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Quantum Tunneling with Dissipation and the Ising Model over $\mathbb{R}$

Herbert Spohn[1] **and Rolf Dümcke**[1]

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We consider a quantum particle in a double-well potential, for simplicity in the two-level approximation, coupled to a phonon field. We show that static and dynamical ground state correlations of the particle and of the field are expressible through expectations in an Ising model over $\mathbb{R}$ (rather than $\mathbb{Z}$). Its free measure is a spin flip process with flip rate ε, the difference in energy between the ground state and the first excited state. The Ising model has a ferromagnetic pair interaction whose form depends on the couplings to the phonon field and on the dispersion relation of the phonon field. In physical applications the interaction is long ranged and decays as t^{-2} for large distances. In this case we prove that for sufficiently strong coupling the particle becomes localized in one of the wells. The effective tunnel rate is zero. The transition to localization is associated with the generation of an infinite number of low momentum phonons. We apply the Ising technology to our problem and discuss the phase diagram in some detail.

KEY WORDS: Two-level system coupled to an ideal heat bath; one-dimensional Ising model with long-range forces; absence and existence of a phase transition (= degeneracy of the ground state).

1. INTRODUCTION

Let us consider the motion of a particle (single degree of freedom) in a double-well potential of the form $V_\lambda(q) = \lambda(1-q^2)^2$, $\lambda > 0$. A low-energy classical particle in this potential simply oscillates around either one of the two minima located at $q = \pm 1$. A quantum particle, however, has the possibility of tunneling through the potential barrier to the other well and will do so with a frequency approximately proportional to

[1] Ludwig-Maximilians-Universität München, Theoretische Physik, Theresienstr. 37, D—8000 München 2, Federal Republic of Germany.

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$\exp\{-\int_{-1}^{1} dq[2V_\lambda(q)]^{1/2}\} = \exp[-\frac{4}{3}(2\lambda)^{1/2}]$; cf., e.g., Ref. 1, $m = 1 = \hbar$. Now let us assume that the particle interacts in addition with a phonon field (or the electromagnetic field; cf. below) in thermal equilibrium. If the thermal energies are much smaller than the height, λ, of the potential barrier, then classically the particle will once in a while be kicked by a large thermal excitation providing enough energy for a jump across the potential barrier into the other well. The particle's dynamics consists of two, in time well separated types of motions: fluctuations in either well and jumps at random (Poisson) times between the two wells. We are interested here in the dynamics of the quantum particle in the limit where thermal excitations are completely suppressed, i.e., the phonon field should be at zero temperature. The problem is then to understand how the quantum mechanical tunneling between the two wells is modified by the interaction with the phonon field.

We are, of course, not the first ones to study this problem. But let us first mold our problem into a standard form and list our main results. In Section 2 we will then discuss the various physical realizations.

The Hamiltonian of the quantum particle, not coupled to the phonon field, is given by

$$H = -\tfrac{1}{2}\Delta + V_\lambda \tag{1.1}$$

(We set the mass $m = 1 = \hbar$.) If λ is large, then the ground state, ψ_0, and the first excited state, ψ_1, are energetically well separated from all other states. This suggests to use of a two-level approximation. We choose the representation where $\binom{1}{0}$ and $\binom{0}{1}$ corresponds to an approximately Gaussian wave packet in the right- and left-hand wells, respectively. Then $\sqrt{2}\,\psi_0 \cong \binom{1}{1}$, $\sqrt{2}\,\psi_1 \cong \binom{1}{-1}$ and the Hamiltonian is approximated by $-\varepsilon\sigma_x$ with 2ε the level splitting, i.e., $2\varepsilon \cong \exp[-\frac{4}{3}(2\lambda)^{1/2}]$. σ_z has the meaning of the position operator. The complete Hamiltonian under consideration is then

$$H = -\varepsilon\sigma_x \otimes 1 + 1 \otimes \int_{\mathbb{R}} dk\, \omega(k)\, a^+(k)\, a(k)$$

$$+\sigma_z \otimes \int_{\mathbb{R}} dk\, \lambda(k)[a^+(k) + a(k)] - h\sigma_z \otimes 1 \tag{1.2}$$

Here $h\sigma_z$ breaks the reflection symmetry of the potential by making the right well deeper ($h > 0$). We are interested in the case $h \downarrow 0$. $\{a^+(k), a(k) \mid k \in \mathbb{R}\}$ is a scalar Bose field with commutation relation $[a(k), a^+(k')] = \delta(k - k')$. $\omega(k)$ is the dispersion relation of the Bose field and $\lambda(k)$ are the couplings. They enter only in the combination

$$\int dk\, \lambda(k)^2\, \delta(\omega(k) - \omega) \equiv \rho(\omega) \tag{1.3}$$

As to be argued, physically, the proper choice is

$$\rho(\omega) = \beta\omega \tag{1.4}$$

for small ω, $\beta > 0$.

The ground state energy of H, the zero point energy of the phonon field already subtracted, should be finite. This is ensured if

$$\int dk\, \lambda(k)^2/\omega(k) = \int_0^\infty d\omega\, \rho(\omega)\, 1/\omega < \infty, \int_0^\infty d\omega \rho(\omega) < \infty \tag{1.5}$$

This includes, in particular, the cases

$$\rho(\omega) = \beta\omega^{1-\gamma} \tag{1.6}$$

for small ω and $\gamma < 1$.

Equation (1.2) should be considered only as a formal expression with the obvious rigorization to be given below. Physically, the Bose field should be over $\mathbb{R}^3$, may have several components, and the couplings could be directionally dependent. This would modify the definition of the frequency density ρ—the quantity which completely determines the physics of the two-level system. Since we discuss ρ in generality, all the mentioned alterations are automatically included. Also the expressions for the field expectations (cf. Section 11) could easily be modified as to include additional features of the Bose field.

We want to study ground state correlations for H. Of particular interest are the static correlations of the particle, $\langle\sigma_z\rangle_+$, $\langle\sigma_x\rangle_+$, ($\langle\sigma_y\rangle_+ = 0$ always), and of the field, $\langle a(f)\rangle_+$, $\langle a^+(f)\, a(g)\rangle_+$ with $a(f) = \int dk\, f(k)\, a(k)$ and the time correlations $\langle\sigma_z(t)\,\sigma_z\rangle_+$, $\langle\sigma_x(t)\,\sigma_x\rangle_+$, etc. Here $\langle\cdot\rangle_+$ refers to the expectation in the ground state of H in the limit $h \downarrow 0$ and $A(t) = e^{itH}Ae^{-itH}$ for some operator A.

The way to attack this problem is implicitly present in the work of Yuval and Anderson[2] on the Kondo problem and, to our knowledge, has been spelled out clearly for the first time by Emery and Luther.[3] The idea is to represent e^{-TH} as a functional integral through the Feynman–Kac formula. $\varepsilon(\sigma_x - 1)$ generates a spin flip process with flip rate ε and $\omega(k)\, a^+(k)\, a(k)$ generates a harmonic oscillator (Ornstein–Uhlenbeck) process. Since the coupling to the field is linear, the Gaussian integration over the harmonic oscillator processes ($\equiv$Bose field) can be carried out producing an effective interaction for the spin process. Ground state correlations are thereby reduced to Ising expectations in the infinite volume limit. The Ising model so obtained differs from the usual one by having spin configurations $t \to \sigma(t) = \pm 1$ over $\mathbb{R}$ rather than over $\mathbb{Z}$.

In essence our paper puts the Emery–Luther observation in the appropriate mathematical context and then applies the modern technology of one-dimensional Ising models with long-range interactions to it. Most of the applications are fairly standard. Basically there are two complications:

(i) Because the model is over $\mathbb{R}$ we have to control short-distance fluctuations.

(ii) The free measure does not correspond to independent spins, but has the finite correlation length $1/2\varepsilon$.

Our main result concerns the analysis of the phase diagram as a function of ε, the level splitting, and of β, the coupling strength to the field; cf. the schematic Fig. 1 for the case of the physical choice (1.4). We consider the ground state in the limit $h \downarrow 0$. In the upper left $\langle \sigma_z \rangle_+ = 0$. This means that the particle is equally likely in either of the two wells. In the lower right $\langle \sigma_z \rangle_+ > 0$ which means that the particle is predominantly in the right well. For sufficiently strong coupling the particle cannot drag the phonon cloud along and the effective height of the potential barrier is infinite. This localization phenomenon is associated with an infinite number of low-momentum phonons. We establish rigorously a region where $\langle \sigma_z \rangle_+ > 0$ by using a corresponding result of Fröhlich and Spencer[4] on the Ising model with $1/r^2$ interaction. Improved mean field bounds yield a region with $\langle \sigma_z \rangle_+ = 0$ and a Gaussian domination of correlation functions. We establish also some results on static field expectations.

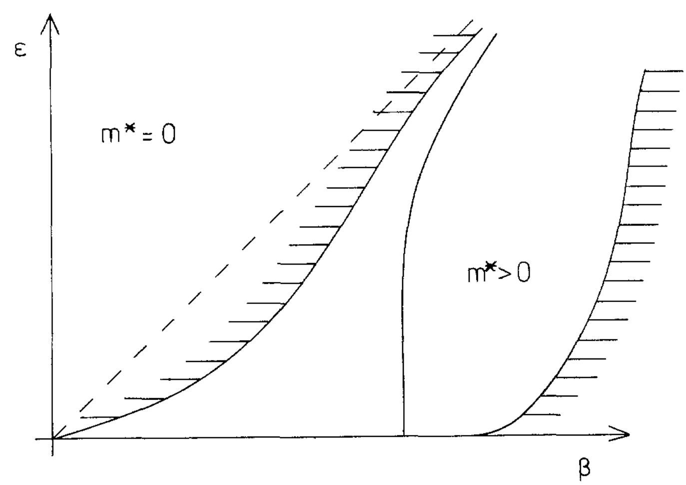

Fig. 1. Schematic form of the phase diagram for the interaction $V(t) \sim 1/t^2 (\rho(\omega) = \beta\omega$ for small $\omega)$. The shaded regions are established in this paper. --- is mean field and the lower part of — is the result of Anderson, Yuval and Hamann.[5]

The unbroken line is the phase boundary obtained from variational calculations and the renormalization group analysis of Anderson, Yuval, and Hamann.[5]

If $\int d\omega\, \rho(\omega)\, \omega^{-2} < \infty$, then $\langle \sigma_z \rangle_+ = 0$ always $(\varepsilon > 0)$. On the other hand if $\rho(\omega) \sim \omega^{1-\gamma}$, $0 < \gamma < 1$, then $\langle \sigma_z \rangle_+ > 0$ for sufficiently strong coupling. In contrast to the case $\gamma = 0$ the phase boundary reaches the origin as $\varepsilon = c\beta^{1/\gamma}$ for small β.

The dynamics of the models of the form (1.2) is well understood in the weak coupling limit.[6] We believe that the technique explained in this paper offers a method also to analyze the intermediate and strong coupling regimes.

2. SOME PHYSICAL REALIZATIONS

The physics of the Hamiltonian (1.2) comes from three somewhat apart areas: solid state physics, quantum chemistry, and the attempt to manufacture experimentally quantum wave packets on macroscopic scales.

(i) The solid state physics context is fairly obvious. We mentioned already the application to the Kondo effect in magnetic alloys. But also spin–phonon relaxation, the dynamics of paraelectric defects in solids and other phenomena are described by (1.2) (cf. Ref. 7 and references therein).

(ii) Pfeifer in his thesis[8] attempts to explain the existence of chiral molecules as a superselection rule which originates in the ever present coupling of the molecule to the radiation field. The phenomenon is that certain molecules, as alanine, with a left–right symmetry are experimentally always found in either $\psi_L (\equiv \psi_{\text{left}})$ or $\psi_R (\equiv \psi_{\text{right}})$ and never in the ground state $(1/\sqrt{2})(\psi_L + \psi_R)$. Furthermore ψ_L and ψ_R are very stable against perturbations. On the other hand other molecules, as, e.g., the isotopically substituted ammonia, whose molecular structure also has the left–right symmetry are found experimentally to be in their ground state. Such substances are optically inactive. Pfeifer argues that this effect is due to the coupling of the molecule to the electromagnetic field. The two states ψ_L and ψ_R of the molecule are represented in the two level approximation. The A^2 term of the nonrelativistically quantized electromagnetic field is neglected. In this approximation the molecule plus radiation field is described by the Hamiltonian (1.2). $\langle \sigma_z \rangle_+ = 0$ corresponds to an achiral molecule (the molecule tunnels between the two molecular states ψ_L and ψ_R, the ground state is nondegenerate), whereas $\langle \sigma_z \rangle_+ > 0$ corresponds to a chiral molecule. In Ref. 8 the Hamiltonian is analyzed as a Schrödinger operator and very useful information is supplied. However, Pfeifer could not establish with rigor the existence of the spontaneous symmetry breaking.

(iii) Caldeira and Leggett[9,10] posed the problem whether such a typical quantum effect as tunneling could be observed on a macroscopic scale. In contrast to the atomic scale, it would then be impossible, in principle, to isolate the system from its surroundings. A calculation based on an isolated system would predict physically incorrect results. Therefore Caldeira and Leggett were led to investigate tunneling in the presence of dissipation: The quantum particle moves in a potential with a local minimum, e.g. $V(q)=q^2(1-q)$ with the large-q behavior not to be taken seriously, and is initially localized in the minimum. To represent dissipation the particle is coupled to a Bose field as in (1.2). One wants to compute the tunnel rate out of the local minimum when the Bose field is in its ground state (zero temperature). For this purpose Caldeira and Leggett use the "bounce trajectory" technique of Coleman.[11,12] Their results triggered a number of further investigations. The tunnel rate at finite temperature is obtained in Ref. 13. If the external potential with a metastable minimum is replaced by a double-well potential, then one arrives at the problem under investigation in this paper. Various aspects of this problem are studied in Refs. 14–17.

To what extent do physical considerations fix the frequency distribution ρ[cf. (1.3)]? In the case of chiral molecules the Bose field is the electromagnetic field which has the dispersion relation $\omega(k)=c\,|k|$. The coupling contains a factor $|k|^{-1/2}$ from the quantization rules of the electromagnetic field and is proportional to the electric dipole matrix element between ψ_L and ψ_R. For the model Hamiltonian to be applicable at all this transition has to be allowed. Therefore the matrix element tends to a constant $\neq 0$ as $k \to 0$ and decreases rapidly for large $|k|$ because of the spatial localization of ψ_L and ψ_R. Altogether this yields $\rho(\omega)\sim\omega$ for small ω(cf. Ref. 8 for details).

For quantum tunneling with dissipation Caldeira and Leggett argue at great length that in order to have linear damping in the classical limit one must have $\rho(\omega)\sim\omega$ for small ω (cf. Ref. 18). For the Kondo effect already Anderson *et al.* argued that $\rho(\omega)\sim\omega$ which translates into a $1/t^2$ decrease for the interaction of the Ising model. In other solid state physics applications it does not seem to have been recognized that the low-frequency behavior of ρ determines essential features of the dynamics of the two-level system.

3. GROUND STATE CORRELATIONS AND ISING EXPECTATIONS/THE ISING MODEL OVER $\mathbb{R}$

We construct the ground state for H in (1.2) by first restricting the phonon field to the finite box $[-L, L]$. This makes the k spectrum discrete. Then thermal expectations at finite temperature are well defined. Subsequently the high-frequency cut off is removed and the box $L \to \infty$. The ground state is obtained in the limit of zero temperature. This is the physically correct order of limits.

We assume that ω and λ are measurable functions satisfying

$$\omega(k) \geqslant 0, \qquad \int dk\, \lambda(k)^2 < \infty, \qquad \int dk\, \lambda(k)^2/\omega(k) < \infty \tag{3.1}$$

It is convenient to introduce the square of the coupling at frequency ω by

$$\rho(d\omega) = \int dk\, \lambda(k)^2\, \delta(\omega(k) - \omega)\, d\omega \tag{1.3}$$

$\rho(d\omega)$ is a measure on $(0, \infty)$. If it has a density we denote it as $\rho(\omega)\, d\omega$. From (3.1) we conclude that

$$\int \rho(d\omega) < \infty, \qquad \int \rho(d\omega)\, \omega^{-1} < \infty \tag{3.2}$$

Let $x(\cdot)$ be standard Brownian motion. $P_x(dx(\cdot))$ is its path measure on $C([0, \infty), \mathbb{R})$ with $x(0) = x$. Let $\sigma(\cdot)$ be a spin flip process, $\sigma(t) = \pm 1$. $\sigma(\cdot)$ changes sign after an exponential holding time with mean $1/\varepsilon$. The flip rate is ε. $e^{-\varepsilon t(1 - \sigma_x)}$ is the transition probability of $\sigma(\cdot)$. We denote the path measure with $\sigma(0) = \sigma$ by $\mu_\sigma^\varepsilon(d\sigma(\cdot))$. It is concentrated on piecewise constant paths taking values ± 1. In (1.2) we replace the integral by a finite sum $j = 1,..., n$ and require $\omega(k_j) > 0$. Then by the standard Feynman–Kac construction the integral kernel of e^{-TH} has the functional integral representation

$$\begin{aligned} &e^{-TH}(\sigma, x_1,..., x_n \mid \sigma', x_1',..., x_n')\, dx_1' \cdots dx_n' \\ &\quad = e^{\varepsilon T} \int \mu_\sigma^\varepsilon(d\sigma(\cdot)) \prod_{j=1}^{n} P_{x_j}(dx_j(\cdot)) \\ &\qquad \times \exp\left[-\int_0^T dt\, V(\sigma(t), x_1(t),..., x_n(t)) \right] \delta_{\sigma'\sigma(T)} \prod_{j=1}^{n} \chi(x_j(T) \in dx_j') \end{aligned} \tag{3.3}$$

where the potential is given by

$$\begin{aligned} V(\sigma, x_1,..., x_n) = \frac{1}{2} \sum_{j=1}^{n} [&\omega(k_j)\, x_j^2 - \omega(k_j) \\ &+ \sigma\lambda(k_j)[2\omega(k_j)]^{1/2}\, x_j - h\sigma] \end{aligned} \tag{3.4}$$

$\chi(A)$ denotes the indicator function of the set A.

In the cut-off Hamiltonian we define thermal expectations. For the sake of concreteness we choose the expectation value of σ_z, i.e.,

$$\langle \sigma_z \rangle_{T,n} = \operatorname{tr} \sigma_z e^{-TH} / \operatorname{tr} e^{-TH} \tag{3.5}$$

with e^{-TH} given by (3.3). We perform the Gaussian integration over $\prod P$. This yields

$$\langle \sigma_z \rangle_{T,n} = Z(T, n)^{-1} \int \sum_{\sigma} \mu_{\sigma}^{\varepsilon}(d\sigma(\cdot))\, \sigma \delta_{\sigma\sigma(T)} \times \exp\left[\frac{1}{2} \int_0^T dt \int_0^T ds\, V_n^T(|t-s|)\, \sigma(t)\, \sigma(s) + h \int_0^T dt\, \sigma(t)\right] \tag{3.6}$$

with

$$V_n^T(t) = \sum_{j=1}^{n} \lambda(k_j)^2 \left(e^{-\omega(k_j)t} + e^{-\omega(kj)(T-t)}\right)/\left(1 - e^{-\omega(kj)T}\right) \tag{3.7}$$

and $Z(T, n)$ the obvious normalization.

For the box quantization of the phonon field with periodic boundary conditions $k_j = \pi j/L$, $j = \pm 1, \pm 2, \ldots$. Then $\lambda(k_j)^2$ in (3.4) should be replaced by $(\pi/L)^{1/2} \lambda(k_j)$. In (3.6) and (3.7) we let $n \to \infty$ and subsequently $L \to \infty$. By our assumptions the Riemann sum (3.7) approximates the integral and we obtain the thermal expectation of σ_z in the infinite-volume limit, $L \to \infty$, as

$$\langle \sigma_z \rangle_T = Z(T)^{-1} \int \sum_{\sigma} \mu_{\sigma}^{\varepsilon}(d\sigma(\cdot))\, \sigma \delta_{\sigma\sigma(T)} \times \exp\left[\frac{1}{2} \int_0^T dt \int_0^T ds\, V^T(|t-s|)\, \sigma(t)\, \sigma(s) + h \int_0^T dt\, \sigma(t)\right] \tag{3.8}$$

with

$$V^T(t) = \int \rho(d\omega)\left(e^{-\omega t} + e^{-\omega(T-t)}\right)/\left(1 - e^{-\omega T}\right) \tag{3.9}$$

We note that from above, by dominated convergence,

$$\lim_{T \to \infty} V^T(t) = V(t) \tag{3.10}$$

with

$$V(t) = \int \rho(d\omega)\, e^{-\omega|t|} \tag{3.11}$$

Clearly V is decreasing for $t \geqslant 0$ and by our assumptions

$$0 \leqslant V(t) \leqslant V(0) < \infty, \qquad \int dt\, V(t) < \infty \tag{3.12}$$

To obtain ground state expectations we have to take the limit $T \to \infty$. We denote the ground state by $\langle \cdot \rangle(\cdots)$. If necessary, we exhibit in the argument its dependence on ε, h, V [i.e., on $\rho(d\omega)$]. The limits $h \downarrow 0$ and $h \uparrow 0$ are distinguished as $\langle \cdot \rangle_+(\cdots)$ and $\langle \cdot \rangle_-(\cdots)$.

It is clear that (3.8) defines an Ising model over $\mathbb{R}$ and that $T \to \infty$ corresponds to its infinite volume limit. We first define the Ising model in its own right. Because $V^T \geqslant 0$ the interaction is ferromagnetic. It may be of long range, however. As the Ising model is over $\mathbb{R}$, we cannot properly refer to known theorems. Since in the following section we will show the validity of Griffiths, FKG, Lebowitz, and other inequalities for this model, we feel entitled to be a bit sloppy here and not to repeat the proofs existing for the Ising model over $\mathbb{Z}$.

We define the +state of the Ising model, since this is the state of interest. The free measure is given by the spin flip process: We place $2n$ points in the interval $[-T, T]$, $-T < q_1 < \cdots < q_{2n} < T$. The corresponding spin configuration $\sigma(t)$ equals to 1 for $q_{2j-2} \leqslant t < q_{2j-1}$ and equals to -1 for $q_{2j-1} \leqslant t < q_{2j}$, $j = 1, 2,..., n+1$ with $q_0 = -\infty$, $q_{2n+1} = \infty$. This spin configuration carries the weight one for $n = 0$ and $\varepsilon^{2n}\, dq_1 \cdots dq_{2n}$ for $n = 1, 2,...$, which defines the free spin measure $\mu^{\varepsilon}_{T,+}(d(\cdot))$ with +boundary conditions. Other boundary conditions are constructed correspondingly. The full finite volume measure is

$$\langle \cdot \rangle_{+,T} = Z_+(T)^{-1} \int \mu^{\varepsilon}_{T,+}\, (d\sigma(\cdot)) \exp\left\{ -\tfrac{1}{2} \int dt ds\, V(t-s)[1 - \sigma(t)\, \sigma(s)] \right\} (\cdot) \tag{3.13}$$

The limit $T \to \infty$ defines the probability measure $\langle \cdot \rangle_+$, the +state, on $\mathscr{D}(\mathbb{R}, \{-1, 1\}) = \mathscr{D}$, the space of piecewise constant functions taken values ± 1. $\langle \cdot \rangle_+$ is translation invariant and mixing with respect to translations.

The connection with the quantum mechanical ground state is given by

$$\langle \sigma_z \rangle_+ = \langle \sigma(0) \rangle_+ \tag{3.14}$$

To see this we define the equilibrium (Gibbs) state with magnetic field h by adding $-h \int dt \sigma(t)$ to the interaction. For $h \neq 0$ the infinite-volume limit exists and is independent of the boundary conditions.[26] Furthermore $\langle \cdot \rangle_+$ is the limit $h \downarrow 0$ of $\langle \cdot \rangle(h)$. Let $\sigma_A = \prod_{j=1}^{n} \sigma(t_j)$ and L be such that $t_j \in [-L, L]$ for all j. The quantum mechanical expectation $\langle \sigma_z \rangle$ at finite temperature $1/2T$ equals the expectation of $\sigma(0)$ in the Gibbs state $\langle\cdot\rangle_{2T,\mathrm{per}}(h)$ with interaction potential V^{2T} and with periodic boundary conditions. Let $T > L$. We impose an infinite external field in $[-T, -L] \cup [L, T]$. Thereby $\langle\sigma_A\rangle$ is increased. We keep L fixed and let $T \to \infty$. Then by (3.10) $\langle\sigma_A\rangle$ converges to $\langle\sigma_A\rangle_{L,+}(h)$, where now the Gibbs state is over $[-L, L]$ and refers to the potential V with $+$boundary conditions as defined above. Therefore

$$\lim_{T\to\infty} \sup\langle\sigma_A\rangle_{2T,\mathrm{per}}(h) \leqslant \langle\sigma_A\rangle_{L,+}(h) \tag{3.15}$$

and similarly for the $-$ state,

$$\lim_{T\to\infty} \inf\langle\sigma_A\rangle_{2T,\mathrm{per}}(h) \geqslant \langle\sigma_A\rangle_{L,-}(h) \tag{3.16}$$

For $L \to \infty$ and $h \neq 0$

$$\langle\sigma_z\rangle(h) = \langle\sigma(0)\rangle(h) \tag{3.17}$$

by uniqueness, which as $h \downarrow 0$ yields (3.14).

Also other ground state correlations of the two-level system may be expressed as Ising expectations. For σ_x there has to be a spin flip at $t = 0$. This yields

$$\langle\sigma_x\rangle_+ = \lim_{t\downarrow 0} -\frac{1}{2\varepsilon}\frac{1}{t}\left[\langle\sigma(0)\,\sigma(t)\rangle_+ - 1\right] \tag{3.18}$$

$\langle\sigma_y\rangle_+ = 0$, since the reduced density matrix of the two-level system is real.

For dynamical correlations let us take as an example $\langle\sigma_z(t)\,\sigma_z\rangle_+$. In the cut-off Hamiltonian one considers

$$\mathrm{tr}\, e^{-(T-t)H}\sigma_z e^{-tH}\sigma_z/\mathrm{tr}\, e^{-TH} = \int \nu_{zz}^{(T)}(d\lambda)\, e^{-\lambda t} \tag{3.19}$$

for $0 \leqslant t \leqslant T$ with some spectral (probability) measure $\nu_{zz}^{(T)}(d\lambda)$ on the real line. From the functional integral representation we know that the left-hand side of (3.19) has a limit as $T \to \infty$ for every $t \geqslant 0$. Since the family of functions $\{e^{-\lambda t} \mid t \geqslant 0\}$ is convergence determining, we conclude that $\nu_{zz}^{(T)}(d\lambda)$ has the weak limit $\nu_{zz}(d\lambda)$, concentrated on $[0, \infty)$ by the KMS condition, and that therefore the two point function has the spectral representation

$$\int_0^\infty \nu_{zz}(d\lambda)\, e^{-\lambda|t|} = \langle\sigma(0)\,\sigma(t)\rangle_+ \tag{3.20}$$

The dynamical correlation $\langle \sigma_z(t)\, \sigma_z \rangle$ for finite temperature is defined as

$$\operatorname{tr} e^{-TH} e^{itH} \sigma_z e^{-itH} \sigma_z / \operatorname{tr} e^{-TH} = \int v_{zz}^{(T)}(d\lambda)\, e^{-i\lambda t} \tag{3.21}$$

Since $v_{zz}^{(T)}(d\lambda)$ tends to $v_{zz}(d\lambda)$ as $T \to \infty$, we finally conclude that in the ground state

$$\langle \sigma_z(t)\, \sigma_z \rangle_+ = \int_0^\infty v_{zz}(d\omega)\, e^{-i\omega t} \tag{3.22}$$

If the system is initially in the ground state and is for $t > 0$ subject to a weak field $e^{i\omega t}\sigma_z$, then for large t, in linear response,

$$\langle \sigma_z(t) \rangle - \langle \sigma_z \rangle \cong \chi(\omega)\, e^{i\omega t} \equiv [\chi'(\omega) + i\chi''(\omega)]\, e^{i\omega t} \tag{3.23}$$

The real and imaginary part of the response function $\chi(\omega)$ is given by

$$\begin{aligned} \chi'(\omega) &= \int_0^\infty v_{zz}(d\lambda)[2\omega/(\lambda^2 - \omega^2)] \\ \chi''(\omega)\, d\omega &= \chi(\{\omega > 0\})\, v_{zz}(d\omega) - \chi(\{\omega < 0\})\, v_{zz}(-d\omega) \end{aligned} \tag{3.24}$$

The usual sum rules (cf., e.g., Ref. 18) are trivially satisfied.

For the other dynamical correlations we observe that

$$[H, \sigma_z] = [-\varepsilon\sigma_x, \sigma_z] = 2i\varepsilon\sigma_y \tag{3.25}$$

Therefore the dynamical correlations for σ_y are obtained from the spectral measures corresponding to σ_z, e.g.,

$$\langle \sigma_y(t)\, \sigma_y \rangle_+ = (1/2\varepsilon)^2 \int_0^\infty v_{zz}(d\omega)\, \omega^2 e^{-i\omega t} \tag{3.26}$$

For the σ_x correlation we use the argument leading to (3.18). For example,

$$\langle \sigma_x(t)\, \sigma_x \rangle_+ = \int_0^\infty v_{xx}(d\omega)\, e^{-i\omega t} \tag{3.27}$$

where for $t > 0$

$$\begin{aligned} \int_0^\infty v_{xx}(d\lambda)\, e^{-\lambda t} &= \lim_{s \downarrow 0} \lim_{s' \downarrow 0} [1/(2\varepsilon)^2 ss'] \\ &\times [\langle \sigma(0)\, \sigma(s)\, \sigma(t)\, \sigma(t+s') \rangle_+ - \langle \sigma(t)\, \sigma(t+s') \rangle_+ - \langle \sigma(0)\, \sigma(s) \rangle_+ + 1] \end{aligned} \tag{3.28}$$

If we define the joint spectral measure for t_1, t_2, $t_3 \geqslant 0$ by

$$\int_0^\infty \nu(d\omega_1, d\omega_2, d\omega_3) \exp[-(\omega_1 t_1 + \omega_2 t_2 + \omega_3 t_3)]$$

$$= \langle \sigma(0)\, \sigma(t_1)\, \sigma(t_1 + t_2)\, \sigma(t_1 + t_2 + t_3) \rangle_+ \tag{3.29}$$

then

$$\nu_{xx}(d\omega) = (1/2\varepsilon)^2 \int_0^\infty \nu(d\omega_1, d\omega, d\omega_2)\, \omega_1 \omega_2 \tag{3.30}$$

In conclusion, all static and dynamic ground state correlations of the two-level system are expressible through correlation functions of the Ising model over $\mathbb{R}$. We will see in Section 11 that this is also the case for field expectations.

We argued in Section 2 that the physics of the model Hamiltonian H forces $\rho(\omega) \cong \omega$ for small ω, which implies

$$V(t) \cong 1/t^2 \tag{3.31}$$

for large t. As is well known for the Ising model over $\mathbb{Z}$ the $1/t^2$ decay of the interaction is exactly on the borderline for the existence of a phase transition.[20] First of all, the pair interaction has to be integrable for the infinite-volume limit to exist. We imposed this in (3.1). If, over $\mathbb{Z}$, the decay is slower than $1/t^2$, in fact if the pair interaction satisfies

$$V(t) \geqslant c(\log\log(|t| + 3))/(t^2 + 1) \tag{3.32}$$

Dyson[21,22] established a nonzero spontaneous magnetization for sufficiently low temperatures. He used the hierarchical model as comparison. If the decay is faster than $1/t^2$, in fact if

$$\lim_{N \to \infty} (\log N)^{-1/2} \sum_{n=1}^{N} nV(n) = 0 \tag{3.33}$$

then the spontaneous magnetization is zero at any interaction strength and $\langle \cdot \rangle_+ = \langle \cdot \rangle_-$.[23–25] For a decay exactly as $1/t^2$ Fröhlich and Spencer[4] prove by a sophisticated entropy–energy argument the existence of a nonzero spontaneous magnetization for sufficiently low temperatures.

One of our aims is to obtain the corresponding results for the Ising model over $\mathbb{R}$ with emphasis on the border line case $1/t^2$. We discuss the phase diagram in dependence on the natural physical parameters: The coupling strength β and the level splitting 2ε($\equiv$ twice the spin flip density of the free measure).

4. LATTICE APPROXIMATION AND INEQUALITIES

One of the helpful facts about ferromagnetic Ising models are inequalities. In general, the natural way to prove them is through a lattice approximation of the continuum model which we do first.

We approximate the free measure of the continuum model by a nearest-neighbor Ising model with lattice spacing δ and coupling $J(\delta)$. To each lattice configuration $\{\sigma_j\}$ we associate a continuum spin configuration by $\sigma(t)=\sigma_j$ for $(j-\frac{1}{2})\,\delta \leqslant t < (j+\frac{1}{2})\,\delta$. This has the advantage of all measures being defined on the same space. The free measure of the continuum model has the two-point function $\langle\sigma(t)\,\sigma(0)\rangle = e^{-2\varepsilon|t|}$. Since the pair correlation of the lattice model

$$\langle\sigma_0\sigma_{j\delta}\rangle = [\tanh J(\delta)]^{|j\delta|} \tag{4.1}$$

$j\in\mathbb{Z}$, for it to approximate the continuum model the nearest-neighbor coupling has to diverge as $J(\delta)=\frac{1}{2}\log\delta\varepsilon$. For each δ this defines then a measure $\langle\cdot\rangle^{(\delta)}_{\text{free}}$ on $\mathscr{D}$ and $\langle\cdot\rangle^{(\delta)}_{\text{free}}$ converges weakly to the free measure of the continuum model as $\delta\to 0$.

We consider now the finite interval $[-T, T]$ and $+$ (or some other) boundary conditions. The Gibbs measure with interaction is approximated by an Ising model with lattice spacing δ, $+$ boundary conditions outside the interval $[-T/\delta, T/\delta]$ and interaction

$$\tfrac{1}{2}J(\delta)\sum_{i,j,|i-j|=1}(1-\sigma_i\sigma_j)+\tfrac{1}{2}\delta^2\sum_{i,j}V((i-j)\,\delta)(1-\sigma_i\sigma_j) \tag{4.2}$$

Then the Ising measure $\langle\cdot\rangle^{(\delta)}_{T,+}$ converges weakly to $\langle\cdot\rangle_{T,+}$, the Gibbs measure with interaction of the continuum model. In particular the correlation functions converge,

$$\lim_{\delta\to 0}\left\langle\prod_{j=1}^{n}\sigma(t_j)\right\rangle^{(\delta)}_{T,+} = \left\langle\prod_{j=1}^{n}\sigma(t_j)\right\rangle_{T,+} \tag{4.3}$$

It is now obvious how inequalities[2] are proved: Whenever an inequality holds for finite δ, it also holds for the limit measure—the one of interest. There is one proviso, however: Some inequalities, such as, e.g., Simon's inequality,[(28)] contain explicitly the pair potential which diverges logarithmically as $\delta\to 0$ and therefore renders the inequality useless as it stands.

The diverging nearest-neighbor coupling teaches us that, in general, it is not a promising strategy for showing some specific property of the con-

[2] For a summary see Ref. 27.

tinuum model to first prove it in the lattice approximation hoping for enough uniformity in the strength of the nearest-neighbor coupling.

It should be remarked that probabilistically our construction is very well known: It corresponds to the approximation of the Poisson process by a two-state Markov chain in the limit of rare events.

5. THE EQUIVALENT SYSTEM OF CHARGES

As exploited already by Yuval and Anderson we may reformulate the Ising model as a system of classical point particles. The particles are located at the points of spin flips, $-T < q_1 \cdots < q_{2n} < T$. Their interaction energy equals, in the case of plus boundary conditions,

$$\begin{aligned}\frac{1}{2} \sum_{\substack{k \neq j = 1 \\ k/j = \text{even/odd}}} \int_{q_j}^{q_{j+1}} dt \int_{q_k}^{q_{k+1}} ds\, V(t-s) + \text{b.c.} \\ = \sum_{j \neq k = 1}^{2n} (-1)^{j-k} U(|q_j - q_k|) + 2nU(0) \\ + \lim_{q \to \infty} \sum_{j=1}^{2n} [(-1)^j U(q_j + q) + (-1)^{j+1} U(q - q_j)] \end{aligned} \qquad (5.1)$$

where

$$\frac{d^2}{dt^2} U(t) = V(t) \qquad (5.2)$$

for $t > 0$. The energy (5.1) does not depend on the constants of integration of (5.2).

There are two equivalent possibilities to interpret (5.1): (5.1) corresponds to a system of classical particles with charges ± 1 constrained to alternate. The fugacity of the gas is $\varepsilon e^{-U(0)}$ and the interaction energy for a pair of charges is $e_j e_k U(|q_j - q_k|)$ with charges $e_j = \pm 1$. Alternatively, we may think of (5.1) as a system of classical uncharged particles. The fugacity is $\varepsilon e^{-U(0)}$, but the interaction is many body of the form

$$\sum_{j \neq k = 1}^{2n} (-1)^{N([q_j, q_k])} U(|q_j - q_k|) \qquad (5.3)$$

where $N([a, b])$ denotes the number of particles in the interval $[a, b]$.

6. THE EQUIVALENT CLASSICAL RANDOM NOISE

In the Ising model the phonon field entered only through the effective interaction. The same interaction could also be obtained from the classical noise $\xi(t)$ with $\xi(\cdot)$ Gaussian, $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\, \xi(s) \rangle = V(t-s)$. The random Hamiltonian is then

$$H(t) = -\varepsilon\sigma_x - h\sigma_z + \xi(t)\, \sigma_z \tag{6.1}$$

Then, e.g.,

$$\langle \sigma(0) \rangle(h) = \lim_{T\to\infty} \mathbb{E} \left\langle \operatorname{tr} \left\{ \exp\left[-\int_{-T}^{0} dt\, H(t) \right] \sigma_z \right.\right.$$
$$\left.\left. \times \exp\left[-\int_0^T dt\, H(t) \right] \right\} \right\rangle \Big/ \mathbb{E} \left\langle \operatorname{tr} \left\{ \exp\left[-\int_{-T}^{T} dt\, H(t) \right] \right\} \right\rangle \tag{6.2}$$

where $\exp[-\int \cdots]$ is understood as time ordered exponential and $\mathbb{E}$ is the average over $\xi(t)$. The averaging over the noise follows the "annealed" prescription. Dynamically of interest are nonthermal, time-dependent expectations as, e.g.

$$\mathbb{E} \left\langle \psi \mid \exp\left[i \int_0^t ds\, H(s) \right] \sigma_z \exp\left[-i \int_0^t ds\, H(s) \right] \psi \right\rangle \tag{6.3}$$

which may be expressed, through analytic continuation, as an expectation in the Ising model. Of course, the physics of the two-level atom coupled to the phonon field and of the Hamiltonian (6.1) are very different. Only certain expectation values are the same.

The example shows that statistical mechanics methods may be used to study the effect of noise on quantum systems. The Hamiltonian (6.1) is an approximation to the noisy Hamiltonian $-\frac{1}{2}\Delta + V_\lambda(q) + \xi(t)\, q$. Fröhlich and Pillet[29] investigated the much more complicated case of $-\frac{1}{2}\Delta + \cos q + \xi(t)\, q$.

7. A VARIATIONAL CALCULATION

We analyze a variational upper bound for the free energy, i.e., for the ground state energy of the quantum system.

The partition function for finite volume is

$$Z(T) = (\cosh 2T)^{-1} \int \mu_T^\varepsilon(d\sigma(\cdot))$$
$$\times \exp\left[-\tfrac{1}{2}\beta \int dt\, ds\, V(t-s)[1 - \sigma(t)\, \sigma(s)] + h \int dt\, \sigma(t) \right] \tag{7.1}$$

As a comparison state we choose the free measure with spin flip density λ and magnetic field α. Then by Jensen's inequality

$$Z(T) \geqslant \operatorname{tr}\{\exp[2T(\lambda\sigma_x + \alpha\sigma_z)]\} \exp[\langle n\rangle_{T,\text{free}}(\lambda, \alpha) \log(\varepsilon/\lambda)$$

$$-\tfrac{1}{2}\beta \int dt\, ds\, V(t-s)[1 - \langle \sigma(t)\, \sigma(s)\rangle_{T,\text{free}}(\lambda, \alpha)]$$

$$+ (h-\alpha) \int dt \langle \sigma(t)\rangle_{T,\text{free}}(\lambda, \alpha)] \tag{7.2}$$

with n the number of spin flips. We evaluate the correlation functions in the limit $T \to \infty$. It is convenient to introduce polar coordinates $\lambda = r\cos\Theta$ and $\alpha = r\sin\Theta$, $r \geqslant 0$, $0 \leqslant \Theta \leqslant \pi/2$. Then the free energy, $f(\beta, \varepsilon, h)$, of the Ising model is bounded by

$$f(\beta, \varepsilon, h) \leqslant \min_{r \geqslant 0, 0 \leqslant \cos\Theta \leqslant 1}$$

$$\times \{-r(\cos\Theta)^2[\log(\varepsilon/r\cos\Theta) + 1] + (\cos\Theta)^2 \beta g(r) - h\sin\Theta\} \tag{7.3}$$

with

$$g(r) = 2r \int \rho(d\omega)[\omega(\omega + 2r)]^{-1} \tag{7.4}$$

We discuss the phase diagram for $h = 0$ associated with the upper bound (7.3). The stationarity conditions are

$$r\cos\Theta = \varepsilon e^{-\beta g'(r)} \tag{7.5}$$

$$r\cos\Theta = \varepsilon \exp\left[\frac{1}{2} - \frac{1}{r}\beta g(r)\right] \tag{7.6}$$

If (7.5), (7.6) allow a solution in the interior of the domain, i.e., $0 < \cos\Theta < 1$, then it has to lie on the circle with radius r satisfying

$$\frac{1}{2} = \beta\left[\frac{1}{r} g(r) - g'(r)\right] \tag{7.7}$$

At such a stationary point the free energy equals

$$-\tfrac{1}{2} r(\cos\Theta)^2 \tag{7.8}$$

On the boundary, $\Theta = 0$, the free energy is

$$-r[\log(\varepsilon/r) + 1] + \beta g(r) \tag{7.9}$$

The stationarity condition is

$$r = \varepsilon e^{-\beta g'(r)} \tag{7.10}$$

with

$$g'(r) = 2 \int \rho(d\omega)(\omega + 2r)^{-2} \tag{7.11}$$

At such a stationary point the free energy equals

$$r \left\{ \beta \left[\frac{1}{r} g(r) - g'(r) \right] - 1 \right\} \tag{7.12}$$

Note that by dominated convergence $g(0) = 0$.

Finally we need the directional derivative, $-d/d \cos \Theta$, in the Θ direction at $\Theta = 0$. It is given by $-2\{-r[\log(\varepsilon/r) + \beta g(r)]\}$. At the point satisfying (7.10) it is then

$$-2r \left\{ \beta \left[\frac{1}{r} g(r) - g'(r) \right] - \frac{1}{2} \right\} \tag{7.13}$$

Now the overall picture is fairly clear. We fix β and discuss the location of the absolute minimum, (r_m, Θ_m), as a function of ε.

The function

$$\frac{1}{r} g(r) - g'(r) = \frac{\int \rho(d\omega)\, 4r}{\omega(\omega + 2r)^2} \tag{7.14}$$

decreases to zero for large r. Therefore for $\varepsilon \to \infty$, in view of (7.8), (7.12), and (7.13), the minimum is at $(r_m, 0)$, r_m large. Let r_c be the largest value at which (7.7) holds. If (7.7) cannot be satisfied, then $\Theta_m = 0$ always, since by (7.13) we have a boundary minimum and since by (7.12) its free energy is always smaller than the one at $r = 0$. The free energy depends smoothly on ε and the spontaneous magnetization remains zero.

Assume then $r_c > 0$ and denote the corresponding value of ε by ε_c. For $\varepsilon \geqslant \varepsilon_c$ the minimum has to be on the boundary according to the previous argument. As $r < r_c$, $\Theta = 0$, the derivative (7.13) changes sign and the minimum has to lie at $(r_m = r_c, \Theta_m > 0)$. ε_c is a critical point. From (7.3) the spontaneous magnetization $m^* = -\sin \Theta$. Inserting we obtain for $\varepsilon \leqslant \varepsilon_c$

$$m^* = [1 - (\varepsilon/\varepsilon_c)^2]^{1/2} \tag{7.15}$$

The phase transition is second order of mean field type.

The phase boundary is

$$\varepsilon_c = r_c e^{\beta g'(rc)} \tag{7.16}$$

with r_c the largest solution to (7.7). For large β

$$\varepsilon_c = 2\beta \int \rho(d\omega)\, \omega^{-1} \tag{7.17}$$

This is the usual mean field solution. For small β the phase boundary depends on the asymptotic decay of $V(t)$. If

$$\int \rho(d\omega)\, \omega^{-2} < \infty \tag{7.18}$$

then $(1/r)\, g(r) - g'(r)$ is bounded and tends to zero as $r \to 0$. Therefore there is a minimal β^* for which (7.7) is satisfied and $r_c > 0$ at that point. Hence $\varepsilon_c(\beta^*) > 0$. For $\beta < \beta^*$ the free energy is smooth. For $0 < \varepsilon < \varepsilon_c(\beta^*)$ the spontaneous magnetization jumps as a function of β. If

$$\frac{1}{r}\, g(r) - g'(r) \to \infty \qquad \text{as} \quad r \to 0 \tag{7.19}$$

then $r_c \to 0$ as $\infty \to 0$. The phase boundary reaches the point $\varepsilon_c = 0$, $\beta_c = 0$. If $\rho(\omega) \cong \omega^{1-\gamma}$, $0 < \gamma < 1$, then $\varepsilon_c \sim \beta^{1/\gamma}$ for small β. $V(t) \cong t^{-2}$ is exactly on the borderline. In this case ε_c tends to zero continuously, but reaches zero at some $\beta^* > 0$.

A schematic phase diagram is plotted in Fig. 2. The variational bound

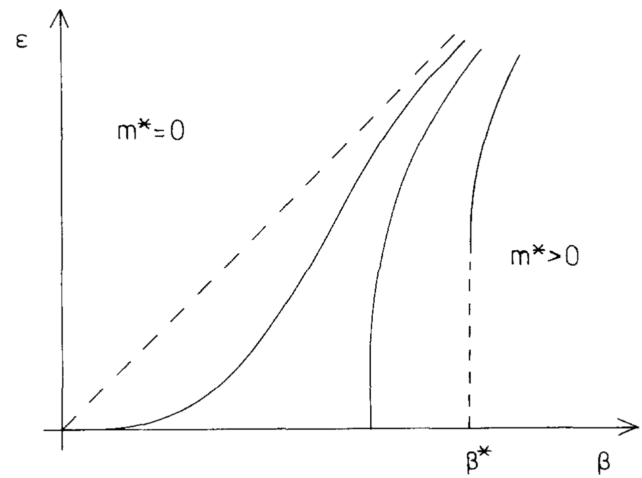

Fig. 2. Phase diagram according to the variational bound for the interaction $V(t) \sim t^{-2+\gamma}$. The left hand curve corresponds to $0 < \gamma < 1$, the middle curve to $\gamma = 0$ and the right hand curve to $\gamma < 0$.

captures some features of the actual phase diagram. But, as expected, it cannot reproduce correctly the difference between the t^{-2} and faster than t^{-2} decay.

8. ABSENCE OF PHASE TRANSITION

If

$$\int \rho(d\omega)\, \omega^{-2} < \infty \tag{8.1}$$

then the spontaneous magnetization is zero and the infinite-volume Gibbs measure is independent of the choice of the boundary conditions (uniqueness of the Gibbs measure). This will be proved in Section 10, where we extend the energy–entropy argument of Simon and Sokal[30] to the present situation. Presumably the slightly sharper bound (3.33) could also be generalized. If (8.1) is satisfied, the quantum particle still tunnels between the two wells even when strongly coupled to the phonon field.

(8.1) yields no information about the physically relevant couplings. One general method to delineate the one phase region are mean field bounds. We present a slightly improved version of Ref. 31.

The interaction is split up into a short-range and long-range part,

$$V(t) = V_s(t) + V_l(t) \tag{8.2}$$

both positive, and we define the interaction

$$V_\lambda(t) = V_s(t) + \lambda V_l(t) \tag{8.3}$$

Let $\langle \cdot \rangle_\lambda$ be the Gibbs measure with interaction $\beta V_\lambda(t)$ and free boundary conditions. As before the free measure has the spin flip density ε. Then

$$\begin{aligned}\frac{d}{d\lambda} \langle \sigma(0)\, \sigma(t) \rangle_\lambda &= \tfrac{1}{2}\beta \int ds \int ds'\, V_l(s-s')[\langle \sigma(0)\, \sigma(t)\, \sigma(s)\, \sigma(s') \rangle_\lambda \\ &\quad - \langle \sigma(0)\, \sigma(t) \rangle_\lambda \langle \sigma(s)\, \sigma(s') \rangle_\lambda] \\ &\leqslant \beta \int ds \int ds'\, V_l(s-s') \langle \sigma(0)\, \sigma(s) \rangle_\lambda \langle \sigma(t)\, \sigma(s') \rangle_\lambda \end{aligned} \tag{8.4}$$

by Lebowitz' inequality.[32] $\langle \sigma(0)\, \sigma(t) \rangle_\lambda$ is then bounded by the solution of the differential equation corresponding to (8.4) with initial conditions $\langle \sigma(0)\, \sigma(t) \rangle_{\lambda=0} = \langle \sigma(0)\, \sigma(t) \rangle_T(\beta V_s)$. Let

$$\alpha(k) = \frac{1}{(2\pi)^{1/2}} \int dt\, e^{ikt} \langle \sigma(0)\, \sigma(t) \rangle (\beta V_s) \tag{8.5}$$

Since $\hat{V}_l(k)$ and $\alpha(k)$ take their supremum at $k=0$, the condition for the solution of the differential equation corresponding to (8.4) to stay bounded for $0 \leqslant \lambda \leqslant 1$ yields, in the infinite-volume limit,

$$\beta\left[\int dt\, V_l(t)\right]\int dt\langle\sigma(0)\,\sigma(t)\rangle(\beta V_s) < 1 \tag{8.6}$$

If (8.6) holds, then

$$\begin{aligned}\langle\sigma(0)\,\sigma(t)\rangle(\beta V) &\leqslant \frac{1}{(2\pi)^{1/2}}\int dk\, e^{-ikt}\alpha(k)[1-2\pi\beta\hat{V}_l(k)\,\alpha(k)]^{-1}\\ &\equiv \langle\sigma(0)\,\sigma(t)\rangle\tilde{}\end{aligned} \tag{8.7}$$

Moreover by the Gaussian inequality [33, 34, 35][36],

$$\begin{aligned}\left\langle\prod_{j\in A}\sigma(t_j)\right\rangle(\beta V) &\leqslant \sum_{\text{pairings}\in A}\prod\langle\sigma(t_i)\,\sigma(t_j)\rangle(\beta V)\\ &\leqslant \sum_{\text{pairings}\in A}\prod\langle\sigma(t_i)\,\sigma(t_j)\rangle\tilde{}\end{aligned} \tag{8.8}$$

i.e., provided (8.6) is satisfied, the correlation functions of $\langle\cdot\rangle(\beta V)$ are bounded by those of the Gaussian measure with mean zero and covariance $\langle\sigma(0)\,\sigma(t)\rangle\tilde{}$. In particular, the spontaneous magnetization is zero and the infinite-volume limit is independent of the boundary conditions (cf. Ref. 31 for details).

The simplest way to use (8.6) is the choice $V_s = 0$. Then $\langle\sigma(0)\,\sigma(t)\rangle(\beta V_s) = \exp(-2\varepsilon\,|t|)$ and (8.6) yields the mean field criterion

$$2\beta\int\rho(d\omega)\,\omega^{-1} < \varepsilon \tag{8.9}$$

for the absence of a phase transition.

The upper bound (8.7) can be supplemented by a lower one. By Griffiths,[37–39]

$$\langle\sigma(0)\,\sigma(t)\rangle(\beta V) \geqslant cV(t) \tag{8.10}$$

In particular for $V(t)\sim t^{-2+\gamma}$, $0 \leqslant \gamma < 1$, in the region defined by (8.9), (8.7), and (8.10) imply the upper and lower bounds

$$c_-(1+t^{2-\gamma})^{-1} \leqslant \langle\sigma(t)\,\sigma(0)\rangle \leqslant c_+(1+t^{2-\gamma})^{-1} \tag{8.11}$$

Equation (8.9) is not a sharp bound on the one phase region. One expects a phase diagram as Fig. 2 with the line corresponding to $t^{-2+\gamma}$,

$\gamma < 0$, omitted. To proceed in this direction a less trivial short range part of the potential has to be used. The only computationally accessible case, besides $V_s = 0$, seems to be $V_s(t) = \lambda^2 \exp(-\alpha\,|t|)$. This corresponds to the one-fermion–one-boson problem

$$H = -\varepsilon\sigma_x + \alpha a^+ a + \lambda\sigma_z(a^+ + a) \tag{8.12}$$

about which rather detailed information is available.[40] If, in the case $V(t) \sim t^{-2}$, we use it in (8.6), then the upper bound on the phase transition drops below the mean field bound as expected. However, even optimizing the exponential, yields only a somewhat smaller, but still finite, slope at $\beta = 0$.

A more sophisticated approach is the use of a low-density expansion. We define

$$V_s(t) = \begin{cases} V(t) & \text{for} \quad |t| \leqslant s \\ 0 & \text{for} \quad |t| > s \end{cases} \tag{8.13}$$

We map the system with interaction V_s onto the system of charges with potential U_s (cf. Section 5). The constants of integration are chosen such that U_s has range s. We assume ε to be small. Then the particles are far (i.e., $\sim 1/\varepsilon$) apart and it is natural to use a low-density expansion. For a classical continuous particle system with pair potential V and fugacity z the convergence radius of the low-density expansion is

$$\beta z e^{\beta B} \, \|V\|_1 < 1/e \tag{8.14}$$

with B the stability constant.[41,42] In our case the potential is many body and it is not clear whether (8.14) still holds. In the spirit that there is no hope to establish a larger convergence radius, let us assume (8.14). The fugacity is

$$z = \varepsilon e^{-\beta V_s(0)} \tag{8.15}$$

The stability bound is a consequence of the positivity of the Ising interaction which implies the stability constant $B = U_s(0)$. If $V(t) \cong t^{-2+\gamma}$, $0 \leqslant \gamma < 1$, then $\|V_s\|_1 \cong s^{1+\gamma}$ for large s and we obtain from (8.14)

$$\beta \varepsilon s^{1+\gamma} \leqslant c \tag{8.16}$$

This means that the low-density expansion should converge provided the range of the potential is of the order of ($\gamma = 0$) or less than ($\gamma > 0$) the mean distance between particles. We evaluate $\int dt \langle \sigma(0)\,\sigma(t)\rangle (\beta V_s)$

approximately by setting $U_s = 0$ and keeping only the change in fugacity due to $U_s(0)$. Then

$$\int dt \langle \sigma(0)\,\sigma(t)\rangle (\beta V_s) \cong \begin{cases} 1/\varepsilon s^{-\beta}, & \gamma = 0 \\ 1/\varepsilon \exp\left(-\dfrac{1}{\gamma} s^{\gamma}\right), & 0 < \gamma < 1 \end{cases} \tag{8.17}$$

within the radius of convergence defined by (8.16). Inserting this into the criterion (8.6) yields, choosing s maximal,

$$\varepsilon > \begin{cases} \exp\left[\dfrac{1}{c}\left(\dfrac{2}{\beta} - 1\right)\log \beta\right], & \gamma = 0 \\ c_+ \beta^{1/\gamma}, & 0 < \gamma < 1 \end{cases} \tag{8.18}$$

β small, for the absence of phase transition. In Section 9 we will show, using the hierarchical model as a lower bound, that for

$$\varepsilon < c_- \beta^{1/\gamma}, \qquad 0 < \gamma < 1 \tag{8.19}$$

the Ising model has a nonzero spontaneous magnetization.

In order to pin down the phase boundary for small β in the case $0 < \gamma < 1$, it may be of some interest to actually prove the convergence of the low-density expansion. We did not push this approach because it fails to give the conventional picture for the border line t^{-2}. We pose the following problem: In the usual Ising model over $\mathbb{Z}$ with $1/t^2$ interaction show that there exist a $\beta^* > 0$ such that for $\beta < \beta^*$ there is no phase transition no matter how strong the nearest-neighbor coupling.

9. EXISTENCE OF PHASE TRANSITION

We establish a nonzero spontaneous magnetization in the cases where the interaction decays as $t^{-2+\gamma}$, $0 \leqslant \gamma < 1$. The existence of a phase transition for the physically relevant t^{-2} interaction is in a way the least obvious result of our paper and we formulate it as follows.

Theorem 1. If the interaction $V(t) \sim t^{-2}$ for large t [in the sense that $\lim_{t\to\infty} t^2 V(t) = c > 0$] and if β is sufficiently large, then

$$\langle \sigma(0)\rangle_+ (\beta V) > 0 \tag{9.1}$$

We show that $\langle \sigma(0)\rangle_+$ is bounded below by the spontaneous magnetization of the usual Ising model with $1/r^2$ interaction, which is strictly positive provided β is large enough by a result of Fröhlich and Spencer.[4]

Proof. The proof consists of two steps. We first average over short distance scales and decouple the free measure. We then use Wells' inequality.

Step 1. We choose a lattice spacing δ and a maximal lower bound $\tilde{V}$ for the potential V such that $\tilde{V}$ is constant on the squares $j\delta \leqslant s < (j+1)\delta$, $i\delta \leqslant t < (i+1)\delta$ and satisfies

$$V(t-s) \geqslant \tilde{V}(t, s) = \begin{cases} \kappa^2 & \text{for } j\delta \leqslant s, t < (j+1)\delta \\ \alpha/j^2 & \text{for } j\delta \leqslant s < (j+1)\delta,\ i\delta \leqslant t < (i+1)\delta,\ i \neq j \end{cases} \tag{9.2}$$

$i, j \in \mathbb{Z}$. α depends on δ as $\alpha \sim V(0)$ for small δ and $\alpha \sim \delta^{-2}$ for large δ. Let

$$m_j = \frac{1}{\delta} \int_{(j-1/2)\delta}^{(j+1/2)\delta} dt\, \sigma(t) \tag{9.3}$$

Then $|m_j| \leqslant 1$. We set $T = (L - 1/2)\delta$ and $m_j = 1$ for $|j| \geqslant L$ (+ boundary conditions). By Griffiths,

$$\langle m_0 \rangle_{T,+} (\beta V) \geqslant \langle m_0 \rangle_{T,+} (\beta \tilde{V}) \tag{9.4}$$

Here the Gibbs measure $\langle \cdot \rangle_{T,+} (\beta \tilde{V})$ can be regarded as defined over the lattice $\mathbb{Z}$. Its interaction is then

$$-\frac{1}{2} \beta\alpha\delta^2 \sum_{\substack{i \neq j \\ |i|, |j| < L}} |i-j|^{-2} m_i m_j + \sum_{|j| < L} \beta\kappa^2\delta^2 m_j^2 + \text{b.c.} \tag{9.5}$$

and its free measure is the joint distribution of the m_j's under the spin flip measure $\mu^{\varepsilon}_{T,+}(d\sigma)$. We recall the lattice approximation of the free measure described in Section 4. In this approximation we suppress the couplings across the points $(j + \frac{1}{2})\delta$, $-L \leqslant j < L$. This further decreases the expectation of m_0 and therefore

$$\langle m_0 \rangle_{T,+} (\beta V) \geqslant \langle m_0 \rangle_{L,+,\mu} (\alpha\delta^2\beta) \tag{9.6}$$

Here $\langle \cdot \rangle_{L,+,\mu}(\beta)$ has the interaction

$$-\tfrac{1}{2} \sum_{i \neq j} |i-j|^{-2} m_i m_j + \text{b.c.} \tag{9.7}$$

and as free measure a product of single site measures μ.

The characteristic function of the single site measure $\mu(dm)$ is given by

$$\int_{-1}^{1} \mu(dm)\, e^{\lambda m} = Z^{-1} \left\langle \exp\left\{\lambda \int_0^1 dt\, \sigma(t) + \left[\kappa \sqrt{\beta} \int_0^1 dt\, \sigma(t)\right]^2\right\}\right\rangle_{[0,1],\varepsilon\delta} \tag{9.8}$$

$\langle \cdot \rangle_{[0,1],\varepsilon\delta}$ refers to the expectation in the spin flip measure with free boundary conditions and density $\varepsilon\delta$. We scaled the interval $[0, \delta]$ to the unit interval here. We may de-Gaussian the square and use again the spin operators. Then

$$\int_{-1}^{1} \mu(dm)\, e^{\lambda m} = Z^{-1} \int d\xi\, e^{-\xi^2/4} \times \sum_{\sigma,\sigma'} \exp[\varepsilon\delta\sigma_x + (\xi\kappa\sqrt{\beta} + \lambda)\,\sigma_z](\sigma \mid \sigma') \tag{9.9}$$

Clearly, $\mu(dm)$ is even.

We note the limits: If $\delta \to 0$, then

$$\mu(dm) = \tfrac{1}{2}[\delta(m+1) + \delta(m-1)], \qquad \int \mu(dm)\, m^2 \to 1 \tag{9.10}$$

and if $\delta \to \infty$, then

$$\mu(dm) = (\varepsilon\delta/2\pi)^{1/2} \exp(-m^2\varepsilon\delta/2), \qquad \int \mu(dm)\, m^2 \to 1/\varepsilon\delta \tag{9.11}$$

Step 2. Wells made the following observation[43,44]: Let μ be an even single site measure and let $a > 0$ be such that

$$\int \mu(d\sigma)(\sigma^2 - a^2)^n \geqslant 0 \tag{9.12}$$

for all $n = 0, 1, \ldots$. A sufficient condition for (9.12) to hold is

$$\mu([0, a]) \leqslant 2\mu([\sqrt{2}\, a, \infty)) \tag{9.13}$$

Let $\langle \cdot \rangle_{+,\mu}$ be the Gibbs state for a general ferromagnetic interaction with single site measure μ and + boundary conditions and let $\langle \cdot \rangle_{+,a}$ be the Gibbs state for the same interaction but with μ replaced by $\frac{1}{2}[\delta(\sigma + a) + \delta(\sigma - a)]$ (Ising model). Then

$$\left\langle \prod_{i \in A} \sigma_i \right\rangle_{+,\mu} \geqslant \left\langle \prod_{i \in A} \sigma_i \right\rangle_{+,a} \tag{9.14}$$

Let $\langle \cdot \rangle_{L,+}(\beta)$ be the Ising model (± 1) with interaction $\beta|i-j|^{-2}$ and $+$ boundary conditions. Let a be such that (9.12) is satisfied with μ defined by (9.8). Then

$$\langle m_0 \rangle_{T,+}(\beta V) \geq \langle \sigma_0 \rangle_{L,+}(a^2\delta^2\alpha\beta) \tag{9.15}$$

From Ref. 4 we know that $\langle \sigma_0 \rangle_+(\beta) > 0$ for $\beta > \beta_c$ with some β_c large enough. Therefore we conclude that

$$\langle \sigma(0) \rangle_+(\beta V) > 0 \tag{9.16}$$

provided

$$a^2\delta^2\alpha\beta > \beta_c \tag{9.17}$$

From the construction it is clear that (9.17) can be achieved provided β is large enough. ▮

The reader may be curious about the shape of the lower bound on $\varepsilon_c(\beta)$. From (9.10), (9.11) we deduce that $a^2 \sim 1$ as $\delta \to 0$ and $a^2 \sim 1/\varepsilon\delta$ as $\delta \to \infty$. We also know that $\alpha \sim c$ as $\delta \to 0$ and $\alpha \sim 1/\delta^2$ as $\delta \to \infty$. We insert in (9.17) and optimize with respect to δ. The resulting curve is qualitively similar to the one of Fig. 1. For β large it is linear. It drops to zero at some finite value of β, however enters there with zero slope.

Our technique can also be applied to potentials decaying as $t^{-2+\gamma}$, $0 < \gamma < 1$. After Step 1 we use the hierarchical model as lower bound.[21,45,46] This establishes a nonzero spontaneous magnetization for β large enough. The condition to be satisfied is again (9.17) with $a^2 = \int \mu(dm)\, m^2$ and β_c a constant coming from the analysis of the hierarchical model. If we again optimize (9.17) with respect to δ, we obtain a lower bound on $\varepsilon_c(\beta)$ which is linear for large β and drops to zero as $\beta^{1/\gamma}$ for $\beta \to 0$.

Note that as $\varepsilon \to 0$ the Gibbs measure $\langle \cdot \rangle(\beta V, \varepsilon)$ tends to the measure giving weight 1/2 to the configurations $\sigma(t) = 1$ and $\sigma(t) = -1$ for all t. Therefore the line $\varepsilon = 0$ corresponds to a zero temperature transition.

10. THE THOULESS EFFECT

The Thouless effect refers to the phenomenon that for the Ising model with $1/t^2$ interaction the spontaneous magnetization jumps at β_c. However, the transition is not first order, since the correlation length diverges for $\beta \to \beta_c$. On the basis of a renormalization group analysis and of numerical data it is predicted that at β_c the two point function decays as $1/\log t$ for large t.[47] We want to apply the technique of Simon and Sokal[30] to our model. It provides a simple proof of zero spontaneous magnetization, if $\int dt\, V(t)\, t < \infty$ and $\varepsilon > 0$. As before, the difficulty in the extension is to properly deal with the fact that the free measure is not a product measure.

We consider the finite system $[-T, T]$. Let Λ be an interval, $\Lambda \subset [-T+\delta, T-\delta]$, $\Lambda = [a, b]$. We define $\partial^\delta \Lambda = \partial \Lambda = [a-\delta, a] \cup [b, b+\delta]$ and $\Lambda^c = [-T, T] \backslash (\Lambda \cup \partial \Lambda)$. To flip spins in directly adjacent intervals costs to much entropy. Therefore we average over intervals of length δ, independently of T, in between. Let σ_I be the spin configuration in the set I. We define the stochastic map

$$(Kf)(\sigma) = \int \mu_{T,+}(d\sigma'_{\partial\Lambda} \mid -\sigma_\Lambda, \sigma_{\Lambda^c})\, f(-\sigma_\Lambda, \sigma'_{\partial\Lambda}, \sigma_{\Lambda^c}) \tag{10.1}$$

for bounded functions $f: \mathscr{D}([-T, T], \{-1, 1\}) \to \mathbb{R}$. Here $\mu^\varepsilon_{T,+}(\cdot \mid \cdot)$ denotes the conditional expectation. The dual of K acts on measures. If they have a density g with respect to $\mu^\varepsilon_{T,+}(d\sigma)$, then

$$K^* g \mu^\varepsilon_{T,+}(d\sigma) \equiv (K^* g)(\sigma)\, \mu^\varepsilon_{T,+}(d\sigma) \tag{10.2}$$

with

$$(K^* g)(\sigma) = R_\Lambda(\sigma) \int \mu^\varepsilon_{T,+}(d\sigma'_{\partial\Lambda} \mid -\sigma_\Lambda, \sigma_{\Lambda^c})\, g(-\sigma_\Lambda, \sigma'_{\partial\Lambda}, \sigma_{\Lambda^c}) \tag{10.3}$$

Let $\mu^\varepsilon_{T,+}(d\sigma_\Lambda, d\sigma_{\Lambda^c})$ be the joint distribution of the spin configuration in Λ and Λ^c. Then $R_\Lambda(\sigma)$ is the Radon–Nikodym derivative of $\mu^\varepsilon_{T,+}(d(-\sigma_\Lambda)),$ $d\sigma_{\Lambda^c})$ relative to $\mu^\varepsilon_{T,+}(d\sigma_\Lambda, d\sigma_{\Lambda^c})$ By a straightforward computation

$$(\tanh \varepsilon\delta)^2 \leqslant R_\Lambda(\sigma) \leqslant (\tanh \varepsilon\delta)^{-2} \tag{10.4}$$

independently of Λ and T.

We define the entropy and the relative entropy for $f, g \geqslant 0$, $\int \mu^\varepsilon_{T,+}(d\sigma)\, f(\sigma) = 1 = \int \mu^\varepsilon_{T,+}(d\sigma)\, g(\sigma)$, as

$$S(f) = -\int \mu^\varepsilon_{T,+}(d\sigma)\, f(\sigma) \log f(\sigma) \tag{10.5}$$

$$S(f \mid g) = -\int \mu^\varepsilon_{T,+}(d\sigma)\, f(\sigma) \log f(\sigma) + \int \mu^\varepsilon_{T,+}(d\sigma)\, f(\sigma) \log g(\sigma) \leqslant 0 \tag{10.6}$$

Under any stochastic map $\bar{K}$ acting on probability measures with density

$$S(\bar{K}f \mid \bar{K}g) \geqslant S(f \mid g) \tag{10.7}$$

(Refs. 48 and 49). Therefore

$$S(K^*g \mid K^*1) \geqslant S(g \mid 1) = S(g)$$

$$\begin{aligned} S(K^*g) &\geqslant S(g) - \int \mu^{\varepsilon}_{T,+}(d\sigma)\, g(\sigma)(K \log R_A)(\sigma) \\ &\geqslant S(g) + 2\log(\tanh \varepsilon\delta) \end{aligned} \tag{10.8}$$

With these preparations the argument of Ref. 30 can be copied. We only sketch the main differences. We pick n disjoint intervals $B_1,\dots, B_n$ of equal length and separated by intervals of fixed length δ. Then $g = Z^{-1}\exp\{-\frac{1}{2}\beta \int dt\, ds\, V(t-s)[1-\sigma(t)\,\sigma(s)] + \text{b.c.}\}$ relative to the free measure $\mu^{\varepsilon}_{T,+}(d\sigma)$ and $f_j = K_j^* g$ with Λ in the definition of K replaced by B_j. A_j is the set of spin configurations such that $\int_{B_j} dt\, \sigma(t) \leqslant 0$. Then

$$\begin{aligned} \int \mu^{\varepsilon}_{T,+}(d\sigma)\, f_j(\sigma)\, \chi(A_j^c) &= \int \mu^{\varepsilon}_{T,+}(d\sigma)\, g(\sigma)\, K\chi(A_j^c) \\ &= \left\langle \left\{ \int_{B_j} dt\, \sigma(t) \leqslant 0 \right\} \right\rangle_{T,+} (\beta V) \end{aligned} \tag{10.9}$$

Therefore K_j^* takes the role of the spin flip operation. We define $f = (1/n)\sum_{j=1}^{n} f_j$. Then

$$\begin{aligned} S(f) &\geqslant \frac{1}{n}\sum_{j=1}^{n} S(f_j) + \log n - \text{const} \\ &\geqslant S(g) + \log n - \text{const} + 2\log(\tanh \varepsilon\delta) \end{aligned} \tag{10.10}$$

Therefore the additional intervals of length δ produce only an error independent of n in the entropy estimate. This does not count, since energy and entropy of order $\log n$ are compared to each other.

We conclude the following.

Theorem 2. If $\int \rho(d\omega)\, \omega^{-2} < \infty$, then for any β and $\varepsilon > 0$

$$\langle \sigma(0) \rangle_{+}(\beta V, \varepsilon) = 0 \tag{10.11}$$

The Gibbs state $\langle \cdot \rangle(\beta V, \varepsilon)$ is independent of the choice of boundary conditions.

Theorem 3. Let $V(t) \sim t^{-2}$ for large t [in the sense that $\lim_{t \to \infty} t^2 V(t) = c > 0$]. Let $m^* = \langle \sigma(0) \rangle_+ (\beta V, \varepsilon)$.

(i) Let $\int dt [\langle \sigma(0)\, \sigma(t) \rangle_+ (\beta V, \varepsilon) - m^{*2}] < \infty$

Then either $m^* = 0$ or

$$4\beta m^{*2} \geqslant 1 \tag{10.12}$$

(ii) Let

$$a^* = \min(1, -\limsup_{t \to \infty} \{\log[\langle \sigma(0)\, \sigma(0) \rangle_+ (\beta V, \varepsilon) - m^{*2}]/\log(1+t)\}) \tag{10.13}$$

Then either $m^* = 0$ or

$$4\beta m^{*2} \geqslant a^{*2} \tag{10.14}$$

If at $(\varepsilon_c(\beta), \beta)$ the truncated two-point function has a power law decay, then by (10.13) the spontaneous magnetization has to jump.

As pointed out by J. Bricmont, (10.12) and (10.14) lend further support for the phase diagram of Fig. 1. If at some point in the region $\{\varepsilon > 0, \beta < 1/4\}$ $m^* > 0$, then necessarily the susceptibility has to diverge because $m^{*2} < 1$. Furthermore by (10.14) there could be no power law decay of the truncated two-point function with an exponent independent of β. Both properties would be rather surprising.

11. GROUND STATE EXPECTATIONS OF THE PHONON FIELD

So far we have directed our effort to $\langle \sigma_z \rangle_+$. We showed that in the physical case, $\rho(\omega) \cong \omega$ for small ω, the quantum particle becomes localized in one of the two wells provided the coupling is strong enough. Here we want to analyze how the phonon field changes its properties when such a transition occurs.

We relate ground state field correlations to expectations in the Ising model. The identification is obtained at finite T. As before, we let then $T \to \infty$ followed by the limit $h \to 0_+$ if necessary. f denotes here a rapidly decreasing test function and $a(f) = \int dk\, f(k)\, a(k)$.

(i) $\langle a^+(f) + a(f) \rangle_+$. The Hamiltonian is perturbed as

$$H_\lambda = H - \frac{\lambda}{T} \sum_j f(k_j) [2\omega(k_j)]^{1/2}\, x_j \tag{11.1}$$

and we want to compute the derivative of $\mathrm{tr}\{\exp[-TH_\lambda]\}$ at $\lambda=0$. Going through the functional integral representation yields

$$\langle a^+(f)+a(f)\rangle_+ = -\langle\sigma(0)\rangle_+ \int dk[\lambda(k)/2\omega(k)]\, f(k) \tag{11.2}$$

(ii) $i\langle a^+(f)-a(f)\rangle_+$. The Hamiltonian is perturbed as

$$H_\lambda = H - \frac{\lambda}{T}\sum_j f(k_j)\{2/[2\omega(k_j)]^{1/2}\}\left(-i\frac{\partial}{\partial x_j}\right) \tag{11.3}$$

We use the Cameron–Martin formula for the functional integral representation. The stochastic integral vanishes because of periodic boundary conditions and the remainder is second order in λ. Therefore

$$i\langle a^+(f)-a(f)\rangle_+ = 0 \tag{11.4}$$

(iii) $\langle a_+(f)\,a(f)\rangle_+$. The Hamiltonian is perturbed as

$$H_\lambda = H - \frac{\lambda}{2T}\sum_{i,j} f(k_i)\, f(k_j)\left\{[\omega(k_i)\,\omega(k_j)]^{1/2}\, x_i x_j - [\omega(k_i)\,\omega(k_j)]^{-1/2}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} - \delta_{ij}\right\} \tag{11.5}$$

and we want to compute the derivative of $\mathrm{tr}[\exp(-TH_\lambda)]$ at $\lambda=0$. The functional integration is no longer with respect to independent Brownian motions. Rather the covariance is

$$\delta_{ij} - \frac{\lambda}{T} f(k_i)\, f(k_j)[\omega(k_i)\,\omega(k_j)]^{-1/2} \tag{11.6}$$

As before we integrate over the Brownian motions. The effective interaction for the Ising model takes the form

$$2\sum_{i,j}\lambda(k_i)\,\lambda(k_j)[\omega(k_i)\,\omega(k_j)]^{1/2}\, G_{ij}^{(\lambda)}(s,t) \tag{11.7}$$

with $G_{ij}^{(\lambda)}(s,t) = G_{ji}^{(\lambda)}(t,s)$ and

$$G_{ij}^{(\lambda)}(s,t) = Z_\lambda^{-1}\,\mathrm{tr}\{\exp[-(T-t)\,H^\lambda]\, x_j \times \exp[-(t-s)\,H^\lambda]\, x_i \exp(-sH^\lambda)\} \tag{11.8}$$

for $t \geqslant s$. Here

$$H^\lambda = \sum_j \omega(k_j)\, a^+(k_j)\, a(k_j) - \frac{\lambda}{T} a^+(f)\, a(f) \tag{11.9}$$

and the trace is over the phonon field. We differentiate at $\lambda = 0$ and take the limit $T \to \infty$. Then

$$\langle a^+(f)\, a(f) \rangle_+ = \int_0^\infty dt \int dk\, \lambda(k)\, f(k) \int dk'\, \lambda(k')\, f(k')$$
$$\times \langle \sigma(0)\, \sigma(t) \rangle_+ \int_0^t d\tau\, e^{-\omega(k)(t-\tau)} e^{-\omega(k')\tau} \quad (11.10)$$

We denote by $m^* = \langle \sigma(0) \rangle_+$. From (11.2) we conclude that if $m^* \neq 0$ the phonon field is polarized. From (11.10) we obtain for the total number, N, of phonons

$$\langle N \rangle_+ = \int_0^\infty dt\, V(t) \langle \sigma(0)\, \sigma(t) \rangle_+ \quad (11.11)$$

If $m^* = 0$, it is reasonable to expect that $\langle \sigma(0)\, \sigma(t) \rangle_+$ decays as the potential (certainly this is the case in the domain of validity of the mean field bounds; cf. Section 8) which implies $\langle N \rangle_+ < \infty$. Also $\langle N \rangle < \infty$ whenever $\int_0^\infty dt\, tV(t) < \infty$. If $V(t) \sim t^{-2}$ or slower and if $m^* \neq 0$, then $\langle N \rangle_+ = \infty$. The localization of the quantum particle is associated with an infinite number of phonons. We discuss their distribution. At that stage, physically, it would be more reasonable to use the three-dimensional field and this could be done without difficulty. But for notational simplicity let us stick to our model.

As before let $v_{zz}(d\lambda)$ be the spectral measure associated with the $\langle \sigma(0)\, \sigma(t) \rangle_+$ correlation; cf. (3.20). Then from (11.10) the number, $n(dk)$, of phonons in momentum interval dk is given by

$$\langle n(dk) \rangle_+ = \int_0^\infty v_{zz}(d\lambda) \{ \lambda(k)/[\lambda + \omega(k)] \}^2\, dk \quad (11.12)$$

For the physical choice, $\omega(k) = |k|$ and $\lambda(k)^2 = \beta\, |k|$ for small k, we obtain

$$\langle n(dk) \rangle_+ \sim \begin{cases} k\, dk, & \text{if} \quad m^* = 0 \\ \dfrac{1}{k}\, dk, & \text{if} \quad m^* \neq 0 \end{cases} \quad (11.13)$$

for small k. For large k the momentum distribution decays faster than $|k|^{-3}$.

Let $n(dx)$ be the number of phonons in the spatial interval dx. From (11.10) we obtain

$$\langle n(dx) \rangle_+ = \int_0^\infty v_{zz}(d\lambda) \left| \int dk\, e^{ikx} \lambda(k)/[\lambda + \omega(k)] \right|^2 dx \quad (11.14)$$

The density of phonons is bounded. For the physical choice of ω and λ it decays for large x as

$$\langle n(dx)\rangle_+ \sim \begin{cases} x^{-3}\,dx, & \text{if } m^*=0 \\ x^{-1}\,dx, & \text{if } m^*\neq 0 \end{cases} \tag{11.15}$$

Both in (11.13) and (11.15) we assumed that $\langle\sigma(0)\,\sigma(t)\rangle_+ \sim t^{-2}$ for $m^*=0$. For $m^*\neq 0$ we only used that $\langle\sigma(0)\,\sigma(t)\rangle_+ \to m^{*2}$ as $t\to\infty$. Finer details of the spatial and momentum density of phonons are then obtained from the rate of decay.

We conclude that the localization of the quantum particle in one of the two wells is associated with the generation of an infinite cloud of infrared phonons located far out in space.

12. MORE GENERAL STATE SPACES

We approximated $-\frac{1}{2}\Delta + V_\lambda$ with $V_\lambda(q)=\lambda(1-q^2)^2$, $\lambda>0$, by a two-level system. From the foregoing analysis it is clear that we could have treated also the full problem. The spin flip measure $\mu^\varepsilon(d\sigma)$ as free measure has to be replaced then by

$$P(dq(\cdot))\exp\left[-\int_T^T dt\; V_\lambda(q(t))\right] \tag{12.1}$$

where $P(dq(\cdot))$ is Brownian motion. If the coupling to the phonon field is of the form $q\otimes\int dk\,\lambda(k)[a^+(k)+a(k)]$, then the effective interaction is still $-\frac{1}{2}\beta\int dt\,ds\,V(t-s)\,q(t)\,q(s)$ with $V(t)\sim t^{-2}$. On a technical level, the properties of the measure (12.1) needed for our purposes are well understood.[27] In particular to establish localization via the existence of a spontaneous magnetization, i.e., $\langle q(0)\rangle_+ > 0$, we would as before average over short distances and use Wells' inequality to reduce ourselves to the Ising model.

In fact a double-well potential is not needed at all. Let us denote the external quantum mechanical potential by V_{qm} in order to distinguish it from the potential V of the effective interaction. If $V_{qm}(q)=\frac{1}{2}aq^2$, $a>0$, then the spectrum of H (zero point energy of the Bose field subtracted) stops to be semibounded at some critical value of β. But if $V_{qm}(q)\geqslant a\,|q|^{2+\gamma}$, $\gamma>0$, then the ground state energy is finite at any coupling strength. Let $V(t)\sim t^{-2}$ and let $V_{qm}(q)=V_{qm}(-q)$. Then for sufficiently strong coupling the ground state is degenerate. The particle is no longer allowed to "oscillate" in the potential. The reason becomes clear if we rewrite the effective interaction in gradient form as

$$-\tfrac{1}{2}\beta \int dt\, ds\, V(t-s)\, q(t)\, q(s) = \tfrac{1}{4}\beta \int dt\, ds\, V(t-s)[q(t)-q(s)]^2$$

$$-\tfrac{1}{2}\beta \left[\int ds\, V(s)\right] \int dt\, q(t)^2 \qquad (12.2)$$

The particular form of the coupling to the phonon field produces an effective potential which drives the particle away from $q=0$.

Physically the coupling $q \otimes \int dk\, \lambda(k)[a^+(k)+a(k)]$ is an oversimplification which, however, does not show up in the two-level approximation. More realistically the coupling is of the form

$$\int dk\, e^{iqk} \lambda(k)[a^+(-k)+a(k)] \qquad (12.3)$$

with $\lambda(k)=\lambda^*(-k)$. Then the effective interaction becomes

$$\int dt\, ds \int dk\, |\lambda(k)|^2\, e^{-\omega(k)|t-s|} e^{ik[q(t)-q(s)]} \qquad (12.4)$$

and the problem of a degenerate ground state has to be analyzed anew.

Once we allow for a continuous external potential there is no reason to model the system only one-dimensional. $q(t)$ is then a vector with the number of components equal to the number of degrees of freedom of the quantum system. The coupling to the phonon field may depend on the direction. Now the corresponding statistical mechanics model becomes more difficult to analyze. If the external potential has two minima of equal depth and if the coupling does not distinguish between them and does not create a new minimum, then the results of this paper should hold. Already for more than two absolute minima the situation becomes rather complicated as discussed in Ref. 50. In addition, with more than one component there is the possibility of a continuous symmetry such as rotations. The picture then changes considerably. For example, if $V(t) \sim t^{-2}$ and with $O(n)$ symmetry, $n \geq 2$, there is no phase transition,[59] (cf. also Ref. 51).

13. CONCLUSIONS AND OPEN PROBLEMS

Our analysis is yet another example for the power of functional integral and statistical mechanics methods in dealing with quantum mechanical problems. It would be of interest to see how other models for matter plus radiation field, as, e.g., those treated in Refs. 52, and 53, would look like in this language. We have not pushed the method to its limits. But we have obtained a fairly complete picture of the static ground state correlations of the two-level atom and the Bose field. In the physical case $\rho(\omega) \cong \omega$ for small ω for fixed level splitting ε in the limit $h \downarrow 0$ the reduced density matrix of the two-level atom is the projection onto $(1/\sqrt{2})\binom{1}{1}$ for zero coupling strength β. As we increase β the reduced density matrix becomes a mixture with some weight given to $(1/\sqrt{2})\binom{1}{-1}$. At a certain critical value β_c the eigenbasis starts to turn and as $\beta \to \infty$ the reduced density matrix becomes again a pure state now corresponding to $\binom{1}{0}$. This is interpreted as a localization of the quantum particle in the right-hand well. The Bose field keeps the particle localized at the expense of generating an infinite number of low-momentum field quanta. Our results do not tell us what happens dynamically in an initial value problem. But in principle this could also be obtained from higher-order correlations of the Ising model.

We list a few problems to which the method of this paper seems to be applicable.

(i) *Return to equilibrium.* As a standard problem the initial state is $\rho \otimes \omega_\beta$ with ρ some state of the two-level system and ω_β the equilibrium (KMS) state of the quasifree Bose field at inverse temperature β. One wants to prove that in the limit $t \to \infty$ the state of the joint system converges to its equilibrium state at inverse temperature β, $\beta < \infty$. To our knowledge only in case the joint system is quasifree this return to equilibrium has been proved. In this case the convergence as $t \to \infty$ can be reduced to a scattering problem in the one-particle space.[54,55] The difficulty in the functional integral approach is to show that the spectral measures at finite volume ($\equiv$ finite β) (cf. Section 3) are absolutely continuous with respect to the Lebesgue measure.

(ii) *Escape probability* (cf. Section 2). The external potential for the quantum particle is of the form $q^2(1-q)$ for small q. Initially the Bose field is in its finite or zero temperature state and the particle in the wave function ψ localized at the metastable minimum. Let P_Λ be the projection onto $\Lambda = [-2/3, 2/3]$. Then one wants to compute the survival probability

$$|\psi\rangle\langle\psi| \otimes \omega_\beta(e^{iHt} P_\Lambda e^{-iHt}) \tag{13.1}$$

at time t. (We do not insist that this is the only way to define a quantum mechanical escape probability.) Coleman's bounce trajectory technique looks rather convincing. But even in the case of no coupling to the Bose field it is not clear to us how the escape probability computed in this fashion is related to (13.1). Certainly the rigorous treatment[1] proceeds differently. One difficulty is of how to deal with resonances.[56]

(iii) *Unconfined motion.* We exploited heavily that the external potential confines the quantum particle and that as a consequence the system has a well-defined ground state. The general problem is whether functional integration offers also an effective tool in case the external potential is nonconfining. (ii) is an example in this direction. An even better known example is the polaron,[57] where the external potential is zero and the coupling is as in (12.3). On a rigorous level only the ground state energy has been investigated.[58] It would be of interest to extract some dynamical information from the functional integral.

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REFERENCES

1. G. Jona-Lasinio, F. Martinelli, and E. Scoppola, *Commun. Math. Phys.* **80**:223 (1981).
2. G. Yuval and P. W. Anderson, *Phys. Rev. B* **9**:1511 (1970).
3. V. J. Emery and A. Luther, *Phys. Rev. B* **9**:215 (1974).
4. J. Fröhlich and T. Spencer, *Commun. Math. Phys.* **84**:87 (1982).
5. P. W. Anderson, G. Yuval, and D. R. Hamann, *Phys. Rev. B* **1**:4464 (1970).
6. E. B. Davies, *Commun. Math. Phys.* **39**:91 (1974).
7. R. Beck, W. Götze, and P. Prelovsek, *Phys. Rev. A* **20**:1140 (1979).
8. P. Pfeifer, Chiral molecules—A superselection rule induced by the radiation field, Ph.D. thesis, ETH Zürich (1980).
9. A. O. Caldeira and A. J. Leggett, *Phys. Rev. Lett.* **46**:211 (1981).
10. A. O. Caldeira and A. J. Leggett, *Ann. Phys. (N.Y.)* **149**:374 (1983).
11. S. Langer, *Ann. Phys. (N.Y.)* **41**:108 (1967).
12. C. G. Callan and S. Coleman, *Phys. Rev. D* **16**:1762 (1977).
13. H. Grabert, U. Weiss, and P. Hänggi, *Phys. Rev. Lett.* **52**:2193 (1984).
14. S. Chakravarty, *Phys. Rev. Lett.* **49**:681 (1982).
15. A. J. Bray and M. A. Moore, *Phys. Rev. Lett.* **49**:1545 (1982).
16. S. Chakravarty and S. Kivelson, *Phys. Rev. Lett.* **50**:1811 (1983).
17. W. Zwerger, *Z. Physik B—Condensed Matter* **53**:53 (1983).
18. W. Zwerger, *Z. Physik B—Condensed Matter* **47**:129 (1982).
19. D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions* (Bejamin, New York, 1975).
20. F. J. Dyson, in *Statistical Mechanics at the Turn of the Decade*, E. G. D. Cohen, ed. (Marcel Dekker, New York, 1971).
21. F. J. Dyson, *Commun. Math. Phys.* **12**:91 (1969).
22. F. J. Dyson, *Commun. Math. Phys.* **21**:269 (1971).
23. D. Ruelle, *Commun. Math. Phys.* **9**:267 (1968).
24. F. J. Dyson, *Commun. Math. Phys.* **12**:212 (1969).
25. J. B. Rogers and C. J. Thompson, *J. Stat. Phys.* **25**:669 (1981).
26. D. Ruelle, *Ann. Phys. (N.Y.)* **69**:364 (1972).

27. B. Simon, *Functional Integration and Quantum Physics* (Academic Press, London, 1979).
28. B. Simon, *Commun. Math. Phys.* **77**:111 (1980).
29. J. Fröhlich and C. A. Pillet, private communication.
30. B. Simon and A. D. Sokal, *J. Stat. Phys.* **25**:679 (1981).
31. A. D. Sokal, *J. Stat. Phys.* **28**:431 (1982).
32. J. L. Lebowitz, *Commun. Math. Phys.* **35**:87 (1974).
33. C. M. Newman, *Z. Wahrscheinlichkeitstheorie verwi. Gebiete* **33**:75 (1975).
34. G. S. Sylvester, *Commun. Math. Phys.* **42**:209 (1975).
35. J. Bricmont, *J. Stat. Phys.* **17**:289 (1977).
36. D. Brydges, J. Fröhlich, and T. Spencer, *Commun. Math. Phys.* **83**:123 (1982).
37. R. B. Griffiths, *J. Math. Phys.* **8**:478 (1967).
38. R. B. Griffiths, *J. Math. Phys.* **8**:484 (1967).
39. R. B. Griffiths, *Commun. Math. Phys.* **6**:121 (1967).
40. F. Leyvraz and P. Pfeifer, *Helv. Phys. Acta* **50**:857 (1977).
41. D. Ruelle, *Statistical Mechanics* (W. A. Benjamin, Reading, Massachusetts, 1969).
42. J. Glimm and A. Jaffe, *Quantum Physics—A Functional Integral Point Of View* (Springer, Berlin, 1981).
43. D. Wells, thesis, Department of Mathematics, Indiana University, 1977, unpublished.
44. J. Bricmont, J. L. Lebowitz, and C. E. Pfister, *J. Stat. Phys.* **24**:269 (1981).
45. G. Gallavotti and H. Knops, *Riv. Nuovo Cimento* **5**:341 (1975).
46. P. Collet and J. P. Eckmann, *A Renormalization Group Analysis of the Hierarchical Model in Statistical Mechanics* (Lecture Notes in Physics No. 74, Springer, Berlin, 1978).
47. J. Bhattacharjee, S. Chakravarty, J. L. Richardson, and D. J. Scalapino, *Phys. Rev. B* **24**:3862 (1981).
48. G. Lindblad, *Commun. Math. Phys.* **40**:147 (1975).
49. J. Voigt, *Commun. Math. Phys.* **81**:31 (1981).
50. J. L. Cardy, *J. Phys. A: Math. Gen.* **14**:1407 (1981).
51. J. M. Kosterlitz, *Phys. Rev. Lett.* **37**:1577 (1976).
52. K. Hepp and E. H. Lieb, *Phys. Rev.* **A8**:2517 (1973).
53. K. Hepp and E. H. Lieb, *Ann. Phys. (N.Y.)* **76**:360 (1973).
54. O. E. Lanford and D. W. Robinson, *Commun. Math. Phys.* **24**:193 (1981).
55. D. W. Robinson, *Commun. Math. Phys.* **31**:171 (1973).
56. E. B. Davies, *Lett. Math. Phys.* **1**:31 (1975).
57. R. P. Feynman, *Statistical Mechanics, Frontiers in Physics* (W. A. Benjamin, Reading, Massachusetts, 1972).
58. M. D. Donsker and S. R. S. Varadhan, *Commun. Pure and Appl. Math.* **36**:505 (1983).
59. B. Simon, *J. Stat. Phys.* **26**:307 (1981).