

On the Validity of an Einstein Relation in Models of Interface Dynamics

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We consider models of interface dynamics derived from Ising systems with Kac interactions and we prove the validity of the "Einstein relation" $\theta = \mu\sigma$, where θ is the proportionality coefficient in the motion by curvature, μ is the interface mobility, and σ is the surface tension.

KEY WORDS: Interface dynamics; motion by curvature; surface tension; mobility.

1. INTRODUCTION

In ref. 2 it is shown that the Glauber dynamics in Ising spin systems with Kac interactions gives rise, in the Lebowitz–Penrose limit, to the equation

$$\frac{\partial m}{\partial t} = -m + \tanh\{\beta(J * m + h)\} \quad (1)$$

($J * m$ being the convolution of J and m), which describes the evolution of the magnetic profile $m = m(r, t)$. In (1), J is the Kac potential, β the inverse temperature, and h the magnetic field. In a companion paper⁽³⁾ it is shown that (1) with $h = 0$ gives rise to a motion by curvature. The result is obtained under some assumptions on J , namely that $J = J(|r|)$, J in C^2 , nonincreasing and identically 0 when $|r| \geq 1$. Furthermore, $\beta\hat{J}(0) > 1$, with $\hat{J}(0) = \int dr J(|r|)$, namely $\beta > \beta_c$, the Lebowitz–Penrose critical temperature with $h = 0$.⁽⁵⁾ The equilibrium magnetization at $\beta > \beta_c$ are $\pm m_\beta$, where m_β is the strictly positive solution of

$$m_\beta = \tanh\{\beta\hat{J}(0)m_\beta\} \quad (2)$$

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The interface dynamics is related to the evolution of an initial magnetic profile which is equal to m_β inside a region A_0 and $-m_\beta$ outside of it. In ref. 3 it is proved that, under a suitable scaling, the evolution is given by a profile which is still m_β inside a region A_t and $-m_\beta$ outside of it, with ∂A_t , the surface of A_t , moving by curvature, namely

$$\frac{dr}{dt} = \frac{\theta}{R(r)} v(r) \tag{3}$$

with $r=r(t)$ the generic point of the surface which moves by curvature; $R(r)^{-1}$ is $(d-1)$ times the mean curvature, and $v(r)$ is the unit normal vector directed toward the concavity. θ is a constant, whose explicit expression is also derived in ref. 3:

$$\theta = \int \mu(dx) [1 - \bar{m}(x)^2] \beta \int dx' \int_{\mathbb{R}^{d-1}} dy J(|(x' - x)^2 + y^2|^{1/2}) \frac{\bar{m}'(x') y_1^2}{\bar{m}'(x) 2} \tag{4}$$

where

$$\mu(dx) = N \frac{\bar{m}'(x)^2}{1 - \bar{m}(x)^2} dx, \quad N^{-1} = \int_{\mathbb{R}} dx \frac{\bar{m}'(x)^2}{1 - \bar{m}(x)^2} \tag{5}$$

with $\bar{m}(x)$ the solution to the $d=1$ problem:

$$\bar{m} = \tanh\{\beta \tilde{J} * \bar{m}\}, \quad \lim_{x \rightarrow \pm\infty} \bar{m}(x) = \pm m_\beta \tag{6}$$

with

$$\tilde{J}(x) = \int_{\mathbb{R}^{d-1}} dy J(|x^2 + y^2|^{1/2}) \tag{7}$$

We refer to ref. 3 for details and notation.

Spohn⁽⁶⁾ has conjectured the validity of an Einstein relation which relates the “transport coefficient” θ appearing in the equation for the motion by curvature, the linear transport coefficient μ , which represent the mobility of the surface, and a thermodynamic quantity which, in this case, is the surface tension σ . As we shall see, it is possible to compute μ and σ independently for the model which gives rise to (1). We will prove that the value of θ obtained in ref. 3 is equal to the product $\mu\sigma$, so that the Einstein relation

$$\theta = \mu\sigma \tag{8}$$

is indeed verified in this model.

2. SURFACE TENSION

The excess free energy associated to m is^(1,5,4)

$$F(m) = \int dr [f(m) - f(m_\beta)] + \frac{1}{4} \int dr dr' J(r-r') [m(r) - m(r')]^2 \quad (9)$$

where

$$\begin{aligned} f(m) &= -\frac{1}{2} \hat{J}(0) m^2 + \beta^{-1} \frac{1+m}{2} \log \frac{1+m}{2} + \beta^{-1} \frac{1-m}{2} \log \frac{1-m}{2} \\ &= -\frac{1}{2} \hat{J}(0) m^2 + \beta^{-1} \frac{m}{2} \log \frac{1+m}{1-m} + \beta^{-1} \frac{1}{2} \log(1-m^2) \end{aligned} \quad (10)$$

$$\int dr dr' J(r-r') [m(r) - m(r')]^2 = 2 \int dr [\hat{J}(0) m^2 - mJ * m] \quad (11)$$

so that

$$F(m) = \int dr [g(m) - g(m_\beta)] \quad (12)$$

where

$$g(m) = \beta^{-1} \frac{m}{2} \log \frac{1+m}{1-m} + \beta^{-1} \frac{1}{2} \log(1-m^2) - \frac{1}{2} mJ * m \quad (13)$$

We point out that $F(m)$ is a positive-definite functional of m . Then it is well defined for every measurable m , but not finite in general.

Since \bar{m} is interpreted as the interface profile connecting the $\pm m_\beta$ phases, the surface tension can be expressed as

$$\begin{aligned} \sigma &= \lim_{L \rightarrow \infty} \frac{1}{(2L)^{d-1}} \lim_{M \rightarrow \infty} \int_{-L}^L dy_1 \cdots \int_{-L}^L dy_{d-1} \int_{-M}^M dx [g(m^*) - g(m_\beta)] \\ &= \int dx [g(m^*) - g(m_\beta)] \end{aligned} \quad (14)$$

where

$$m^*(r) = \bar{m}(x) \quad (15)$$

if $r = (x, y_1, \dots, y_{d-1})$ in a coordinate frame with the x axis orthogonal to the equilibrium interface.

A more microscopic definition of the surface tension (see ref. 6 and references therein) involves the computation of the logarithm (normalized by the surface area) of the ratio of two partition functions with different boundary conditions. The second one has boundary conditions $+$ on the two opposite faces of a cube and periodic conditions on the other ones; the first one is defined by conditions $+$ and $-$ instead of $+$ and $+$. The correct procedure for obtaining the surface tension is to take first the thermodynamic limit, then the limit as $\gamma \rightarrow 0$, γ being the scalus parameter in the Kac potential. To my knowledge, there is no proof that this gives rise to the value (14). However, if one takes the thermodynamic limit and simultaneously $\gamma \rightarrow 0$, in a suitable fashion, then (14) can be proven to hold, as it follows from the analysis of ref. 1 and from results recently obtained by Cassandro and Vares.

From (6) and (15) it follows easily that

$$g(m^*)(r) = \frac{1}{2}(\bar{m}\tilde{J} * \bar{m} + \beta^{-1} \log(1 - \bar{m}^2))(x) \quad (16)$$

But Eq. (6) implies also

$$(1 - \bar{m}^2) \beta \tilde{J} * \bar{m}' = \bar{m}' \quad (17)$$

so that

$$\frac{d}{dx} g(m^*) = \frac{1}{2} (\bar{m}' \tilde{J} * \bar{m} - \bar{m} \tilde{J} * \bar{m}') \quad (18)$$

Integrating by parts in (14), we finally obtain

$$\begin{aligned} \sigma &= -\frac{1}{2} \int dx \, x \frac{d}{dx} g(m^*) \\ &= \frac{1}{2} \int dx \, dx' (x' - x) \bar{m}'(x) \tilde{J}(x - x') \bar{m}(x') \end{aligned} \quad (19)$$

3. MOBILITY

We are looking for a planar traveling wave solution of (1),

$$m_h(r, t) = m_h(x - v(h)t) \quad (20)$$

for small h . E. Orlandi and L. Triolo (private communication) have shown the existence of a solution for small h which is close to the $h=0$ stationary solution m^* . Avoiding the uniqueness problem, we take this solution and expand

$$v(h) = v_1 h + O(h^2), \quad m_h = \bar{m} + h\psi + O(h^2) \quad (21)$$

From (1), at first order in h , we obtain the following identity:

$$-v_1 \bar{m}' = -\psi + (1 - \bar{m}^2) \beta \tilde{J} * \psi + \beta(1 - \bar{m}^2) \quad (22)$$

We multiply both sides of (22) by $\bar{m}'(x)/[1 - \bar{m}(x)^2]$ and then integrate; using (17), we obtain

$$v_1 = -2N\beta m_\beta \quad (23)$$

But, by the definition of the mobility, we must have

$$v(h) = -2m_\beta \mu h + O(h^2) \quad (24)$$

Equations (23) and (24) imply then

$$\mu = N\beta \quad (25)$$

4. CONCLUSIONS

We can now prove Eq. (8). By substituting (5) in (4) we have the following expression for θ :

$$\theta = \frac{1}{2}N\beta \int dx \bar{m}'(x) \int dx' dy J(|x' - x|^2 + y^2)^{1/2} \bar{m}'(x') y_1^2 \quad (26)$$

This expression seems quite different from the product $\mu\sigma$. In order to obtain (8) it is convenient to eliminate the dependence on the y_1 variable to have θ expressed in terms of \bar{m} and \tilde{J} . We note that

$$\frac{\partial}{\partial x'} J(|x' - x|^2 + y^2)^{1/2} = \frac{x' - x}{y_1} \frac{\partial}{\partial y_1} J(|x' - x|^2 + y^2)^{1/2} \quad (27)$$

Integrating by parts in dx' , using (27), and then integrating by parts in dy_1 , we obtain

$$\theta = \frac{1}{2}N\beta \int dx dx' (x' - x) \bar{m}'(x) \tilde{J}(x - x') \bar{m}(x') \quad (28)$$

Equation (8) follows then from (19), (25), and (28).

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