Journal of Statistical Physics, Vol. 53, Nos. 3/4, 1988

The Free Energy of the Spin-Boson Model

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Received February 15, 1988; revision received May 16, 1988

For n spins 1/2 coupled linearly to a boson field in a volume V_n, the existence of the specific free energy is proved in the limit $n \to \infty$, $V_n \to \infty$ with $n/V_n = \text{const}$. The interaction is essentially of the mean field type, in as much as it is proportional to $1/\sqrt{V_n}$; the coupling constants are allowed to be spin dependent. A variational expression is obtained for the limiting specific free energy, and a critical temperature is identified above which the system behaves as if there were no coupling at all.

KEY WORDS: Spins coupled to a boson field; thermodynamics of two-level atoms interacting with radiation; phase transition.

1. INTRODUCTION AND MAIN RESULT

Consider the Hamiltonian

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

for n spins 1/2—described by the spin operators $\{S_{(j)}^\alpha : j = 1, 2,..., n; \alpha = x, y, z\}$, with $[S_{(j)}^x, S_{(k)}^y] = i\delta_{jk} S_{(j)}^z$ and cyclic permutations—interacting linearly with a countable number of bosonic degrees of freedom described by creation/annihilation operators $\{a_\nu^*, a_\nu : \nu \geqslant 1\}$, with $[a_\nu, a_{\nu'}^*] \subset \delta_{\nu,\nu'}$. The *strictly positive* bosonic frequencies $\omega_n(\nu)$ are assumed to satisfy

$$\sum_{\nu \geqslant 1} e^{-\beta \omega_n(\nu)} < \infty \qquad \text{for} \quad \beta > 0$$

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the coupling constants $\{\lambda_n(j; \nu): \nu \geqslant 1, j = 1, 2,..., n\}$ are complex numbers satisfying

$$\sum_{\nu \geqslant 1} |\lambda_n(j; \nu)|^2 < \infty \qquad \text{for every} \quad j = 1, 2,..., n$$

and the $\{\varepsilon_n(j): j = 1, 2,..., n\}$ are real. The Hamiltonian arises in a realistic model of atoms (or molecules) interacting with radiation if one accepts to treat the atoms in a two-level approximation and neglects terms that are quadratic in creation or annihilation operators.[9]

The problem is to determine the specific free energy of the system in the thermodynamic limit $n \to \infty$, where V_n, the volume of the system, is proportional to n, that is, $\rho = n/V_n$, the density of the spins, is constant. This problem has been solved in a number of particular cases. Hepp and Lieb[8] treated the case of one bosonic mode, using a rotating-wave approximation for the coupling (Dicke maser model). These same authors then[9] removed the latter approximation and treated finitely many bosonic modes in the *homogeneous* case, where the coupling constants and spin frequencies are independent of the spins: $\lambda_n(j; \nu) = \lambda_n(\nu)$ and $\varepsilon_n(j) = \varepsilon_n$ for every $j = 1, 2,..., n$. Hepp and Lieb also obtained results on the thermodynamic stability for the general (i.e., *heterogeneous*) model, leaving open the question of the existence of the thermodynamic limit.[9] Subsequently, the "approximating Hamiltonian method" has been used on the Hamiltonian H_n and its variants.[2,3,12] The homogeneous case with countably many bosonic modes has been treated in detail[10] using large-deviation methods developed in ref. 4.

Here, the problem is solved for the heterogeneous model using a method developed by Duffield and Pulè in their treatment of the BCS model[6] supplemented with an idea of Bogoljubov and Plechko.[3] It is shown that under certain specified conditions H_n is thermodynamically equivalent (in the sense that the difference of the specific free energies vanishes in the thermodynamic limit) to the Hamiltonian

$$\tilde{H}_n = \sum_{\nu \geqslant 1} \omega_n(\nu)\, a_\nu^* a_\nu + \sum_{j=1}^{n} \varepsilon_n(j)\, S^z_{(j)} - V_n^{-1} \sum_{j,k=1}^{n} \Lambda_n(j, k)\, S^x_{(j)} S^x_{(k)}$$

where the spin–boson interaction is replaced by an effective quadratic spin–spin interaction:

$$\Lambda_n(j, k) = \operatorname{Re} \sum_{\nu \geqslant 1} \omega_n(\nu)^{-1}\, \overline{\lambda_n(j; \nu)}\, \lambda_n(k; \nu), \qquad j, k = 1, 2,..., n$$

Moreover, $\tilde{H}_n$ is thermodynamically equivalent to the Hamiltonian

$$\hat{H}_n(x) = \sum_{\nu \geqslant 1} \omega_n(\nu)\, a_\nu^* a_\nu + \sum_{j=1}^{n} \varepsilon_n(j)\, S_{(j)}^z + \sum_{j,k=1}^{n} \Lambda_n(j,k)\, x_j \{ V_n x_k 1 - 2S_{(k)}^x \}$$

if the real n-vector x is chosen so as to minimize the corresponding specific free energy.

The result is then the following:

Theorem 1. Suppose there exist real-valued continuous functions ε on $[0, 1]$ and Λ on $[0, 1] \times [0, 1]$ such that the following conditions hold:

$$\text{(C1)} \qquad \lim_{n \to \infty} \sup_{j \in \{1,2,\ldots,n\}} |\varepsilon_n(j) - \varepsilon(j/n)| = 0$$

$$\text{(C2)} \qquad \lim_{n \to \infty} \sup_{j,k \in \{1,2,\ldots,n\}} |\Lambda_n(j,k) - \Lambda(j/n, k/n)| = 0$$

If

$$\text{(C3)} \qquad f^0 = \lim_{\substack{n \to \infty \\ \rho = \text{const}}} (-\beta V_n)^{-1} \log \operatorname{tr} \exp\left\{ -\beta \sum_{\nu \geqslant 1} \omega_n(\nu)\, a_\nu^* a_\nu \right\}$$

exist for some $\beta > 0$ and if

$$\text{(C4)} \qquad \lim_{n \to \infty} n^{-3/2} \sum_{\nu \geqslant 1} \omega_n(\nu)^{-1/2} \sum_{j=1}^{n} |\lambda_n(j; \nu)| = 0$$

then

$$\lim_{\substack{n \to \infty \\ \rho = \text{const}}} (-\beta V_n)^{-1} \log \operatorname{tr} \exp(-\beta H_n)$$

$$= f^0 - \rho \sup_{\substack{r,s \in L_{\mathbb{R}}^\infty([0,1]) \\ |s| \leqslant r \leqslant 1}} \left(\int_0^1 \{ \beta^{-1} I(r(t)) + \tfrac{1}{2} |\varepsilon(t)|\, [r(t)^2 - s(t)^2]^{1/2} \}\, dt + \tfrac{1}{4}\rho \int_0^1 \int_0^1 \Lambda(t,u)\, s(t)\, s(u)\, dt\, du \right)$$

where

$$I(x) = -\tfrac{1}{2}(1+x) \log[\tfrac{1}{2}(1+x)] - \tfrac{1}{2}(1-x) \log[\tfrac{1}{2}(1-x)] \qquad \text{for} \quad 0 \leqslant x \leqslant 1$$

This is proved in Section 3, after introducing notation in Section 2. The solution of the variational problem, following Duffield and Pulè,[6] is presented and briefly discussed in Section 4.

2. NOTATION AND DEFINITIONS

It will be convenient to use Fock-space notation. For each $n=1, 2, 3,\ldots$, let $\mathscr{A}_n$ be a bounded region in $\mathbb{R}^d$ of volume (i.e., Lebesgue measure) V_n. Let $\mathfrak{h}_n$ be a positive, *injective*, self-adjoint operator on $L^2(\mathscr{A}_n)$ such that $\exp(-\beta\mathfrak{h}_n)$ is trace-class for $\beta>0$. It follows that $\mathfrak{h}_n$ has a bounded inverse. Write $\mathfrak{K}_n$ for the n-fold tensor product of $\mathbb{C}^2$ and let $S_{(j)}$ be a copy of the spin operator of magnitude 1/2 acting on the jth component of $\mathfrak{K}_n$ ($j=1, 2,\ldots, n$). Let $\mathfrak{F}_n$ be the symmetric Fock space over $L^2(\mathscr{A}_n)$ and consider the Hamiltonian[2]

$$H_n = d\Gamma(\mathfrak{h}_n) + \sum_{j=1}^{n} \{(V_n)^{-1/2}\{a^*(\lambda_n(j)) + a(\lambda_n(j))\} S^x_{(j)} + \varepsilon_n(j) S^z_{(j)}\} \qquad (2.1)$$

acting on $\mathfrak{F}_n \otimes \mathfrak{K}_n$, where $\{\varepsilon_n(j)\} \subset \mathbb{R}$, $\{\lambda_n(j)\} \subset L^2(\mathscr{A}_n)$, $a(\cdot)$ is the familiar annihilation operator, and $d\Gamma$ denotes the second-quantization map. The quadratures formula[5]

$$W[f]^*\, d\Gamma(\mathfrak{h})\, W[f] = d\Gamma(\mathfrak{h}) + a^*(\mathfrak{h}f) + a(\mathfrak{h}f) + \langle f, \mathfrak{h}f\rangle \cdot 1 \qquad (2.2)$$

valid for $f\in \mathrm{Dom}(\mathfrak{h})$, where $W[f] \equiv \exp\{\overline{a^*(f) - a(f)}\}$ is the unitary Weyl operator, enables one to write

$$H_n = \sum_{j=1}^{n} \{n^{-1} U_n(j)^*\, d\Gamma(\mathfrak{h}_n)\, U_n(j) + \varepsilon_n(j) S^z_{(j)} - \tfrac{1}{4}\rho\, \|\mathfrak{h}_n^{-1/2}\lambda_n(j)\|^2\, 1\} \qquad (2.3)$$

where the unitaries $U_n(j)$, $j=1, 2,\ldots, n$, are given by

$$U_n(j) := W[\tfrac{1}{2}n(V_n)^{-1/2}\, \mathfrak{h}_n^{-1}\lambda_n(j)]\, P^+_{(j)} + W[\tfrac{1}{2}n(V_n)^{-1/2}\, \mathfrak{h}_n^{-1}\lambda_n(j)]^*\, P^-_{(j)} \qquad (2.4)$$

where $P^{\pm}_{(j)}$ is the spectral projection of $S^x_{(j)}$ to the eigenvalue $\pm\frac{1}{2}$. Formula (2.3) can now be used to prove the self-adjointness of H_n.

Two free energy densities are associated with H_n:

$$\exp(-\beta V_n f_n) = \mathrm{tr}_{\mathfrak{F}_n\otimes\mathfrak{K}_n}[\exp(-\beta H_n)] \qquad (2.5)$$

$$\exp(-\beta V_n f_n^0) = \mathrm{tr}_{\mathfrak{F}_n}[\exp[-\beta\, d\Gamma(\mathfrak{h}_n)]] \qquad (2.6)$$

Of interest is the limit $n\to\infty$, such that V_n diverges but $\rho = n/V_n$ remains constant.

The Hamiltonian (2.1) has the following symmetry. Let the self-adjoint, unitary operator L_n on $\mathfrak{F}_n \otimes \mathfrak{K}_n$ be given by $L_n = \Gamma(-1)(\prod_{j=1}^n 2S^z_{(j)})$; then

[2] Tensor notation for operators is not used, i.e., $S_{(j)} = 1\otimes S_{(j)}$, $a(\cdot) = a(\cdot)\otimes 1$, etc.

$L_n S^z_{(j)} L_n = S^z_{(j)}$ and $L_n S^x_{(j)} L_n = -S^x_{(j)}$ for every $j = 1, 2,..., n$, and $L_n\, d\Gamma(\cdot)\, L_n = d\Gamma(\cdot)$, $L_n a(\cdot)\, L_n = -a(\cdot)$. In particular, L_n commutes with H_n.

Consider the Hamiltonian $H_n(h)$, $h \in \mathbb{R}^n$, defined by

$$H_n(h) = H_n + \sum_{j=1}^{n} h_j S^x_{(j)} \tag{2.7}$$

where the symmetry of H_n implemented by L_n is broken if the external field vector h is nonzero. The free energy density associated with $H_n(h)$ is written $f_n(h)$ and is a concave function of each of the n components of h. Expectation values with respect to the canonical state associated with $H_n(h)$ are denoted by $\langle \cdot \rangle_h$.

The $n \times n$ matrix A_n is defined by its matrix elements

$$A_n(j, k) \equiv \mathrm{Re}\langle \lambda_n(j), \mathfrak{h}_n^{-1} \lambda_n(k) \rangle_{L^2(\mathscr{A}_n)}, \quad j, k \in \{1, 2,..., n\} \tag{2.8}$$

It is readily seen that A_n is positive semidefinite and the multiplicity of the eigenvalue 0 is equal to n minus the number of vectors in $\{\lambda_n(j): j = 1, 2,..., n\}$ which are real-linearly independent.

3. THE PROOFS

Introduce a bosonic Hamiltonian $H^b_n(x)$, $x \in \mathbb{R}^n$, on $\mathfrak{F}_n$ by

$$H^b_n(x) = d\Gamma(\mathfrak{h}_n) + V_n \sum_{j=1}^{n} x_j \left\{ V_n^{-1/2} [a^*(\lambda_n(j)) + a(\lambda_n(j))] + \sum_{k=1}^{n} A_n(j, k)\, x_k 1 \right\} \tag{3.1}$$

and two spin Hamiltonians $\tilde{H}^s_n(h)$ and $\hat{H}^s_n(h; x)$, $h, x \in \mathbb{R}^n$, on $\mathfrak{K}_n$ by

$$\tilde{H}^s_n(h) = \sum_{j=1}^{n} \left[\varepsilon_n(j)\, S^z_{(j)} + h_j S^x_{(j)} - V_n^{-1} \sum_{k=1}^{n} A_n(j, k)\, S^x_{(j)} S^x_{(k)} \right] \tag{3.2}$$

$$\hat{H}^s_n(h; x) = \sum_{j=1}^{n} \left\{ \varepsilon_n(j)\, S^z_{(j)} + \left[h_j - 2 \sum_{k=1}^{n} A_n(j, k)\, x_k \right] S^x_{(j)} \right\} + V_n x A_n x 1 \tag{3.3}$$

Write $\tilde{f}^s_n(h)$ and $\hat{f}^s_n(h; x)$ for the free energy densities associated with (3.2) and (3.3), respectively. Expectation values with respect to a canonical state will be written as angular brackets indexed by the corresponding Hamiltonian or distinctive parameters characterizing it.

Lemma 1:

$$(-\beta V_n)^{-1} \log \operatorname{tr}_{\mathfrak{F}_n} \exp[-\beta H_n^{\mathrm{b}}(x)] = f_n^0 \qquad \text{for every} \quad x \in \mathbb{R}^n$$

$$\hat{f}_n^{\mathrm{s}}(h; x) = x\Lambda_n x - (V_n\beta)^{-1} \times \sum_{j=1}^{n} \log\left[2\cosh\left(\tfrac{1}{2}\beta\left\{\varepsilon_n(j)^2 + \left[h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k)\, x_k\right]^2\right\}^{1/2}\right)\right]$$

Proof. An application of (2.2) shows that (3.1) is unitarily equivalent to $d\Gamma(\mathfrak{h}_n)$ for every $x \in \mathbb{R}^n$ (see the proof of Lemma 2A). Up to the constant term $V_n x\Lambda_n x 1$, the Hamiltonian (3.3) is the sum of n pairwise commuting operators

$$\varepsilon_n(j)\, S^z + \left(h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k)\, x_k\right) S^x$$

on $\mathbb{C}^2$, each of which has

$$\pm\tfrac{1}{2}\left[\varepsilon_n(j)^2 + \left(h_j - 2\sum_{k=1}^{n} \Lambda_n(j,k)\, x_k\right)^2\right]^{1/2}$$

as its eigenvalues. ∎

Lemma 2A:

$$\bar{f}_n^{\mathrm{s}}(h) - \inf_{x \in \mathbb{R}^n} \hat{f}_n^{\mathrm{s}}(h; x) \leqslant f_n^0 + \bar{f}_n^{\mathrm{s}}(h) - f_n(h)$$

Proof. Equivalently,

$$f_n^0 + \inf_{x \in \mathbb{R}^n} \hat{f}_n^{\mathrm{s}}(h; x) - f_n(h) \geqslant 0 \tag{*}$$

By the first part of Lemma 1, $f_n^0 + \hat{f}_n^{\mathrm{s}}(h; x)$ is the specific free energy associated with the Hamiltonian $\hat{H}_n(h; x) = H_n^b(x) + \hat{H}_n^{\mathrm{s}}(h; x)$; by Bogoljubov's inequality (see ref. 7 for a proof),

$$f_n^0 + \hat{f}_n^{\mathrm{s}}(h; x) - f_n(h) \geqslant V_n^{-1}\langle \hat{H}_n(h; x) - H_n(h)\rangle_{\hat{H}_n(h;x)} \tag{**}$$

Now by (3.1), (3.2), and (2.7), the right-hand side of (**) is given by

$$\sum_{j=1}^{n}\left\{\left[V_n^{-1/2}\langle a^*(\lambda_n(j)) + a(\lambda_n(j))\rangle_{H_n^b(x)} + 2\sum_{k=1}^{n} \Lambda_n(j,k)\, x_k\right] \times [x_j - V_n^{-1}\langle S_{(j)}^x\rangle_{\hat{H}_n^{\mathrm{s}}(h;x)}]\right\}$$

By (2.2),

$$H_n^{\mathrm{b}}(x) = W\left[-V_n^{1/2} \sum_{j=1}^{n} x_j \mathfrak{h}_n^{-1} \lambda_n(j) \right] d\Gamma(\mathfrak{h}_n)\, W\left[V_n^{1/2} \sum_{j=1}^{n} x_j \mathfrak{h}_n^{-1} \lambda_n(j) \right]$$

Using the formula $W[f]^*\, a(g)\, W[f] = a(g) + \langle g, f \rangle\, 1$ and (2.8), one finds

$$\begin{aligned}
&\langle a^*(\lambda_n(k)) + a(\lambda_n(k)) \rangle_{H_n^{\mathrm{b}}(x)} \\
&\quad = \Big\langle W\Big[V_n^{1/2} \sum_{j=1} x_j \mathfrak{h}_n^{-1} \lambda_n(j) \Big] \\
&\qquad \times [a^*(\lambda_n(k)) + a(\lambda_n(k))]\; W\Big[-V_n^{1/2} \sum_{j=1} x_j \mathfrak{h}_n^{-1} \lambda_n(j) \Big] \Big\rangle_{d\Gamma(\mathfrak{h}_n)} \\
&\quad = -V_n^{1/2} \sum_{j=1}^{n} x_j \big(\overline{\langle \lambda_n(k), \mathfrak{h}_n^{-1} \lambda_n(j) \rangle} + \langle \lambda_n(k), \mathfrak{h}_n^{-1} \lambda_n(j) \rangle \big) \\
&\qquad + \langle a^*(\lambda_n(k)) + a(\lambda_n(k)) \rangle_{d\Gamma(\mathfrak{h}_n)} \\
&\quad = -2 V_n^{1/2} \sum_{j=1}^{n} \Lambda_n(j, k)\, x_j
\end{aligned}$$

Thus, the right-hand side of (**) is zero for every $x \in \mathbb{R}^n$; (*) follows by taking the infimum with respect to x. ∎

Bogoljubov's inequality also gives an upper bound on $f_n^0 + \tilde{f}_n^{\mathrm{s}}(h) - f_n(h)$; this involves

$$V_n^{-3/2} \sum_{\nu \geq 1} \sum_{j=1}^{n} \langle [\lambda_n(j; \nu)\, a_\nu^* + \overline{\lambda_n(j; \nu)}\, a_\nu]\, S_{(j)}^x \rangle_h \tag{3.4}$$

Bogoljubov and Plechko[3] have devised an alternative method which avoids the problem of estimating (3.4). Fix an arbitrary n, and consider an arbitrary finite number N of boson modes with strictly positive frequencies $\{\omega_n(\nu): 1 \leq \nu \leq N\}$ and associated coupling constants $\{\lambda_n(j; \nu): 1 \leq \nu \leq N, j = 1, 2,..., n\}$. The Hamiltonian $H_n(h; N)$ is that obtained from $H_n(h)$ by considering only these N modes, and the associated specific free energy will be written $f_n(h; N)$; accordingly, write $f_n^0(N)$, and $\tilde{f}_n^{\mathrm{s}}(h; N)$.

Let $\mathbb{A} = \{\nu: 1 \leq \nu \leq N,\ \ \lambda_n(j; \nu) = 0$ for every $j = 1, 2,..., n\}$, and $\mathbb{B} = \{1, 2,..., N\} \setminus \mathbb{A}$. For any set $\tau = \{\tau_\nu: \nu \in \mathbb{B}\}$ of real numbers in the open interval (0, 1), one has the identity

$$\begin{aligned}
H_n(h; N) = {} & \sum_{\nu \in \mathbb{A}} \omega_n(\nu)\, a_\nu^* a_\nu + \sum_{\nu \in \mathbb{B}} (1 - \tau_\nu)\, \omega_n(\nu)\, a_\nu^* a_\nu + \tilde{H}_n^{\mathrm{s}}(h; N; \tau) \\
& + \sum_{\nu \in \mathbb{B}} \tau_\nu \omega_n(\nu)\, \mathfrak{b}_\nu(\tau)^* \mathfrak{b}_\nu(\tau)
\end{aligned} \tag{3.5}$$

where

$$\tilde{H}_n^s(h; N; \tau) = \sum_{j=1}^{n} \left[\varepsilon_n(j)\, S^z_{(j)} + h_j S^x_{(j)} - V_n^{-1} \sum_{k=1}^{n} A_n^N(j, k; \tau)\, S^x_{(j)} S^x_{(k)} \right] \qquad (3.6)$$

$$A_n^N(j, k; \tau) = \mathrm{Re} \sum_{v \in \mathbb{B}} [\tau_v \omega_n(v)]^{-1}\, \overline{\lambda_n(j; v)}\, \lambda_n(k; v) \qquad (3.7)$$

$$\mathrm{b}_v(\tau) = a_v + V_n^{-1/2} [\tau_v \omega_n(v)]^{-1} \sum_{j=1}^{n} \lambda_n(j; v)\, S^x_{(j)} \qquad (3.8)$$

Let $f_n^0(N; \tau)$ be the specific free energy of

$$\sum_{v \in \mathbb{A}} \omega_n(v)\, a_v^* a_v + \sum_{v \in \mathbb{B}} (1 - \tau_v)\, \omega_n(v)\, a_v^* a_v$$

and write $\tilde{f}_n^s(h; N; \tau)$ for that of (3.6). Since the last term in (3.5) is positive, $f_n^0(N; \tau) + \tilde{f}_n^s(h; N; \tau) \leqslant f_n(h; N)$ by Bogoljubov's inequality. Thus,

$$\begin{aligned} &f_n^0(N) + \tilde{f}_n^s(h; N) - f_n(h; N) \\ &\quad \leqslant [f_n^0(N) - f_n^0(N; \tau)] + [\tilde{f}_n^s(h; N) - \tilde{f}_n^s(h; N; \tau)] \end{aligned} \qquad (3.9)$$

Using Bogoljubov's inequality and the familiar formula for $f_n^0(N; \tau)$, one has

$$\begin{aligned} &f_n^0(N) - f_n^0(N; \tau) \\ &\quad \leqslant V_n^{-1} \sum_{v \in \mathbb{B}} \tau_v \omega_n(v) \langle a_v^* a_v \rangle_{(N; \tau)} \\ &\quad = -\sum_{v \in \mathbb{B}} \tau_v (\partial f_n^0 / \partial \tau_v)(N; \tau) \\ &\quad = V_n^{-1} \sum_{v \in \mathbb{B}} \tau_v \omega_n(v) (e^{\beta(1 - \tau_v)\omega_n(v)} - 1)^{-1} \\ &\quad \leqslant (\beta V_n)^{-1} \sum_{v \in \mathbb{B}} \tau_v (1 - \tau_v)^{-1} \end{aligned} \qquad (3.10)$$

Also using Bogoljubov's inequality and $-\frac{1}{2}1 \leqslant S^x \leqslant \frac{1}{2}1$, one finds

$$\begin{aligned} &\tilde{f}_n^s(h; N) - \tilde{f}_n^s(h; N; \tau) \\ &\quad \leqslant V_n^{-2} \sum_{v \in \mathbb{B}} \Bigg[(\tau_v^{-1} - 1)\, \omega_n(v)^{-1} \\ &\qquad \times \mathrm{Re} \sum_{j,k=1}^{n} \overline{\lambda_n(j; v)}\, \lambda_n(k; v) \langle S^x_{(j)} S^x_{(k)} \rangle_{(h; N; \tau)} \Bigg] \\ &\quad \leqslant (2V_n)^{-2} \sum_{v \in \mathbb{B}} (1 - \tau_v)\, \tau_v^{-1} \omega_n(v)^{-1} \left[\sum_{j=1}^{n} |\lambda_n(j; v)| \right]^2 \end{aligned} \qquad (3.11)$$

Inserting (3.10) and (3.11) into (3.9), one obtains

$$
\begin{aligned}
&[f_n^0(N)+\bar{f}_n^{\mathrm{s}}(h;N)]-f_n(h;N)\\
&\quad\leqslant(\beta V_n)^{-1}\sum_{v\in\mathbb{B}}\tau_v(1-\tau_v)^{-1}\\
&\quad+(2V_n)^{-2}\sum_{v\in\mathbb{B}}(1-\tau_v)\,\tau_v^{-1}\omega_n(v)^{-1}\left[\sum_{j=1}^{n}|\lambda_n(j;v)|\right]^2
\end{aligned}
\tag{3.12}
$$

The infimum of the right-hand side of (3.12) with respect to τ is assumed at

$$
\tau_v=\frac{\beta^{1/2}\omega_n(v)^{-1/2}\sum_{j=1}^{n}|\lambda_n(j;v)|}{2V_n^{1/2}+\beta^{1/2}\omega_n(v)^{-1/2}\sum_{j=1}^{n}|\lambda_n(j;v)|}
\tag{3.13}
$$

which lies in (0, 1) by virtue of the definition of $\mathbb{B}$. Thus,

$$
\begin{aligned}
&f_n^0(N)+\bar{f}_n^{\mathrm{s}}(h;N)-f_n(h;N)\\
&\quad\leqslant V_n^{-1}(\beta V_n)^{-1/2}\sum_{v\geqslant 1}^{N}\omega_n(v)^{-1/2}\sum_{j=1}^{n}|\lambda_n(j;v)|
\end{aligned}
\tag{3.14}
$$

For fixed n, it follows that $f_n^0(N)$, $\bar{f}_n^{\mathrm{s}}(h;N)$, and $f_n(h;N)$ converge to f_n^0, $\bar{f}_n^{\mathrm{s}}(h)$, and $f_n(h)$ respectively, as $N\to\infty$, so that the following result is proved.

Lemma 2B:

$$
f_n^0+\bar{f}_n^{\mathrm{s}}(h)-f_n(h)\leqslant V_n^{-1}(\beta V_n)^{-1/2}\sum_{v\geqslant 1}\omega_n(v)^{-1/2}\sum_{j=1}^{n}|\lambda_n(j;v)|
$$

The limit of $\bar{f}_n^{\mathrm{s}}(h)$ has been recently obtained by Duffield and Pulè[6] in their analysis of the BCS model. Their result, which combines large-deviation methods with Berezin–Lieb bounds, is the following.

Theorem 2 (Duffield and Pulè). If conditions (C1) and (C2) are satisfied and there exists a real-valued continuous function h on [0, 1] such that

$$
\text{(C0)}\qquad \lim_{n\to\infty}\ \sup_{j\in\{1,2,\dots,n\}}|h_j-h(j/n)|=0
$$

then

$$
\begin{aligned}
\bar{f}^{\mathrm{s}}(h)&=\lim_{\substack{n\to\infty\\ \rho=\text{const}}}\bar{f}_n^{s}(h)\\
&=\rho\inf_{\substack{r,s\in L_{\mathbb{R}}^{\infty}([0,1])\\ |s|\leqslant r\leqslant 1}}\left(\int_0^1\{-\beta^{-1}I(r(t))+\tfrac{1}{2}h(t)\,s(t)\right.\\
&\quad-\tfrac{1}{2}|\varepsilon(t)|\,[r(t)^2-s(t)^2]^{1/2}\}\,dt\\
&\quad\left.-\tfrac{1}{4}\rho\int_0^1\int_0^1 A(t,t')\,s(t)\,s(t')\,dt\,dt'\right)
\end{aligned}
$$

Remark 1. The proofs of ref. 6 apply without change under the slightly stronger assumptions $h_j = h(j/n)$, $\varepsilon_n(j) = \varepsilon(j/n)$, and $\Lambda_n(j,k) = \Lambda(j/n, k/n)$, but can be adapted to accommodate (C0)–(C2).

The $\inf_{x \in \mathbb{R}^n} \hat{f}_n^s(h; x)$ is discussed in Appendix A; one has the following result:

Lemma 3. Under the assumptions (C0)–(C2),

$$\lim_{\substack{n \to \infty \\ \rho = \text{const}}} \inf_{x \in \mathbb{R}^n} \hat{f}_n^s(h; x) = \bar{f}^s(h)$$

Proof. Let $M_n = \inf_{x \in \mathbb{R}^n} \hat{f}_n^s(h; x)$; by Lemma A1, setting $s_j = r_j \sin(\vartheta_j)$,

$$M_n = \inf_{|s_j| \leqslant r_j \leqslant 1} \left(V_n^{-1} \sum_{j=1}^{n} \left[-\beta^{-1} I(r_j) - \tfrac{1}{2} |\varepsilon_n(j)| \, (r_j^2 - s_j^2)^{1/2} + \tfrac{1}{2} h_j s_j \right] \right.$$
$$\left. - \tfrac{1}{4} V_n^{-2} \sum_{j=1}^{n} \sum_{k=1}^{n} \Lambda_n(j,k)\, s_j s_k \right)$$

Define L_n by replacing $\varepsilon_n(j)$, h_j, and $\Lambda_n(j,k)$ in the above expression for M_n by $\varepsilon(j/n)$, $h(j/n)$, and $\Lambda(j/n, k/n)$, respectively, where $\varepsilon(\cdot)$, $h(\cdot)$, and $\Lambda(\cdot,\cdot)$ are the functions given by conditions (C0)–(C2). As in Theorem 3 of ref. 6, one proves that $L_n \to \bar{f}^s(h)$ as $n \to \infty$ with $\rho = \text{const}$. Now,

$$|M_n - L_n| \leqslant \sup_{|s_j| \leqslant r_j \leqslant 1} \left| V_n^{-1} \sum_{j=1}^{n} \left\{ \tfrac{1}{2} [|\varepsilon(j/n)| - |\varepsilon_n(j)|] (r_j^2 - s_j^2)^{1/2} \right. \right.$$
$$\left. + \tfrac{1}{2} [h_j - h(j/n)]\, s_j \right\}$$
$$\left. + \tfrac{1}{4} V_n^{-2} \sum_{j=1}^{n} \sum_{k=1}^{n} \{ [\Lambda(j/n, k/n) - \Lambda_n(j,k)]\, s_j s_k \} \right|$$
$$\leqslant \tfrac{1}{2} \rho n^{-1} \sum_{j=1}^{n} \{ \| \varepsilon(j/n)| - |\varepsilon_n(j)\| + |h_j - h(j/n)| \}$$
$$+ \tfrac{1}{4} \rho^2 n^{-2} \sum_{j=1}^{n} \sum_{k=1}^{n} |\Lambda(j/n, k/n) - \Lambda_n(j,k)|$$

so that, by (C0)–(C2), $M_n - L_n \to 0$ as $n \to \infty$ with $\rho = \text{const}$. ∎

Remark 2. One can prove

$$\lim_{n \to \infty} [\bar{f}_n^s(h) - \inf \hat{f}_n^s(h; x)] = 0$$

directly by the "approximating Hamiltonian method," using an idea of ref. 1; one has to assume that n^{-1} (number of nonzero eigenvalues of $\Lambda_n) \to 0$ as $n \to \infty$; moreover, the positivity of Λ_n is used.[11]

The proof of Theorem 1 is obtained by combining Lemmas 2A, 2B, and 3 and Theorem 2.

One can recover the results of ref. 10, which are valid for the homogeneous case: $\varepsilon_n(j)=\varepsilon_n$, $\lambda_n(j;v)=\lambda_n(v)$, and $h_j=h$, for all $j=1,2,\dots,n$.[3] Condition (CO) is trivially met; conditions (C1) and (C2) demand the existence of real numbers ε and Λ ($\geqslant 0$) such that $\varepsilon_n\to\varepsilon$ and $\langle\lambda_n,\mathfrak{h}_n^{-1}\lambda_n\rangle_{L^2(\mathscr{A}_n)}\to\Lambda$.

Lemma 4. In the homogeneous case

$$\mathcal{F}^s(h)=-\rho\sup_{0\leqslant z,u\leqslant 1}\left[\beta^{-1}I(u)+\tfrac{1}{2}|h|\,u(1-z^2)^{1/2}+\tfrac{1}{2}|\varepsilon|\,uz+\tfrac{1}{4}\rho\Lambda u^2(1-z^2)\right]$$

Proof. By Theorem 2, choosing $r(t)=r$ and $s(t)=s$ a.e., one has

$$\begin{aligned}-\mathcal{F}^s(h)/\rho &\geqslant \sup_{|s|\leqslant r\leqslant 1}\left[\beta^{-1}I(r)-\tfrac{1}{2}hs+\tfrac{1}{2}|\varepsilon|\,(r^2-s^2)^{1/2}+\tfrac{1}{4}\rho\Lambda s^2\right]\\ &=\sup_{0\leqslant x,r\leqslant 1}\left[\beta^{-1}I(r)+\tfrac{1}{2}|h|\,rx\right.\\ &\qquad\left.+\tfrac{1}{2}|\varepsilon|\,r(1-x^2)^{1/2}+\tfrac{1}{4}\rho\Lambda r^2x^2\right]\end{aligned}$$

For r and s in $L^\infty_{\mathbb{R}}([0,1])$ with $|s|\leqslant r\leqslant 1$ (all integrals are over $[0,1]$),

$$\begin{aligned}&\int[r(t)^2-s(t)^2]^{1/2}\,dt\\ &\quad=\int[r(t)-s(t)]^{1/2}\,[r(t)+s(t)]^{1/2}\,dt\\ &\quad\leqslant\left\{\int[r(t)-s(t)]\,dt\cdot\int[r(t)+s(t)]\,dt\right\}^{1/2}\\ &\quad=\left\{\left[\int r(t)\,dt\right]^2-\left[\int s(t)\,dt\right]^2\right\}^{1/2}\end{aligned}$$

by the Schwarz inequality; since I is concave,

$$\begin{aligned}-\mathcal{F}^s(h)/\rho &\leqslant \sup_{\substack{r,s\in L^\infty_{\mathbb{R}}([0,1])\\ |s|\leqslant r\leqslant 1}}\left(\beta^{-1}I\left(\int r(t)\,dt\right)\right.\\ &\qquad-\tfrac{1}{2}h\int s(t)\,dt+\tfrac{1}{4}\rho\Lambda\left[\int s(t)\,dt\right]^2\\ &\qquad\left.+\tfrac{1}{2}|\varepsilon|\left\{\left[\int r(t)\,dt\right]^2-\left[\int s(t)\,dt\right]^2\right\}^{1/2}\right)\\ &=\sup_{|s|\leqslant r\leqslant 1}\left[\beta^{-1}I(r)-\tfrac{1}{2}hs+\tfrac{1}{2}|\varepsilon|\,(r^2-s^2)^{1/2}+\tfrac{1}{4}\rho\Lambda s^2\right]\quad\blacksquare\end{aligned}$$

[3] Condition (C4) is not needed for the results of ref. 10.

4. THE PHASE TRANSITION

The variational problem determining $\bar{f}^s(h)$, and thus $f(h)$, is

$$\mathscr{I}(h) = \sup_{\substack{r,s \in L^\infty_{\mathbb{R}}([0,1]) \\ |s| \leqslant r \leqslant 1}} \left(\int_0^1 \{\beta^{-1} I(r(t)) + \tfrac{1}{2} |\varepsilon(t)| \, [r(t)^2 - s(t)^2]^{1/2} - \tfrac{1}{2} h(t) \, s(t)\} \, dt + \tfrac{1}{4}\rho \int_0^1 \int_0^1 A(t, t') \, s(t) \, s(t') \, dt \, dt' \right) \tag{4.1}$$

For $A(t, t') \geqslant 0$ (and $h = \text{const}$) this problem[4] is solved by Duffield and Pulè[6]; most of their arguments apply to the case of arbitrary A.

Notice that if $h = 0$ and (r, s) is a maximizer for (4.1), then so is $(r, -s)$. The function I is concave, with derivative $-\text{arctanh}$. The r variation can be done as in ref. 6; for $s \in L^\infty_{\mathbb{R}}([0, 1])$ with $|s| \leqslant 1$, let $r_s\colon [0, 1] \to \mathbb{R}$ be defined (a.e.) to be 1 where $|s| = 1$, and otherwise as the largest zero in the interval $[|s(t)|, 1]$ of the function[5]

$$x \to \tfrac{1}{2}\beta \, |\varepsilon(t)| \, x - [x^2 - s(t)^2]^{1/2} \, \text{arctanh}(x) \tag{4.2}$$

Then, if $\mathscr{B}$ denotes the unit ball of $L^\infty_{\mathbb{R}}([0, 1])$, one has

$$\mathscr{I}(h) = \sup_{s \in \mathscr{B}} \{\mathscr{V}(s; h)\} \tag{4.3}$$

where

$$\mathscr{V}(s; h) = \int_0^1 \{\beta^{-1} I(r_s(t)) + \tfrac{1}{2} |\varepsilon(t)| \, [r_s(t)^2 - s(t)^2]^{1/2} - \tfrac{1}{2} h(t) \, s(t)\} \, dt + \tfrac{1}{4}\rho \int_0^1 \int_0^1 A(t, t') \, s(t) \, s(t') \, dt \, dt' \tag{4.4}$$

For $h = 0$, one has inversion symmetry, $\mathscr{V}(s; 0) = \mathscr{V}(-s; 0)$. Let K be the self-adjoint, integral operator on $L^2_{\mathbb{R}}([0, 1])$ defined by the kernel A; K is compact. Consider the continuous function g_β on $[0, 1]$ given by

$$g_\beta(t) = \begin{cases} (\beta/2)^{1/2}, & \text{if } \varepsilon(t) = 0 \\ (\{\tanh[\tfrac{1}{2}\beta \, |\varepsilon(t)|]\}/|\varepsilon(t)|)^{1/2} & \text{if } \varepsilon(t) \neq 0 \end{cases} \tag{4.5}$$

[4] The kernel need not be positive; it defines a positive operator. $A(t, t') > 0$ is used in the uniqueness results of ref. 6.

[5] Notice that $r_0(t) = \tanh[\tfrac{1}{2}\beta \, |\varepsilon(t)|]$ a.e., that $r_{-s} = r_s$, and that $r_s = |s|$ on the set where $\varepsilon(t) = 0$.

and let G_β be the (bounded, positive) operator on $L^2_{\mathbb{R}}([0,1])$ of multiplication by g_β. Let $U^\rho_\beta = \rho G_\beta K G_\beta$, i.e.,

$$\{U^\rho_\beta \psi\}(t) = \rho g_\beta(t) \int_0^1 g_\beta(t')\, A(t,t')\, \psi(t')\, dt' \tag{4.6}$$

Define $\Phi^\rho_\beta(s;t)$ (a.e.) by

$$\Phi^\rho_\beta(s;t) = \rho\{Ks\}(t) - \begin{cases} 2\beta^{-1} \operatorname{arctanh} s(t) & \varepsilon(t)=0 \\ |\varepsilon(t)|\, s(t)/[r_s(t)^2 - s(t)^2]^{1/2} & \varepsilon(t)\neq 0 \end{cases} \tag{4.7}$$

and notice that $\Phi^\rho_\beta(-s;\cdot) = -\Phi^\rho_\beta(s;\cdot)$.

The solution of (4.1) for $h=0$ is obtained from the following two results, which will be proved in Appendix B by adjusting the arguments of ref. 6:

Theorem 3. If $\|U^\rho_\beta\| \leqslant 1$, then

$$\mathscr{I}(0) = \mathscr{V}(0;0) = \beta^{-1} \int_0^1 \log\{2\cosh[\tfrac{1}{2}\beta\varepsilon(t)]\}\, dt$$

Theorem 4. If $\|U^\rho_\beta\| > 1$, then there exists a nonzero $s_* \in \mathscr{B}$ such that $\mathscr{I}(0) = \mathscr{V}(s_*;0) = \mathscr{V}(-s_*;0)$, where s_* and $-s_*$ are solutions of the Euler–Lagrange equation $\Phi^\rho_\beta(s;\cdot)=0$. Moreover,

$$\begin{aligned} \mathscr{I}(0) &= \mathscr{V}(\pm s_*;0) \\ &= \beta^{-1}\int_0^1 \log(2\cosh\{\tfrac{1}{2}\beta[\varepsilon(t)^2 + k_\beta(t)^2]^{1/2}\})\, dt \\ &\quad - \frac{1}{4}\int_0^1 \frac{\tanh\{\tfrac{1}{2}\beta[\varepsilon(t)^2 + k_\beta(t)^2]^{1/2}\}}{[\varepsilon(t)^2 + k_\beta(t)^2]^{1/2}}\, k_\beta(t)^2\, dt \end{aligned}$$

where $k_\beta \neq 0$ satisfies

$$k_\beta(t) = \rho \int_0^1 A(t,t')\, \frac{\tanh\{\tfrac{1}{2}\beta[\varepsilon(t')^2 + k_\beta(t')^2]^{1/2}\}}{[\varepsilon(t')^2 + k_\beta(t')^2]^{1/2}}\, k_\beta(t')\, dt'$$

Remark 3. Most likely, s_* and $-s_*$ are the only nonzero solutions of the Euler–Lagrange equation if K is positive, but I am unable to prove this.

The map $\beta \to \|U^\rho_\beta\|$ is strictly increasing with $\lim_{\beta\downarrow 0}\|U^\rho_\beta\| = 0$, so that one can identify a possibly infinite critical reciprocal temperature β_c such that if $\beta < \beta_c$, then $\|U^\rho_\beta\| < 1$, and if $\beta > \beta_c$, then $\|U^\rho_\beta\| > 1$. For $\beta \leqslant \beta_c$, $\bar{f}^s$ (and thus f) is independent of the interaction: the system is thermodynamically equivalent to a noninteracting system of bosons and spins. Qualitatively, the results are identical to those of refs. 9 and 10.

As an illustration, in the homogeneous case, one has

$$\| U_\beta^\rho \| = \rho \Lambda \begin{cases} \frac{1}{2}\beta & \text{if} \quad \varepsilon = 0 \\ \tanh(\frac{1}{2}\beta\, |\varepsilon|)/|\varepsilon| & \text{if} \quad \varepsilon \neq 0 \end{cases}$$

and thus, as in ref. 10,

$$\beta_c = \begin{cases} 2\,\mathrm{arctanh}(|\varepsilon|/\rho\Lambda)/|\varepsilon| & \text{if} \quad \varepsilon \neq 0 \text{ and } |\varepsilon| < \rho\Lambda \\ +\infty & \text{if} \quad \varepsilon \neq 0 \text{ and } |\varepsilon| \geqslant \rho\Lambda \\ 2/\rho\Lambda & \text{if} \quad \varepsilon = 0 \end{cases}$$

Finally, one can proceed, as in ref. 6, to obtain the thermodynamic limit of the equilibrium expectation of the average spin polarization in x direction when $h(t) = \hbar$ (by symmetry, this limit is zero for $\hbar = 0$), and then consider the limit $\hbar \to 0$. The result is qualitatively the same as that for the homogeneous case,[10] namely: the limit is zero for $\beta \leqslant \beta_c$ and *not* zero if $\beta > \beta_c$, with different sign depending on whether $\hbar \uparrow 0$ or $\hbar \downarrow 0$.

APPENDIX A. DISCUSSION OF $\inf_{x \in \mathbb{R}^n} \hat{f}_n^s(h; x)$

Lemma A1. Let I on $[0, 1]$ be defined as in Theorem 1. Then,

$$\inf_{x \in \mathbb{R}^n} \hat{f}_n^s(h; x)$$

$$= \inf_{\substack{r_j \in [0,1] \\ \vartheta_j \in [0, 2\pi]}} \left\{ V_n^{-1} \sum_{j=1}^{n} \left[-\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j)\, r_j \cos(\vartheta_j) + \tfrac{1}{2} h_j r_j \sin(\vartheta_j) - \tfrac{1}{4} V_n^{-1} \sum_{k=1}^{n} \Lambda_n(j, k)\, r_j r_k \sin(\vartheta_j) \sin(\vartheta_k \right] \right\}$$

$$= \inf_{\substack{r_j \in [0,1] \\ \vartheta_j \in [-1/2\pi, 1/2\pi]}} \left\{ V_n^{-1} \sum_{j=1}^{n} \left[-\beta^{-1} I(r_j) - \tfrac{1}{2}\, |\varepsilon_n(j)|\, r_j \cos(\vartheta_j) + \tfrac{1}{2} h_j r_j \sin(\vartheta_j) - \tfrac{1}{4} V_n^{-1} \sum_{k=1}^{n} \Lambda_n(j, k)\, r_k \sin(\vartheta_j) \sin(\vartheta_k) \right] \right\}$$

Proof. One verifies that for a and b real,

$$\inf_{\substack{r \in [0,1] \\ y^2 + z^2 = 1}} \left[-\beta^{-1} I(r) + \tfrac{1}{2} a r z + \tfrac{1}{2} b r y \right]$$

$$= -\beta^{-1} \log\{2 \cosh[\tfrac{1}{2}\beta(a^2 + b^2)^{1/2}]\}$$

Thus, by Lemma 1,

$$\hat{f}_n^{s}(h; x) = V_n^{-1} \inf_{\substack{r_j \in [0,1] \\ z_j^2 + y_j^2 = 1}} \sum_{j=1}^{n} \Big\{ -\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j)\, r_j z_j + \tfrac{1}{2} r_j y_j \Big[h_j - 2 \sum_{k=1}^{n} A_n(j,k)\, x_k \Big] \Big\} + x A_n x$$

The variation over $x \in \mathbb{R}^n$ can be done explicitly (for this, it is convenient to diagonalize A_n); it follows that

$$\inf_{x \in \mathbb{R}^n} \hat{f}_n^{s}(h; x) = V_n^{-1} \inf_{\substack{r_j \in [0,1] \\ z_j^2 + y_j^2 = 1}} \sum_{j=1}^{n} \Big[-\beta^{-1} I(r_j) + \tfrac{1}{2}\varepsilon_n(j)\, r_j z_j + \tfrac{1}{2} h_j r_j\, y_j - \tfrac{1}{4} V_n^{-1} \sum_{k=1}^{n} r_j r_k\, y_j\, y_k A_n(j,k) \Big]$$

which proves the first claim upon setting $z_j = \cos(\vartheta_j)$, $\vartheta_j \in [0, 2\pi]$. The second claim is obvious. ∎

APPENDIX B. SOLUTION OF THE VARIATIONAL PROBLEM FOLLOWING DUFFIELD AND PULÈ[6]

Write $\mathscr{I}$ for $\mathscr{I}(0)$ and $\mathscr{V}(s)$ for $\mathscr{V}(s; 0)$.

Proof of Theorem 3. This is a minor adjustment of the corresponding result of ref. 6, to accommodate the fact that the present variation is over $\mathscr{B}$ and not its positive part. Let A be the support of ε. For arbitrary $s \in \mathscr{B}$ and $0 < p < 1$, put $F(p) = \mathscr{V}(ps)$. Now, F is differentiable with derivative (integrals with unspecified domain are over $[0, 1]$)

$$F'(p) = \tfrac{1}{2} p\rho \iint A(t, t')\, s(t)\, s(t')\, dt\, dt' - \tfrac{1}{2} p \int_A |\varepsilon(t)|\; s(t)^2\, [r_{ps}(t)^2 - p^2 s(t)^2]^{-1/2}\, dt - \beta^{-1} \int_{A^c} \operatorname{arctanh}[p\, |s(t)|]\; |s(t)|\, dt$$

Using the inequalities

$$|s(t)| \operatorname{arctanh}[p\, |s(t)|] \geqslant p s(t)^2$$
$$[r_s(t)^2 - s(t)^2]^{1/2} \leqslant \tanh[\tfrac{1}{2}\beta\, |\varepsilon(t)|]$$

one obtains

$$F'(p) \leqslant \tfrac{1}{2} p \langle \hat{s}, \{U_\beta^\rho - 1\}\, \hat{s} \rangle_{L^2_{\mathbb{R}}([0,1])}$$

where $\hat{s}(t) = s(t)/g_\beta(t)$. The assumption $\|U_\beta^\rho\| \leqslant 1$ implies $F'(p) \leqslant 0$, so that $\mathscr{V}(ps) \leqslant \mathscr{V}(0)$, and by continuity $\mathscr{V}(s) \leqslant \mathscr{V}(0)$. One can compute $\mathscr{V}(0)$ using $r_0(t) = \tanh[\tfrac{1}{2}\beta\, |\varepsilon(t)|]$. ∎

The proof of Theorem 4 is broken up into a series of lemmas all of which have their origins in ref. 6.

Lemma B1. There exists $s \in \mathscr{B}$ such that $\mathscr{I}(h) = \mathscr{V}(s; h)$.

Proof. See Theorem 5 of ref. 6. ∎

Lemma B2. If $\|U_\beta^\rho\| > 1$, then $\mathscr{I} > \mathscr{V}(0)$.

Proof. Let $s \in \mathscr{B}$ with $\mathscr{V}(s) = \mathscr{I}$. Since U_β^ρ is compact, $\|U_\beta^\rho\|$ is an eigenvalue; let ξ be a corresponding eigenvector. Define $\xi_n \in L^\infty_{\mathbb{R}}([0, 1])$ by

$$\xi_n(t) = \begin{cases} \xi(t) & \text{if } |\xi(t)| \leqslant n \\ 0 & \text{otherwise} \end{cases}$$

a.e. It follows that

$$\langle \xi_n, \{U_\beta^\rho - 1\}\, \xi_n \rangle_{L^2_{\mathbb{R}}([0,1])} \to \|U_\beta^\rho\| - 1 (>0!) \qquad \text{as} \quad n \to \infty$$

Choose m such that

$$\langle \xi_m, \{U_\beta^\rho - 1\}\, \xi_m \rangle_{L^2_{\mathbb{R}}([0,1])} > 0$$

and let $\hat{s} = \xi_m g_\beta$. The proof then proceeds as in Lemma 3 of ref. 6. ∎

Lemma B3. If $s \in \mathscr{B}$ and $\mathscr{I} = \mathscr{V}(s)$, then $\{t \in [0, 1]: |s(t)| = 1\}$ has zero measure.

Proof. Proceed as in the proof of Lemma 2 of ref. 6, with the set $\{t \in [0, 1]: |s(t)| = 1\}$. ∎

Lemma B4. If $s \in \mathscr{B}$ and $\mathscr{I} = \mathscr{V}(s)$, then $\Phi_\beta^\rho(s; \cdot) = 0$.

Proof. This is an adaptation of the proof of Theorem 6 of ref. 6. Let $0 < \delta < 1$, and take $\xi \in L^\infty_{\mathbb{R}}([0, 1])$ with essential support contained in

$A_\delta \equiv \{t \in [0, 1]: |s(t)| \langle 1 - \delta\}$. For $|p|$ sufficiently small, $s_p = s(1 + p\xi)$ lies in $\mathscr{B}$. Let $F(t) = \mathscr{V}(s_p)$. Taking the derivative at $p = 0$, one obtains

$$\frac{1}{2} \int_{A_\delta} \xi(t)\, s(t)\, \Phi_\beta^\rho(s; t)\, dt = 0 \tag{*}$$

Now take $\xi = s\Phi_\beta^\rho(s; \cdot)$ on A_δ and $\xi = 0$ on A_δ^c; (*) implies that $s\Phi(s; \cdot) = 0$ on A_δ. Since δ was arbitrary, Lemma B3 implies that $s\Phi_\beta^\rho(s; \cdot) = 0$. Thus, $\Phi_\beta^\rho(s; \cdot) = 0$ on B, the essential support of s; but by the definition of $\Phi_\beta^\rho(s; \cdot)$, $\Phi_\beta^\rho(s; \cdot) = 0$ on B^c. ∎

The first part of Theorem 4 follows from Lemmas B2–B4; the rest of the claim follows as in ref. 6.

ACKNOWLEDGMENTS

I am grateful to N. G. Duffield and J. V. Pulè for generously providing and explaining their results, and thank them and J. T. Lewis for discussions and encouragement.

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