function $I^j(\cdot)$, which is differentiable on $(0, 1)$ with strictly decreasing derivative $(I^j)'$ satisfying

$$\lim_{u \downarrow 0} (I^j)'(u) = 0, \qquad \text{and} \qquad \lim_{u \uparrow 1} (I^j)' = -\infty$$

We first identify a *critical spin density*

$$\rho_c = |\varepsilon|/2j\Lambda$$

and a j- and density-dependent, *critical reciprocal temperature*[7]

$$\beta_c := \begin{cases} +\infty & \text{if} \quad \rho \leqslant \rho_c \\ (-j\,|\varepsilon|)^{-1}(I^j)'\,(|\varepsilon|/2j\Lambda\rho) & \text{if} \quad \rho > \rho_c \end{cases}$$

For every $\beta > 0$, the equation

$$j\,|\varepsilon| + \beta^{-1}(I^j)'(u) = 0, \qquad u \in [0, 1]$$

admits a unique solution $\mu(\beta)$.[8] The function $\mu(\cdot)$ is increasing and continuous on $(0, \infty)$ with $\lim_{\beta \downarrow 0} \mu(\beta) = 0$ and $\lim_{\beta \uparrow \infty} \mu(\beta) = 1$ when $\varepsilon \neq 0$. If $\rho > \rho_c$, then for every $\beta \geqslant \beta_c$, the equation

$$2j^2\rho\Lambda u + \beta^{-1}(I^j)'(u) = 0, \qquad u \in [0, 1]$$

admits a unique *nonzero* solution $\xi(\beta)$. The function $\xi(\cdot)$ is increasing and

[6] $\Lambda \geqslant 0$ by definition; if $\Lambda = 0$, then the system is thermodynamically equivalent to the non-interacting system obtained by setting $\lambda_n = 0$ in the Hamiltonian.

[7] If $\varepsilon = 0$, then $\rho_c = 0$ and $\beta_c = 3/2j(j+1)\,\rho\Lambda$. All our results are correct also in the case $\varepsilon = 0$.

[8] Set $\mu(\beta) = 0$ if $\varepsilon = 0$.

continuous on $[\beta_c, \infty)$ and satisfies $\xi(\beta_c) = |\varepsilon|/2j\Lambda\rho$, $\lim_{\beta\uparrow\infty} \xi(\beta) = 1$. We let

$$\eta = |\varepsilon|/2j\rho\Lambda$$

The quantity η acts as an order parameter: $\eta \geqslant 1$ for $\rho \leqslant \rho_c$, and $\eta < 1$ for $\rho > \rho_c$.

When $j = 1/2$ the above can be made more explicit, since

$$I^{1/2}(u) = -\tfrac{1}{2}(1+u)\log[\tfrac{1}{2}(1+u)] - \tfrac{1}{2}(1-u)\log[\tfrac{1}{2}(1-u)]$$
$$(I^{1/2})'(u) = -\tfrac{1}{2}\log[(1+u)/(1-u)] = -\operatorname{arctanh}(u)$$

One has $\rho_c = |\varepsilon|/\rho\Lambda$, $\beta_c = (2/|\varepsilon|)\operatorname{arctanh}(|\varepsilon|/\rho\Lambda)$ for $\rho > \rho_c$,

$$\mu(\beta) = \tanh(\tfrac{1}{2}\beta\,|\varepsilon|)$$

and ξ is the solution of

$$u = \tanh(\tfrac{1}{2}\beta\rho\Lambda u), \qquad \beta > \beta_c$$

2.1. The Free Energy and Entropy Densities

We use (6). The solution of the variational problem for $\alpha = 0$, $\mathbf{t} = \mathbf{0}$, is discussed in Appendix B; the result is[9]

$$\Delta f(\beta) = -\rho \begin{cases} j\,|\varepsilon|\,\mu(\beta) + \beta^{-1} I^j(\mu(\beta)) & \text{for} \quad \beta \leqslant \beta_c \\ j^2\rho\Lambda[\xi(\beta)^2 + \eta^2] + \beta^{-1} I^j(\xi(\beta)) & \text{for} \quad \beta > \beta_c \end{cases}$$

For $j = \frac{1}{2}$, this reads

$$\Delta f(\beta) = -\rho\beta^{-1}\log[2\cosh(\tfrac{1}{2}\beta\varepsilon)] \qquad \beta \leqslant \beta_c$$
$$\Delta f(\beta) = -\rho\beta^{-1}\log\{2\cosh[\tfrac{1}{2}\beta\rho\Lambda\xi(\beta)]\} + \tfrac{1}{4}\rho^2\Lambda[\xi(\beta)^2 - (\varepsilon/\rho\Lambda)^2], \qquad \beta > \beta_c$$

The entropy density s is given by $k\beta^2\,\partial f/\partial\beta$; we obtain

$$\Delta s(\beta) = k\rho \begin{cases} I^j(\mu(\beta)) & \text{for} \quad \beta \leqslant \beta_c \\ I^j(\xi(\beta)) & \text{for} \quad \beta > \beta_c \end{cases}$$

We recover, but for infinitely many boson modes and arbitrary spins, the second-order phase transition discovered by Hepp and Lieb[(4)]: The second derivative of Δf is discontinuous at β_c. Notice also that Δf does not depend on the coupling (i.e., on Λ) above the critical temperature, this being always the case if the density is below the critical density.

[9] Here and in what follows Δ denotes the excess with respect to the free boson field; e.g., $\Delta f = f - f^0$.

2.2. The Spin Polarizations and Their Fluctuations

We have already remarked that P^x and P^y are both zero; to compute P^z, we use (7), verify that $f(\beta)$ is differentiable with respect to ε, and use Griffiths' lemma (see, e.g., Lemma 1 in the Appendix of Ref. 5) on the sequence $f_n(\beta)$ of functions which are concave in ε. We obtain

$$P^z(\beta) = \begin{cases} -j\,\mathrm{sgn}(\varepsilon)\,\mu(\beta) & \text{for} \quad \beta \leqslant \beta_c \\ -\varepsilon/2\rho\Lambda & \text{for} \quad \beta > \beta_c \end{cases}$$

P^z is a continuous function of β with a discontinuous derivative at β_c. Notice that below the critical temperature, P^z is *independent of the temperature and of the spin magnitude j.* Figure 1 shows P^z for $j = \frac{1}{2}$.[10]

To obtain the dispersions $\mathfrak{D}^{aa}$ $(a = x, y, z)$, we use (8); the functions $f_n(\beta, \alpha, \mathbf{t})$ are concave in the components of $\mathbf{t}$. We set $\alpha = 0$ and all components of $\mathbf{t}$ equal to zero except t_a in the variational problem of the

[10] $P^z(\beta) = -\frac{1}{2}\tanh(\frac{1}{2}\beta\varepsilon)$ for $\beta \leqslant \beta_c$ and $-\frac{1}{2}\varepsilon/\rho\Lambda$ for $\beta > \beta_c$.

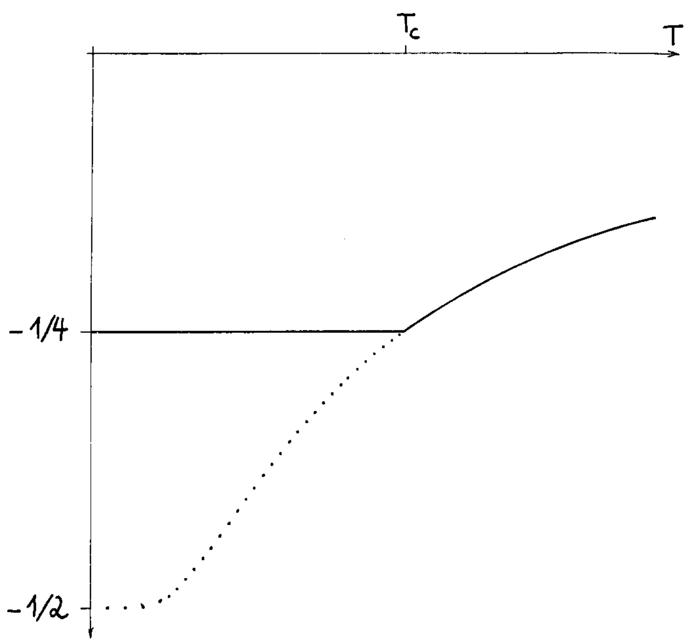

Fig. 1. Plot of P^z versus T for $j = \frac{1}{2}$ and $\varepsilon = 1$. $(\cdots)$ $\eta \geqslant 1$; (—) $\eta = \frac{1}{2}$ $[kT_c = (2\,\mathrm{arctanh}\,\frac{1}{2})^{-1} \simeq 0.910]$.

theorem, then verify differentiability with respect to t_a, and use Griffiths' lemma. The results are

$$\mathfrak{D}^{yy}(\beta) = \mathfrak{D}^{zz}(\beta) = 0$$

$$\mathfrak{D}^{xx}(\beta) = \begin{cases} 0 & \text{for} \quad \beta \leqslant \beta_c \\ j^2[\xi(\beta)^2 - \eta^2] & \text{for} \quad \beta > \beta_c \end{cases}$$

Figure 2 shows $\mathfrak{D}^{xx}$ for $j = \frac{1}{2}$.[11]

Since the y and z polarizations are dispersion-free, we conclude from the Schwarz inequality for states, that

$$\mathfrak{D}^{ab}(\beta) = 0 \quad \text{for all } \beta > 0$$
$$\text{and all } a, b \in \{x, y, z\} \text{ except } a = b = x$$

With these results, we can compute the limiting value of the energy density $u_n(\beta) = V_n^{-1} \langle H_n \rangle_n$. We obtain

$$\Delta u(\beta) = \rho \varepsilon P^z(\beta) - \rho^2 \Lambda \mathfrak{D}^{xx}(\beta) \tag{9}$$

Figure 3 shows Δu for $j = \frac{1}{2}$.

[11] $\mathfrak{D}^{xx}(\beta) = 0$ for $\beta \leqslant \beta_c$ and $\frac{1}{4}[\xi(\beta) - (\varepsilon/\rho\Lambda)^2]$ for $\beta > \beta_c$.

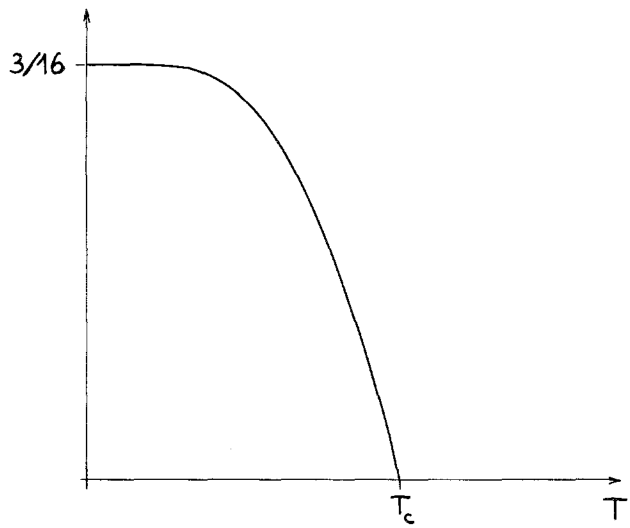

Fig. 2. Plot of $\mathfrak{D}^{xx}$ versus T for $j = \frac{1}{2}$, $\varepsilon = 1$, and $\eta = \frac{1}{2}$ ($kT_c \simeq 0.910$).

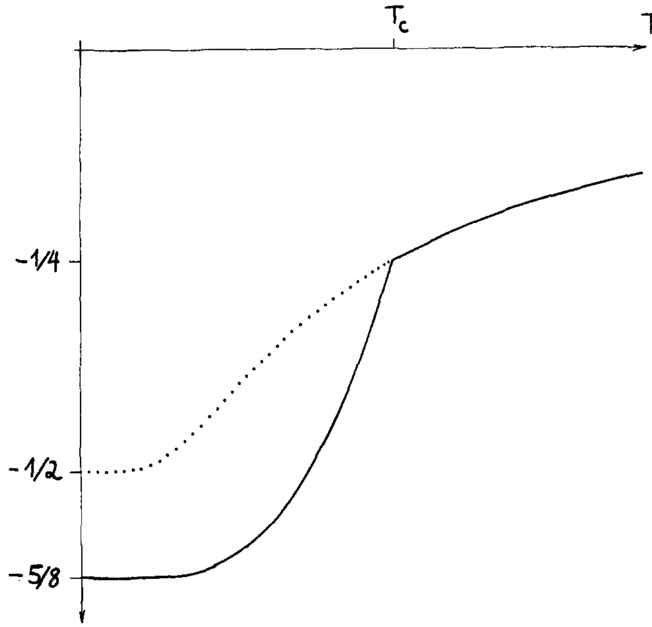

Fig. 3. Plot of $\rho^{-1}\Delta u$ versus T for $j=\frac{1}{2}$ and $\varepsilon=1$. $(\cdots)$ $\eta \geqslant 1$; (—) $\eta=\frac{1}{2}$ ($kT_c \simeq 0.910$).

To make the phase transition more transparent, we consider the x polarization for the Hamiltonian H_n perturbed by $\alpha(1 \otimes S_n^x)$:

$$P_n^x(\beta, \alpha) \equiv n^{-1}\langle 1 \otimes S_n^x \rangle_{K_n(\alpha, \mathbf{0})} = (\partial f_n/\partial \alpha)(\beta, \alpha, \mathbf{0})$$

We find (see Appendix B) that $f(\beta, \cdot, \mathbf{0})$ is a function of $|\alpha|$, and is differentiable on $\mathbb{R}\backslash\{0\}$. For $\beta \leqslant \beta_c$, $\lim_{\alpha \to 0} P^x(\beta, \alpha)=0$; but for $\beta > \beta_c$ [$P^x(\beta, \cdot)$ is odd]

$$-\lim_{\alpha \uparrow 0} P_n^x(\beta, \alpha) = \lim_{\alpha \downarrow 0} P^x(\beta, \alpha) = j[\xi(\beta)^2 - \eta^2]^{1/2}$$

Figure 4 shows P^x for $j=\frac{1}{2}$.

2.3. The Contribution of the Bosons to the Energy

For finite volume, the contribution of the bosons to the energy density is $u_n^b(\beta) = V_n^{-1}\langle d\Gamma(\mathfrak{h}_n) \otimes 1 \rangle_n$. We proceed as before and let $g_n(\beta, \gamma)$ be the specific free energy for the Hamiltonian obtained from H_n by multiplying $\mathfrak{h}_n$ with $\gamma > 0$. We have

$$u_n^b(\beta) = (\partial g_n/\partial \gamma)(\beta, 1) \tag{10}$$

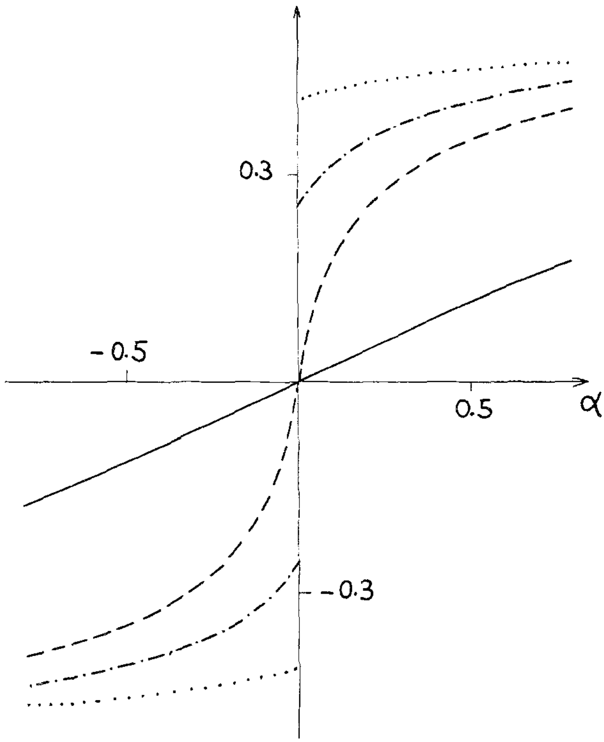

Fig. 4. Plot of P^x versus α for $j=\frac{1}{2}$, $\varepsilon=1$, and $\eta=\frac{1}{2}$ ($kT_c \simeq 0.910$). (···) $kT=0.5$ (-·-) $kT=0.8$; (- -) $kT=1$; (—) $kT=2$.

We have already computed the limit $g(\beta, \gamma)$ of $g_n(\beta, \gamma)$; by concavity of g_n in γ, we obtain from (10) that

$$\Delta u^b(\beta) = \rho^2 \Lambda \mathfrak{D}^{xx}(\beta) \tag{11}$$

Combining (11) and (9), we obtain

$$\lim_{\substack{n \to \infty \\ \rho = \text{const}}} V_n^{-3/2} \langle [a^*(\lambda_n) + a(\lambda_n)] \otimes S_n^x \rangle_n = -2\rho^2 \Lambda \mathfrak{D}^{xx}(\beta) \tag{12}$$

We see that (12) factorizes to

$$\lim_{\substack{n \to \infty \\ \rho = \text{const}}} V_n^{-1/2} \langle [a^*(\lambda_n) + a(\lambda_n)] \otimes 1 \rangle_n \lim_{\substack{n \to \infty \\ \rho = \text{const}}} V_n^{-1} \langle 1 \otimes S_n^x \rangle_n \quad (\equiv 0)$$

for $\beta \leqslant \beta_c$ but *does not factorize for* $\beta > \beta_c$.

2.4. The Boson-Number Density

For $\omega \in [0, \infty]$, let

$$\vartheta_\omega(x) = \begin{cases} 1 & \text{if } x < \omega \\ 0 & \text{if } x \geqslant \omega \end{cases} \qquad (x \in \mathbb{R})$$

The number operator for the bosons of energy strictly less than ω is given by

$$N_n(\omega) = d\Gamma(\vartheta_\omega(\mathfrak{h}_n))$$

Notice that $N_n(0) = 0$ and $N_n(\infty) = N_n$ is the total boson number operator. Consider the number density for the bosons of energy strictly less than ω:

$$\sigma_n(\beta; \omega) = V_n^{-1} \langle N_n(\omega) \otimes 1 \rangle_n$$

Introducing the auxiliary Hamiltonian

$$M_n(\mu; \omega) = H_n - \mu N_n(\omega) \otimes 1, \qquad \mu \leqslant 0$$

and the associated "pressure"

$$p_n(\beta, \mu; \omega) = (\beta V_n)^{-1} \log \operatorname*{trace}_{\mathfrak{F} \otimes \mathfrak{K}_n} \exp[-\beta M_n(\mu; \omega)]$$

we have

$$\sigma_n(\beta; \omega) = (\partial p_n / \partial \mu)(\beta, 0; \omega) \tag{13}$$

Since $M_n(\mu; \omega)$ is obtained from H_n by replacing $\mathfrak{h}_n$ by $\mathfrak{h}_n - \mu \vartheta_\omega(\mathfrak{h}_n)$, which is again a strictly positive self-adjoint operator, we may apply the theorem, replacing Λ_n by

$$\Lambda_n(\mu; \omega) = \langle \lambda_n, [\mathfrak{h}_n - \mu \vartheta_\omega(\mathfrak{h}_n)]^{-1} \lambda_n \rangle$$

and thus condition (4) by

$$p^0(\beta, \mu; \omega) = \lim_{n \to \infty} (\beta V_n)^{-1} \log \operatorname*{trace}_{\mathfrak{F}} \exp\{-\beta [d\Gamma(\mathfrak{h}_n) - \mu N_n(\omega)]\}$$

$$\Lambda(\mu; \omega) = \lim_{n \to \infty} \Lambda_n(\mu; \omega)$$

both exist. This guarantees the existence of $p(\beta, \mu; \omega)$, and gives us a variational formula for $\Delta p(\beta, \mu; \omega)$:

$$\Delta p(\beta, \mu; \omega) = \rho \sup_{u \in [0,1]} \sup_{\mathbf{e} \in S^2} [-j\varepsilon uz + j^2 \rho \Lambda(\mu; \omega)\, u^2 x^2 + \beta^{-1} I^j(u)]$$

In order to proceed, we disregard the subtleties, which could appear already for free bosons (see Ref. 15), and *assume that* $\sigma(\beta;\omega)$ *exists* (for some $\beta>0$ and $\omega>0$). We also assume that $p^0(\beta,\cdot;\omega)$ and $\Lambda(\cdot;\omega)$ exist for μ in an arbitrarily small interval $[-a, 0]$, $a>0$. By convexity,[12] these functions are continuous in the open interval $(-a, 0)$. We suppose that they are continuous from the left at $\mu=0$. Finally, we assume that $\Lambda(\cdot;\omega)$ is differentiable in $(-a, 0)$ with derivative $\Lambda'(\cdot;\omega)$ and that

$$\lim_{\mu\uparrow 0} \Lambda'(\mu;\omega)=\Lambda'(\omega)$$

exists. Solving the variational problem and using (13), we can now claim

$$\Delta\sigma(\beta;\omega)=\rho^2\mathfrak{D}^{xx}(\beta)\,\Lambda'(\omega)$$

We observe a (positive) contribution from the spins to the boson number density only below the critical temperature, and this contribution is nondecreasing in ω.

APPENDIX A

For completeness, we comment on the self-adjointness of the Hamiltonian H_n defined by (1). We drop the index n. Assuming that $\exp(-\beta\mathfrak{h})$ is trace-class, we could proceed by rewriting H in the form of Section 1; we consider the general case where $\mathfrak{h}$ is assumed to be positive and injective (i.e., $\mathfrak{h}^{-1}$ exists), and λ lies in the domain of $\mathfrak{h}^{-1/2}$

Lemma. Let $\mathfrak{h}$ be a positive, injective self-adjoint operator on the Hilbert space $\mathfrak{h}$; let $\lambda\in\mathrm{Dom}(\mathfrak{h}^{-1/2})$ and set $\Lambda=\|\mathfrak{h}^{-1/2}\lambda\|^2$. For complex c, the operator

$$\mathscr{H}=d\Gamma(\mathfrak{h})+ca^*(\lambda)+\bar{c}a(\lambda)$$

on the symmetric Fock space built upon $\mathfrak{h}$ is self-adjoint on $\mathrm{Dom}(d\Gamma(\mathfrak{h}))$, and bounded below by $-|c|^2\Lambda$. If, more restrictively,[13] $\lambda\in\mathrm{Dom}(\mathfrak{h}^{-1})$, then

$$\mathscr{H}=W(-c\mathfrak{h}^{-1}\lambda)\,d\Gamma(\mathfrak{h})\,W(c\mathfrak{h}^{-1}\lambda)-|c|^2\Lambda 1$$

where the unitary operator W is given by

$$W(f)=\exp[\overline{a^*(f)-a(f)}],\qquad f\in\mathfrak{h}$$

[12] It is easily seen that $\Lambda_n(\cdot;\omega)$ is convex and nondecreasing.

[13] Recall that $\mathrm{Dom}(\mathfrak{h}^{-1})$ is a core for $\mathfrak{h}^{-1/2}$.

Proof. The obvious operator inequality $|\mathfrak{h}^{-1/2}\lambda\rangle\langle\mathfrak{h}^{-1/2}\lambda| \leqslant \Lambda 1$ entails $|\lambda\rangle\langle\lambda| \leqslant \Lambda\mathfrak{h}$, which in turn implies that $a^*(\lambda)\, a(\lambda) \leqslant \Lambda d\Gamma(\mathfrak{h})$. From this one concludes that for $f \in \mathrm{Dom}(d\Gamma(\mathfrak{h}))$,

$$\|[a^*(\lambda) + a(\lambda)]\, f\| \leqslant a\, \|d\Gamma(\mathfrak{h})\, f\| + (\Lambda a^{-1} + \|\lambda\|)\, \|f\| \qquad \text{for all } 0 < a < 1$$

The Kato–Rellich theorem then establishes the self-adjointness claim. Moreover, if $\lambda \neq 0$,

$$\begin{aligned} \mathscr{H} &\geqslant \Lambda^{-1} a^*(\lambda)\, a(\lambda) + c a^*(\lambda) + \bar{c} a(\lambda) \\ &= \Lambda^{-1}[a(\lambda) + c\Lambda]^*[a(\lambda) + c\Lambda] - |c|^2\, \Lambda \end{aligned}$$

which gives the lower bound. If $\lambda \in \mathrm{Dom}(\mathfrak{h}^{-1})$, then the claim follows from the quadratures formula[16]:

$$W(f)^*\, d\Gamma(\mathfrak{h})\, W(f) = d\Gamma(\mathfrak{h}) + a^*(\mathfrak{h} f) + a(\mathfrak{h} f) + \langle f, \mathfrak{h} f\rangle, \quad f \in \mathrm{Dom}(\mathfrak{h}) \quad \blacksquare$$

Consider H ($\equiv H_n$); it suffices to consider $H^0 = H - \varepsilon(1 \otimes S_n^z)$, since H is a bounded perturbation of H^0. The spectrum of S_n^x consists of simple eigenvalues $\{E(k)\colon k = 1, 2,..., (2j+1)^n \equiv N\}$; let $P(k)$ denote the associated spectral projections. We may then write

$$H^0 = \sum_{k=1}^{N} \{d\Gamma(\mathfrak{h}) + V^{-1/2} E(k)[a^*(\lambda) + a(\lambda)]\} \otimes P(k)$$

If, then, $\lambda \in \mathrm{Dom}(\mathfrak{h}^{-1/2})$, we conclude from the lemma that H^0 is self-adjoint on $\mathrm{Dom}(d\Gamma(\mathfrak{h}) \otimes 1)$ and bounded below by

$$-(\Lambda/V) \sum_{k=1}^{N} E(k)^2[1 \otimes P(k)] = -(\Lambda/V)\, 1 \otimes (S_n^x)^2$$

which is in turn bounded below by $-(\Lambda n^2 j^2/V)$.

If $\lambda \in \mathrm{Dom}(\mathfrak{h}^{-1})$, then we have

$$H^0 = U^*[d\Gamma(\mathfrak{h}) \otimes 1]\, U - (\Lambda/V)[1 \otimes (S_n^x)^2]$$

where the unitary U is given by

$$U = \sum_{k=1}^{N} W(V^{-1/2} E(k)\, \mathfrak{h}^{-1}\lambda) \otimes P(k)$$

Finally, if $\exp(-\beta\mathfrak{h})$ is trace-class, then so is $\exp[-\beta d\Gamma(\mathfrak{h})]$; since $\mathfrak{h}^{-1}$ is bounded, the above formulas combined with, say, the Golden–Thompson inequality show that $\exp(-\beta H)$ is trace-class.

APPENDIX B

We comment briefly on the solution of the variational problem obtained in the theorem. We give some details only in the case $\mathbf{t}=\mathbf{0}$.

The I^j defined by (5) is clearly concave and decreasing. Moreover, I^j is differentiable in (0, 1) with derivative $(I^j)'$ given by

$$(I^j)'(u) = -a(u), \qquad u \in (0, 1)$$

where $a(u)$ is the unique positive solution of the equation

$$[(2j+1)/2j] \coth[a(2j+1)/2j] - (1/2j) \coth(a/2j) = u$$

$(I^j)'$ is strictly decreasing, negative, with $\lim_{u \downarrow 0} (I^j)'(u) = 0$ and $\lim_{u \uparrow 1} (I^j)'(u) = -\infty$. One has $I^j(0) = \log(2j+1)$, $I^j(1) = 0$, and

$$I^j(u) = -ua(u) + \log \frac{\sinh[a(u)(2j+1)/2j]}{\sinh[a(u)/2j]}$$

Moreover, $(I^j)'$ behaves as $[-3j/(j+1)]\, u$ when $u \downarrow 0$, and $\lim_{u \downarrow 0} (I^j)''(u) = -3j/(j+1)$.

Let

$$\mathscr{S}(\varepsilon, \alpha, \beta) \equiv \sup_{u \in [0,1]} \sup_{\mathbf{e} \in S^2} [\beta^{-1} I^j(u) - ju(\varepsilon z + \alpha x) + j^2 \rho \Lambda u^2 x^2]$$

where ε and α are real, $\rho\Lambda > 0$, and $\beta > 0$. Clearly,

$$\mathscr{S}(\varepsilon, \alpha, \beta) = \sup_{u,z \in (0,1)} [\beta^{-1} I^j(u) + M^j(u, z)]$$

where the function M^j on $(0, 1) \times (0, 1)$ is defined as

$$M^j(u, z) = ju[|\varepsilon|\, z + |\alpha|\, (1-z^2)^{1/2}] + j^2 \rho \Lambda u^2 (1-z^2)$$

The derivative of $M^j(u, \cdot)$ with respect to z is [notice that we are now working in the *open* interval (0, 1)]

$$M^j_z(u, z) = ju[|\varepsilon| - |\alpha|\, z(1-z^2)^{-1/2} - 2j\rho\Lambda uz]$$

We discuss the solutions z of $M^j_z(u, z) = 0$. If $\varepsilon = 0$, then $M^j_z(u, \cdot) < 0$. If $\varepsilon \neq 0$, $\alpha = 0$, then $M^j_z(u, \cdot) > 0$ if $|\varepsilon| \geqslant 2j\rho\Lambda u$, and if $|\varepsilon| < 2j\rho\Lambda u$, then $M^j_z(u, z) = 0$ if $z = (|\varepsilon|/2j\rho\Lambda u)$. If ε and α are not zero, then there is a *unique* solution, which we denote by $\zeta(u; \varepsilon, \alpha)$. We verify that

$$\zeta(u; \varepsilon, \alpha) \leqslant \min\{(|\varepsilon|/2j\rho\Lambda u),\ |\varepsilon|/(\varepsilon^2 + \alpha^2)^{1/2}\}$$

and that

$$\lim_{u\downarrow 0} \xi(u, \varepsilon, \alpha) = |\varepsilon|/(\varepsilon^2+\alpha^2)^{1/2}, \qquad \lim_{\varepsilon\to 0} \zeta(u, \varepsilon, \alpha) = 0$$

$$\lim_{\alpha\to 0} \zeta(u, \varepsilon, \alpha) = \begin{cases} |\varepsilon|/2j\rho\Lambda u & \text{if} \quad u \geqslant |\varepsilon|/2j\rho\Lambda \\ 1 & \text{if} \quad u \leqslant |\varepsilon|/2j\rho\Lambda \end{cases}$$

We *define* $\zeta(u; \varepsilon, \alpha)$ for arbitrary real ε and α using the above limits for $\zeta(u; 0, \alpha)$ and $\zeta(u; \varepsilon, 0)$, and *verify* that indeed

$$\sup_{z\in(0,1)} M^j(u, z) = M^j(u, \zeta(u; \varepsilon, \alpha)) \qquad \text{for all} \quad u \in (0, 1)$$

Moreover, $\zeta(\cdot; \varepsilon, \alpha)$ is decreasing and differentiable, $\zeta(u; \cdot, \alpha)$ is even, increasing in $|\varepsilon|$, and differentiable, and $\zeta(u; \varepsilon, \cdot)$ is even, decreasing in $|\alpha|$, and differentiable.

We can now write

$$\mathscr{S}(\varepsilon, \alpha, \beta) = \sup_{u\in(0,1)} \{\beta^{-1}I^j(u) + M^j(u, \zeta(u; \varepsilon, \alpha))\}$$

The condition for the maximum is then

$$j\,|\varepsilon|\,\zeta(u; \varepsilon, \alpha) + j\,|\alpha|\,[1-\zeta(u; \varepsilon, \alpha)^2]^{1/2} + 2j^2\rho\Lambda u[1-\zeta(u; \varepsilon, \alpha)^2] = -\beta^{-1}(I^j)'(u) \qquad (*)$$

The left-hand side of (*) is a positive, increasing function of u, converging to $j(\varepsilon^2+\alpha^2)^{1/2}$ when $u\downarrow 0$, and having a finite, nonzero limit as $u\uparrow 1$.

If either ε or α is not zero, the properties of $(I^j)'$ imply that (*) has a *unique* solution $\psi \equiv \psi(\varepsilon, \alpha, \beta)$ for every $\beta > 0$. We then verify that $\mathscr{S}(\varepsilon, \alpha, \beta) = \beta^{-1}I^j(\psi) + M^j(\psi, \zeta(\psi; \varepsilon, \alpha))$. It follows that

$$\{\partial\mathscr{S}/\partial\varepsilon\}(\varepsilon, \alpha, \beta) = j\,\mathrm{sgn}(\varepsilon)\,\psi\zeta(\psi; \varepsilon, \alpha)$$

$$\{\partial\mathscr{S}/\partial\alpha\}(\varepsilon, \alpha, \beta) = j\,\mathrm{sgn}(\alpha)\,\psi[1-\zeta(\psi; \varepsilon, \alpha)^2]^{1/2}$$

$$\{\partial\mathscr{S}/\partial\beta\}(\varepsilon, \alpha, \beta) = -\beta^{-2}I^j(\psi)$$

If both ε and α are zero, then (*) reads

$$2j^2\rho\Lambda u = -\beta^{-1}(I^j)'(u) \qquad (**)$$

which, by the properties of $(I^j)'$, admits a solution $\xi(\beta)$ in $(0, 1)$ if and only if

$$2j^2\rho\Lambda > -\beta^{-1}\lim_{u\downarrow 0}(I^j)''(u) = 3\beta^{-1}j/(j+1)$$

We infer that $\beta > \beta_c^0 \equiv 3/2j(j+1)\rho\Lambda$. The function $\xi(\cdot)$ is increasing and continuous on (β_c^0, ∞), with

$$\lim_{\beta \downarrow \beta_c^0} \xi(\beta) = 0 \qquad \text{and} \qquad \lim_{\beta \uparrow \infty} \xi(\beta) = 1$$

We have

$$\mathscr{S}(0, 0, \beta) = \begin{cases} \beta^{-1} I^j(0) & \text{for} \quad \beta \leqslant \beta_c^0 \\ \beta^{-1} I^j(\xi(\beta)) + j^2 \rho\Lambda \xi(\beta)^2 & \text{for} \quad \beta > \beta_c^0 \end{cases}$$

We now discuss the case $\alpha = 0$. We have $\mathscr{S}(\varepsilon, 0, \beta) = \max\{A, B\}$, where [using the definition of $\zeta(u, \varepsilon, 0)$ and $\eta \equiv |\varepsilon|/2j\rho\Lambda$]

$$A \equiv \sup_{u \in [0, \min\{\eta, 1\}]} \{ j\,|\varepsilon|\, u + \beta^{-1} I^j(u) \}$$

$$B \equiv \sup_{u \in (\min\{\eta, 1\}, 1]} \{ (\varepsilon^2/4\rho\Lambda) + j^2 \rho\Lambda u^2 + \beta^{-1} I^j(u) \}$$

Consider A. If $\varepsilon = 0$, then $\eta = 0$ and $A = \beta^{-1} I^j(0)$. Let $\varepsilon \neq 0$; the extremal condition (*) reads

$$j\,|\varepsilon| = -\beta^{-1} (I^j)'(u) \qquad (***)$$

which admits a unique solution $\mu(\beta)$ in (0, 1) for every $\beta > 0$. The function $\mu(\cdot)$ is strictly increasing, and, when $\eta < 1$, $\mu(\beta) \leqslant \eta$ if and only if $\beta \leqslant \beta_c$, where β_c is the solution of $\mu(\beta_c) = \eta$, that is,

$$\beta_c\, j\,|\varepsilon| = -(I^j)'(\eta), \qquad \eta < 1$$

We verify that indeed $\lim_{\varepsilon \to 0} \beta_c = \beta_c^0$. We incorporate the case $\varepsilon = 0$ consistently by putting $\mu(\beta) \equiv 0$ for $\varepsilon = 0$. We have then

$$A = \begin{cases} j\,|\varepsilon|\, \mu(\beta) + \beta^{-1} I^j(\mu(\beta)) & \text{for} \quad \beta \leqslant \beta_c \\ j\,|\varepsilon|\, \eta + \beta^{-1} I^j(\eta) & \text{for} \quad \beta > \beta_c \quad (\text{hence } \eta < 1) \end{cases}$$

Consider B, which does not trivialize only when $\eta < 1$. The extremal condition is then (**), with solutions as discussed previously. Since $u = \eta$ (< 1) solves (**) at β_c, we have $\xi(\beta_c) = \eta$ and $\beta_c \geqslant \beta_c^0$. We may conclude that if $\eta < 1$, then

$$B = \begin{cases} j\,|\varepsilon|\, \eta + \beta^{-1} I^j(\eta) & \text{if} \quad \beta \leqslant \beta_c \\ \varepsilon^2/2\rho\Lambda + j^2\rho\Lambda \xi(\beta)^2 + \beta^{-1} I^j(\xi(\beta)) & \text{if} \quad \beta > \beta_c \end{cases}$$

We conclude that

$$\mathscr{S}(\varepsilon, \alpha, \beta) = \begin{cases} j\,|\varepsilon|\, \mu(\beta) + \beta^{-1} I^j(\mu(\beta)) & \beta \leqslant \beta_c \\ \varepsilon^2/2\rho\Lambda + j^2\rho\Lambda \xi(\beta)^2 + \beta^{-1} I^j(\xi(\beta)) & \beta > \beta_c \end{cases}$$

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