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Tunnelling in the equilibrium state of a spin–boson model†

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Abstract. For a two-level spin-boson system describing a quantum particle in a double-well potential coupled to a quantised radiation field, we prove the unicity of the equilibrium state at all positive temperatures. We are also able to compute rigorously the transition probability between the thermal wavefunctions of the two wells.

1. Introduction

Spin-boson models are studied in many areas of physics, such as solid state physics, quantum chemistry and problems of quantum tunnelling in superconducting devices. A fairly good introduction to their physics can be found in [1]. There are many different types of models in the literature. Here we are interested in the following Hamiltonian:

$$H = \mu\sigma_x + \int_{\mathbb{R}} \mathrm{d}k\,\varepsilon(k) a_k^+ a_k + \sigma_z \int_{\mathbb{R}} \mathrm{d}k\,\lambda(k)(a_k^+ + a_k) \tag{1}$$

describing a two-level atom in a boson field; $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices and a_k^+, a_k the boson creation and annihilation operators. In most applications, the functions ε and λ behave like $\varepsilon(k) \simeq |k|$, $\lambda(k) \simeq |k|^{1/2}$ at $k = 0$. More generally, we assume that ε and λ are $\mathbb{R}$-valued continuous functions satisfying the following conditions, including the physically interesting case:

$$\begin{aligned} &\int_{\mathbb{R}} \mathrm{d}k\,\lambda(k)^2 < \infty && \int_{\mathbb{R}} \mathrm{d}k \frac{\lambda^2(k)}{\varepsilon(k)} < \infty && \\ &\varepsilon(k) \geqslant C|k|^\gamma && C, \gamma \in \mathbb{R}^+ && \text{for large } |k| \\ &0 < \varepsilon(k) \leqslant C'|k| && C' \in \mathbb{R}^+ && \text{for small } |k| \neq 0. \end{aligned} \tag{2}$$

The Hamiltonian H originates from the description of a particle in a double-well potential $V(x)$ with potential barrier of height Δ. The Schrödinger problem has two lowest energy levels $E_\pm$, with wavefunctions $\psi_\pm = (1/\sqrt{2})(\psi_{\mathrm{L}} \pm \psi_{\mathrm{R}})$, where ψ_{L}, ψ_{R} are wavepackets localised in the left and right wells. The ground state ψ_+ is non-degenerate, exhibits reflection symmetry $(x \to -x)$ and, because Δ is finite, describes tunnelling between the two wells. The question is now whether this tunnelling is decreased or enhanced when friction is added.

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To arrive at the Hamiltonian (1) one makes a two-level approximation, i.e. one replaces the above Schrödinger particle by $\mu\sigma_x$ with $-2\mu = |E_+ - E_-|$ and puts it in a boson bath with linear coupling.

There are many other models related in one or another sense to the above one. Here we limit ourselves to mentioning the Dicke-Maser models (one-mode case [2] and infinite-mode case [3]), which are lattice formulations of this problem.

As far as we know, there exist only a few rigorous results for the model (1). In [4] some results on the spectrum of the proposed Hamiltonian are discussed, and in [5] a thorough analysis is made of the finite-mode approximation of the Hamiltonian. In particular, the Hartree-Fock solutions are found to show breaking of symmetry under the condition $\mu < 2\int (\lambda(k)^2/\varepsilon(k))\,dk$. In [6] the ground state of the model is partially analysed. By functional integration techniques it is shown that no spontaneous symmetry breaking appears if λ/ε is square integrable (in fact in $k=0$). Otherwise, if the coupling λ is large enough there is symmetry breaking.

Our contribution [7] consists in the computation of all temperature states and hence in actually solving the problem for $T>0$. Our method consists in considering the term $\mu\sigma_x$ as a perturbation. This point of view was already present in [4, 5]. Then we work towards a rigorous formulation of the KMS equation for the so-called unperturbed model and we are able to solve it completely. Then the perturbation theory is applied at the level of the cyclic vector of the unperturbed system. The proof is based on the stability theory of KMS states under symmetry transformations. Here we give an independent proof which looks mathematically more elegant, but is physically less transparent (see § 3). Section 4 contains the explicit rigorous computation of the transition probability between the thermal wavefunctions of the two minima, a result which was announced in [8]. For all temperatures $T>0$ the transition probability turns out to be strictly larger than zero. This result is used to get more physical insight in the phenomenon for finite temperatures as well as for the ground state.

2. Mathematical structure

Because of the type of system, an interaction between a spin and a Bose field, the algebra of observables is of the form

$$\mathcal{B} = \mathcal{A} \otimes M_2 \tag{3}$$

where $\mathcal{A}$ is a $C^\star$ algebra and M_2 the set of 2×2 complex matrices.

A general element of $\mathcal{B}$ is of the form

$$X = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \qquad X_{ij} \in \mathcal{A} \tag{4}$$

and a state ω of $\mathcal{B}$ can be described by a set $\{\omega_{ij} \mid i,j=1,2\}$ of linear functionals of $\mathcal{A}$. A useful notation is the following:

$$\omega = \begin{pmatrix} \omega_{11} & \omega_{21} \\ \omega_{12} & \omega_{22} \end{pmatrix}. \tag{5}$$

Then the expectation value of the observable X is computed by

$$\omega : X \to \omega(X) = \sum_{i,j=1}^{2} \omega_{ij}(X_{ij}). \tag{6}$$

A functional ω of the form (5) is a state of $\mathscr{B}$ if and only if it is normalised and positive, which is expressed by the following conditions on the functionals ω_{ij} of $\mathscr{A}$:

$$\omega_{11}(\mathbb{1})+\omega_{22}(\mathbb{1})=1$$

$$\omega_{ii}(x^\star x)\geqslant 0 \qquad |\omega_{12}(x^\star y)|^2\leqslant \omega_{11}(x^\star x)\omega_{22}(y^\star y)$$

$$\overline{\omega_{12}(x)}=\omega_{21}(x^\star)$$

for all $x, y\in\mathscr{A}$.

First we treat the particular case of (1) with $\mu=0$, i.e.

$$H_0=\int \mathrm{d}k\, \varepsilon(k)a_k^+a_k+\int \mathrm{d}k\, \lambda(k)(a_k^++a_k)\sigma_z. \tag{7}$$

We now specify $\mathscr{A}$.

Let $\mathscr{H}_\sim$ be the completion of the continuous complex functions of compact support on $\mathbb{R}$ vanishing on a neighbourhood of zero with respect to the scalar product

$$(f,g)_\sim=\int\left(1+\frac{1}{\varepsilon(k)}\right)\bar{f}(k)g(k)\,\mathrm{d}k.$$

Now for $\mathscr{A}$ we choose the $CCR-C^\star$ algebra $\Delta(\mathscr{H}_\sim)$ which is generated by the Weyl operators

$$W(f) \qquad f\in\mathscr{H}_\sim\subset L^2(\mathbb{R})$$

satisfying the commutation relations

$$W(f)^\star=W(-f)$$

$$W(f)\,W(g)=W(f+g)\exp(-\mathrm{i}\,\mathrm{Im}(f,g))$$

with

$$(f,g)=\int \mathrm{d}k\,\bar{f}(k)g(k).$$

Therefore the $C^\star$ algebra of observables $\mathscr{B}$ is given by $\Delta(\mathscr{H}_\sim)\otimes M_2$ and we define the unperturbed dynamics ($\mu=0$) by a group of *-automorphisms $(\alpha_t^0)_{t\in\mathbb{R}}$ on $\mathscr{B}$. We define α_t^0 on the generators of $\mathscr{B}$ as follows:

$$\alpha_t^0(\sigma_\pm)=\sigma_\pm W\left(\pm\frac{2\mathrm{i}\lambda}{\varepsilon}(1-\mathrm{e}^{\mathrm{i}t\varepsilon})\right) \tag{8a}$$

where

$$\sigma_\pm=\tfrac{1}{2}(\sigma_x\pm\mathrm{i}\sigma_y)$$

$$\alpha_t^0(\sigma_z)=\sigma_z \tag{8b}$$

$$\alpha_t^0(W(f))=W(\mathrm{e}^{\mathrm{i}t\varepsilon}f)\exp[2\mathrm{i}\sigma_z\,\mathrm{Re}(\lambda/\varepsilon,(\mathrm{e}^{\mathrm{i}t\varepsilon}-1)f)]. \tag{8c}$$

Because of the conditions (2) and the special choice of $\mathscr{A}=\Delta(\mathscr{H}_\sim)$, the evolution α_t^0 is well defined on the $C^\star$ algebra $\mathscr{B}$.

In order to define the full dynamics we limit ourselves to a particular class of states satisfying the following conditions.

(i) Regularity of the states, i.e. for all $f,g\in\mathscr{H}_\sim$, the map

$$z\in\mathbb{R}\to\omega_{ij}(W(f+zg))$$

is analytic. This condition implies the existence of fields and of the correlation functions:

$$\omega_{ij}(a^{\#}(f_1)\dots a^{\#}(f_n)) \qquad f_k\in\mathcal{H}_{\sim};\ k=1,\dots,n;\ n\in\mathbb{N}$$

where $a^{\#}$ stands for a or a^{+}.

(ii) Continuity of the correlation functions: we suppose that there exists a constant $C\in\mathbb{R}^{+}$ such that for all finite sets $\{f_1,\dots,f_n\}\subset\mathcal{H}_{\sim}$:

$$|\omega_{ij}(b(f_1)\dots b(f_n))|^2\leqslant C^n n!\prod_{i=1}^{n}\|f_i\|_{\sim}^2$$

where $b(f)=a^{+}(f)+a(f)$ for all $f\in\mathcal{H}_{\sim}$.

For any state ω of $\mathcal{B}$ we consider its GNS triplet $(\mathcal{H}_\omega,\pi_\omega,\Omega_\omega)$. For notational convenience we identify the algebra and the representation for the elements of $\mathcal{B}$, i.e. $x=\pi_\omega(x)$ for all $x\in\mathcal{B}$. We denote by $\mathcal{B}''$ the von Neumann algebra generated by $\pi_\omega(\mathcal{B})$.

(iii) Existence of the dynamics: we assume that the dynamics α_t^0 extends to a weakly continuous one-parameter group of *-automorphisms of $\mathcal{B}''$ for all states under consideration.

From condition (iii) it follows that the group $\{\alpha_t^0, t\in\mathbb{R}\}$ defines an infinitesimal generator $\delta_0:\alpha_t^0=\exp(\mathrm{i}t\delta_0)$ such that δ_0 is formally given by

$$\delta_0=[H_0,\cdot\,]$$

where H_0 is given by (7).

We now define the full model using the Dyson expansion: for all $x\in\mathcal{B}''$

$$\alpha_t(x)=\alpha_t^0(x)+\sum_{n\geqslant1} i^n\mu^n\int_{0\leqslant s_n\leqslant\dots\leqslant s_1\leqslant t}\dots\int \mathrm{d}s_1\dots\mathrm{d}s_n \times[\alpha_{s_n}^0(\sigma_x),[\alpha_{s_{n-1}}^0(\sigma_x),\dots[\alpha_{s_1}^0(\sigma_x),\alpha_t^0(x)]\dots]] \tag{9}$$

for $t\geqslant0$, and a similar expansion for $t<0$. As the perturbation $[\mu\sigma_x,\cdot\,]$ is a bounded derivation of $\mathcal{B}''$ the series is uniformly convergent and defines a weak *-continuous group of *-automorphisms of $\mathcal{B}''$. The infinitesimal generator δ of the group is formally given by

$$\delta=[H,\cdot\,]$$

where

$$H=H_0+\mu\sigma_x.$$

Remark that by formulae (8) and (9) we have arrived at a rigorous definition of the dynamics of the model on the appropriate von Neumann algebra of observables taking into account the conditions

$$\int\lambda(k)^2\,\mathrm{d}k<\infty \qquad \int\frac{\lambda(k)^2}{\varepsilon(k)}\,\mathrm{d}k<\infty.$$

3. Equilibrium states

We are interested in the equilibrium states at fixed inverse temperature $\beta\geqslant0$ for the full dynamics $\{\alpha_t|t\in\mathbb{R}\}$ defined in (9). The strategy consists in constructing the equilibrium states for the unperturbed dynamics α_t^0, then we use the known stability properties of KMS states for bounded perturbations to obtain the equilibrium states of the full dynamics.

For any state ω satisfying (i)-(iii), we define ω to be a (α^0, β) KMS state if for all $x, y \in \mathscr{B}''_{\alpha^0}$, a weakly dense α^0-invariant subalgebra of $\mathscr{B}''$ holds [9]:

$$\omega(x\alpha^0_{i\beta}(y)) = \omega(yx). \tag{10}$$

We prove first that this equilibrium condition has a unique solution for the unperturbed evolution α^0.

Theorem 3.1. There exists a unique (α^0, β) KMS state ω^0_β of $\mathscr{B}$ satisfying conditions (i)-(iii). Using the notation (5), it is given by

$$\omega^0_\beta = \begin{pmatrix} \frac{1}{2}\omega_+ & 0 \\ 0 & \frac{1}{2}\omega_- \end{pmatrix} \tag{11}$$

where $\omega_\pm$ are the states of the CCR algebra $\Delta(\mathscr{H}_\sim)$ given by

$$\omega_\pm(W(f)) = \exp[\pm 2\mathrm{i}\ \mathrm{Im}(\mathrm{i}\lambda/\varepsilon, f) - \tfrac{1}{2}(f, \coth(\tfrac{1}{2}\beta\varepsilon)f)]. \tag{12}$$

Proof. First we prove that the off-diagonal components of ω^0_β vanish. Therefore apply (10) with $x = \sigma_x W(f)$ and $y = \sigma_z$. Using (8*b*) one gets

$$\omega^0_\beta(\sigma_x W(f)\alpha^0_{i\beta}(\sigma_z)) = \omega^0_\beta(\sigma_z\sigma_x W(f))$$

and

$$\omega^0_\beta(\sigma_x\sigma_z W(f)) = \omega^0_\beta(\sigma_z\sigma_x W(f))$$

or

$$\omega^0_\beta(\sigma_y W(f)) = 0.$$

Analogously,

$$\omega^0_\beta(\sigma_x W(f)) = 0.$$

Therefore ω^0_β is of the form

$$\omega^0_\beta = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}$$

where

$$\omega_1(W(f)) = \omega^0_\beta(\tfrac{1}{2}(\mathbb{1} + \sigma_z)W(f)) \qquad f \in \mathscr{H}_\sim$$

$$\omega_2(W(f)) = \omega^0_\beta(\tfrac{1}{2}(\mathbb{1} - \sigma_z)W(f)) \qquad f \in \mathscr{H}_\sim.$$

Define the automorphism groups $\{\alpha_t^\mp \mid t \in \mathbb{R}\}$ of $\Delta(\mathscr{H}_\sim)$ by

$$\alpha_t^\mp(W(f)) = W(\mathrm{e}^{\mathrm{i}\varepsilon t}f)\exp[\pm 2\mathrm{i}\ \mathrm{Re}(\lambda/\varepsilon, (\mathrm{e}^{\mathrm{i}\varepsilon t} - 1)f)].$$

From (8*b*) one has

$$\tfrac{1}{2}(\mathbb{1} \pm \sigma_z)\alpha_t^\mp(W(f)) = \tfrac{1}{2}(\mathbb{1} \pm \sigma_z)\alpha_t^0(W(f)).$$

Remark that for all x, y analytic elements for the evolution α^+

$$\begin{aligned}\omega_1(x\alpha^+_{i\beta}y) &= \omega^0_\beta(x\tfrac{1}{2}(\mathbb{1}+\sigma_z)\alpha^+_{i\beta}(y))\\ &= \omega^0_\beta(x\tfrac{1}{2}(\mathbb{1}+\sigma_z)\alpha^0_{i\beta}(y))\\ &= \omega^0_\beta(yx\tfrac{1}{2}(\mathbb{1}+\sigma_z))\\ &= \omega_1(yx)\end{aligned}$$

hence ω_1 is a (α^+, β) KMS state, and similarly ω_2 is a (α^-, β) KMS state.

The automorphisms $\alpha^\pm$ are up to a displacement the free Bose-gas automorphisms. Under our general conditions λ^2/ε and $\lambda^2 \in L^1(\mathbb{R})$, (i)-(iii), they yield the unique KMS states $\omega_\pm$ given by (12) [10]. Hence there exists $\eta \in [0, 1]$ such that

$$\omega_1 = \eta\omega_+ \qquad \omega_2 = (1-\eta)\omega_-$$

where $\eta = \omega_1(\mathbb{1})$ and denote

$$\omega_\eta = \begin{pmatrix} \eta\omega_+ & 0 \\ 0 & (1-\eta)\omega_- \end{pmatrix}. \tag{13}$$

We have to prove that there exists only one solution, namely corresponding to the value $\eta = \frac{1}{2}$. Therefore define the reflection symmetry automorphism τ on $\mathscr{B}$ by the following relations:

$$\begin{aligned}&\tau(\sigma_1) = \sigma_1 \qquad \tau(\sigma_2) = -\sigma_2 \qquad \tau(\sigma_3) = -\sigma_3\\ &\tau(W(f)) = W(-f) \qquad f \in \mathscr{H}_\sim\end{aligned} \tag{14}$$

and remark that $\omega_\eta \circ \tau = \omega_{1-\eta}$. The state ω_η with $\eta = \frac{1}{2}$ is then precisely the unique τ-invariant state in (13). To prove this we use (10) again. Remark that using the explicit formulae for the evolution α^0_t (8) and for the state ω_+ (12) the function $t \to \omega_\eta(\sigma^+\alpha^0_t\sigma^-)$ extends analytically to the complex plane and takes the value η at $t = i\beta$. The function $t \to \omega_\eta(\alpha^0_t(\sigma^-)\sigma^+)$ takes the value $1-\eta$ at $t = 0$. By (10) $\eta = \frac{1}{2}$.

The equilibrium state of the full model can now be computed by a perturbation of the equilibrium state of the solvable model $\{\alpha^0_t \mid t \in \mathbb{R}\}$. In order to do this we need the perturbation technique on von Neumann algebras developed in the context of stability theory for KMS states.

Theorem 3.2. Under the conditions $\int \mathrm{d}k\lambda^2\varepsilon^{-1} < \infty$ and $\int \mathrm{d}k\lambda^2 < \infty$ the full model defined in (9) admits for every positive β a unique (α, β) KMS state ω_β which satisfies (i)-(iii). Furthermore ω_β is normal WRT the unique (α^0, β) KMS state ω^0_β and is given by the following strongly convergent perturbation expansion. Let $(\mathscr{H}_0, \pi_0, \Omega_0)$ be the GNS triplet of ω^0_β then

$$\omega_\beta(x) = \frac{\langle\Omega \mid \pi_0(x)\Omega\rangle}{\|\Omega\|^2} \qquad x \in \mathscr{B} \tag{15}$$

where

$$\Omega = \Omega_0 + \sum_{n\geq 1} (-\beta\mu)^n \int_{0\leq s_n\leq\ldots\leq s_1\leq 1/2} \mathrm{d}s_1 \ldots \mathrm{d}s_n\, \alpha^0_{i\beta s_1}(\sigma_x) \ldots \alpha^0_{i\beta s_n}(\sigma_x)\Omega_0.$$

It follows that ω_β is τ invariant where τ is defined in (14), and in particular $\omega_\beta(\sigma_z) = 0$.

Proof. Using [9, theorem 5.4.4] one constructs a KMS state ω_β for a perturbed dynamics α (9) from the unperturbed α^0 (8). The full dynamics α is obtained by adding a bounded operator $\mu\sigma_x$ to the Hamiltonian.

The state ω_β is given by its cyclic vector which is constructed in terms of a series expansion (15). As the unperturbed state ω_β^0 is the unique (α^0, β) KMS state (theorem 3.1), it is a factor state [9, theorem 5.3.30]. Hence by [9, theorem 5.4.4] ω_β is the unique (α, β) KMS state. The τ invariance of ω_β is then immediate.

This theorem proves that for all finite temperatures $T > 0$, there exists a unique temperature state. Hence there is no spontaneous breaking of the reflection symmetry τ. Therefore the possible ground-state symmetry breaking [6] turns off abruptly at arbitrarily small temperatures.

4. Transition probabilities

In the preceding section we gave the mathematical proof of the existence and uniqueness of the equilibrium state of the model at any temperature $T > 0$. In view of the kind of physical system described by the model (see the introduction) the proof might be supplemented by more physically transparent arguments which can be provided by the computation of transition probabilities between the two states with fixed value of the spin. Clearly the explicit form of the solution ω_β (theorem 3.2) is constructed by means of the states $\omega_\pm$ (theorem 3.1) of the Bose field representing the two spin states.

The unicity of the solution yields intrinsically that there is always tunnelling from one state to the other.

In this section we show explicitly that in the spirit of the technique used in § 3 and neglecting the bounded perturbation, the transition probability $\omega_+ \to \omega_-$ is non-vanishing for all $T > 0$.

First we define the mathematical notion of the transition probability between two arbitrary states of a C^* algebra.

Transition probabilities between wavefunctions in the Hilbert space $\mathscr{H}$ of quantum mechanics are well known. Take ψ_1, ψ_2 normalised vectors in $\mathscr{H}$, defining the states

$$\omega_i(\cdot) = (\psi_i, \cdot\, \psi_i) \qquad i = 1, 2$$

and the transition probability for the transition $\psi_1 \to \psi_2$ is then given by

$$P(\omega_1, \omega_2) = |(\psi_1, \psi_2)|^2.$$

This notion has been generalised to arbitrary states of a C^* algebra as follows [11-13].

Let ω_i $(i = 1, 2)$ be two arbitrary states of a C^* algebra $\mathscr{A}$, suppose that π is a representation of $\mathscr{A}$ in $\mathscr{B}(\mathscr{H})$ and Ω_i $(i = 1, 2)$ elements of $\mathscr{H}$ such that

$$\omega_i(A) = (\Omega_i, \pi(A)\Omega_i) \qquad (i = 1, 2). \tag{16}$$

Then the transition probability $P(\omega_1, \omega_2)$ is defined by

$$P(\omega_1, \omega_2) = \sup|(\Omega_1, \Omega_2)|^2 \tag{17}$$

where the sup is taken over all representations π and vectors Ω_i for which (16) holds.

Now we compute rigorously the transition probability $P(\omega_+, \omega_-)$ where $\omega_\pm$ are defined in (12), as states of the CCR algebra $\mathscr{A} = \Delta(\mathscr{H}_-)$.

Theorem 4.1. With the above notations

$$P(\omega_+, \omega_-) = \exp\left[-4 \int \mathrm{d}k \left(\frac{\lambda(k)}{\varepsilon(k)}\right)^2 \tanh \tfrac{1}{2}\beta\varepsilon(k)\right]. \tag{18}$$

Proof. First we construct the representations for the states $\omega_\pm$. As representation space take $\mathcal{H} = \mathcal{H}_F \otimes \mathcal{H}_F$ where $\mathcal{H}_F$ is the Fock space built on the test function space $L^2(\mathbb{R})$. As representation consider the map

$$\pi: W(f) \to \pi(W(f)) = \exp(2\mathrm{i}\,\mathrm{Im}(\mathrm{i}\lambda/\varepsilon, f))\, W((\tfrac{1}{2}(A+\mathbb{1}))^{1/2} f) \otimes W(\overline{(\tfrac{1}{2}(A-\mathbb{1}))^{1/2} f})$$

where A is the multiplication operator by $\coth \frac{1}{2}\beta\varepsilon$ and where $\overline{}$ denotes the complex conjugate.

Take $\Omega_+ = \Omega_F \otimes \Omega_F$, where Ω_F is the Fock vacuum; then $(\mathcal{H}, \pi, \Omega_+)$ is the GNS triplet of ω_+ and

$$\omega_+(x) = (\Omega_+, \pi(x)\Omega_+) \qquad x \in \Delta(\mathcal{H}_-).$$

Denote

$$\Omega_-(W(g_1) \otimes W(g_2))\Omega_+$$

with

$$g_1 = -\mathrm{i}\frac{(2(A+\mathbb{1}))^{1/2}}{A}\frac{\lambda}{\varepsilon}$$

$$g_2 = -\mathrm{i}\frac{(2(A-\mathbb{1}))^{1/2}}{A}\frac{\lambda}{\varepsilon}.$$

Then one easily checks that

$$\omega_-(x) = (\Omega_-, \pi(x)\Omega_-) \qquad x \in \Delta(\mathcal{H}_-)$$

and by (17) one has that

$$P(\omega_+, \omega_-) \geq |(\Omega_+, \Omega_-)|^2 = \exp\left(-4 \int \mathrm{d}k \left(\frac{\lambda}{\varepsilon}(k)\right)^2 \tanh \tfrac{1}{2}\beta\varepsilon(k)\right)$$

yielding a lower bound for the transition probability.

Now we derive an upper bound, using the property [12]

$$P(\omega_{+|\mathcal{A}}, \omega_{-|\mathcal{A}}) \leq P(\omega_{+|\mathcal{A}_1}, \omega_{-|\mathcal{A}_1})$$

where $\mathcal{A}_1$ is any C^* subalgebra of $\mathcal{A}$. Here we will use Abelian subalgebras. Take as subalgebra the von Neumann algebra generated by the spectral family $\{e(B) \mid B$ Borel subset of $\mathbb{R}\}$ of the element $W(f)$ for some fixed $0 \neq f \in \mathcal{H}_-$, i.e.

$$W(f) = \int e^{\mathrm{i}t}\, \mathrm{d}e((-\infty, t]).$$

One defines the measures $\mu_\pm$ over the Borel sets of $\mathbb{R}$:

$$\mu_\pm(B) = \omega_\pm(e(B)).$$

A straightforward computation, using the explicit formulae (12), yields

$$\mu_\pm(B) = \int_B \mathrm{d}t \frac{1}{(2\pi y)^{1/2}} \exp\left(-\frac{1}{2}\frac{(t \mp 2x)^2}{y}\right)$$

with

$$x = \operatorname{Im}(\mathrm{i}\lambda/\varepsilon, f)$$
$$y = (f, Af) > 0.$$

Hence both measures $\mu_\pm$ are absolutely continuous with respect to the Lebesgue measure $\mathrm{d}t$ and by [13]

$$P(\omega_+, \omega_-) \leqslant \left[\int \left(\frac{\mathrm{d}\mu_+}{\mathrm{d}t}\right)^{1/2} \left(\frac{\mathrm{d}\mu_-}{\mathrm{d}t}\right)^{1/2} \mathrm{d}t\right]^2.$$

We choose

$$f = (\lambda/\varepsilon) \tanh \tfrac{1}{2}\beta\varepsilon \in \mathcal{H}_-$$

and compute

$$\int \left(\frac{\mathrm{d}\mu_+}{\mathrm{d}t}\right)^{1/2} \left(\frac{\mathrm{d}\mu_-}{\mathrm{d}t}\right)^{1/2} \mathrm{d}t = \exp\left[-2 \int \mathrm{d}k \left(\frac{\lambda}{\varepsilon}(k)\right)^2 \tanh \tfrac{1}{2}\beta\varepsilon(k)\right].$$

Combining the upper and lower bounds yields the proof of the theorem.

This theorem yields an understanding of the fact that, under the conditions (2), for finite temperature $T > 0$ there always exists a finite transition probability between the two spin states, there is no infinite barrier, the states do not represent distinct phases, there is no symmetry breaking and one should have a unique equilibrium state, as was proved in § 3. In fact, although the computation of the theorem above is meant for a better physical understanding of the phenomenon, it is also possible to use it as the basis of a rigorous proof. Indeed, a strictly positive transition probability implies the quasi-equivalence of the states ω_+ and ω_-, which is the basic mathematical argument behind the property of theorem 3.1 [7].

Furthermore, formula (18) indicates that for the ground state ($T = 0$), there is still quantum tunnelling ($P(\omega_+, \omega_-) > 0$) as long as $\lambda/\varepsilon \in L^2$. The transition probability vanishes if $\lambda/\varepsilon \notin L^2$. This condition turns up in [6] as a sufficient condition for symmetry breaking. This condition is also suggested by a first-order perturbation calculation in the parameter μ. Indeed, if $\mu = 0$, the ground state is two-fold degenerate and the two states are explicitly given by

$$\omega^0_{\infty,\pm}(W(f) \otimes X) = e_\pm(X) \exp[\pm 2\mathrm{i} \operatorname{Im}(\mathrm{i}\lambda/\varepsilon, f) - \tfrac{1}{2}\|f\|^2]$$

where

$$X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}$$

$$e_\pm(X) = \begin{cases} x_{11} & \text{for } e_+ \\ x_{22} & \text{for } e_-. \end{cases}$$

The states $\omega^0_{\infty,\pm}$ are orthogonal vector states

$$\omega^0_{\infty,\pm}(\cdot) = (\psi_\pm, \cdot\, \psi_\pm)$$

represented by the vectors

$$\psi_+ = \begin{pmatrix} \Omega_+ \\ 0 \end{pmatrix} \qquad \psi_- = \begin{pmatrix} 0 \\ \Omega_- \end{pmatrix}$$

where $\Omega_\pm$ are the cyclic vectors of $\omega_\pm$ and satisfying

$$|(\Omega_+, \Omega_-)|^2 = \exp\left[-4 \int \mathrm{d}k \left(\frac{\lambda}{\varepsilon}(k)\right)^2\right].$$

If E_0 is the ground-state energy in the states $\omega_\pm$, the first-order Rayleigh-Ritz perturbation calculation of the perturbed energy yields the values

$$E_{\mu,\pm} = E_0 \pm \mu \exp\left[-2 \int \mathrm{d}k \left(\frac{\lambda}{\varepsilon}(k)\right)^2\right]$$

showing that the degeneracy disappears if $\lambda/\varepsilon \in L^2$, and remains if $\lambda/\varepsilon \notin L^2$.

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