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Tunnelling in Nonlocal Evolution Equations

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Abstract

We study "tunnelling" in a one-dimensional, nonlocal evolution equation by assigning a penalty functional to orbits which deviate from solutions of the evolution equation. We discuss the variational problem of computing the minimal penalty for orbits which connect two stable, stationary solutions.

1 Introduction

Tunnelling is a phenomenon which describes transitions between two stable states of a system. It appears in nature in the most various contexts and for the most different causes. It is frequently observed in quantum mechanics, where its prototype is a Schrödinger particle subject to a symmetric double-well potential. Unlike its classical analogue, due to intrinsic quantum indeterminacy, there is a delocalization of the ground state with the wave function spreading over both wells. This causes a splitting of the energy levels which is well observed experimentally and with important practical applications.

The phenomenon is not restricted to atomic physics. It appears also in macroscopic systems. Its most known aspect is maybe metastability, where an apparently stable state after a long time suddenly and unexpectedly changes into a new, more stable one. Analogous to metastability is the tunnelling between two pure phases of a same system. In both cases the origin of the phenomenon is ascribed to stochastic fluctuations which are due to "intrinsic randomness" in the system, to "random external forces" or to both. In all cases one is interested in the waiting time for the tunnelling to take place, the nature of the forces which drive the tunnelling and the specific pattern of the tunnelling event. As we will see, such questions involve interesting problems of mathematical engineering.

As a schematic model of the phenomenon we consider here a nonlocal evolution equation which has been introduced in connection with the analysis of Ising systems with Kac potentials. Our setting is one-dimensional for which the analysis is much simpler. The state of the system is then described by a function $u = u(x,t)$, $|x| \le L$, $L > 1$, $t \ge 0$, which has the physical meaning of a magnetization density at point x and time t. We suppose that u evolves according to the evolution equation

$$u_t = f_L(u), \qquad u(\cdot,0) \text{ given}, \tag{1.1}$$

with u_t the t-derivative of u and the "force field" $f_L(u)$ given by

$$f_L(u) = -\frac{1}{\beta} \operatorname{arctanh} u + J^{\text{neum}} * u, \quad \beta > 1; \qquad J^{\text{neum}} * u(x) = \int_{-L}^{L} J^{\text{neum}}(x,y)u(y)\,dy$$

$$J^{\text{neum}}(x,y) = J(x,y) + J(x,R_L(y)) + J(x,R_{-L}(y)), \tag{1.2}$$

with $R_\xi(y) = \xi - (y - \xi)$ the reflection of y around ξ. We finally suppose that $J(x,y)$, $(x,y) \in \mathbb{R} \times \mathbb{R}$, is a smooth, symmetric, translationally invariant probability kernel supported in $|y - x| \le 1$. We also assume that $J(0,x)$ is a nonincreasing function whenever restricted to $x \ge 0$.

A solution $u(x,t)$, $|x| \le L$, $t \ge 0$, of (1.1) is mapped under reflections around all nL, $n = \pm 1, \pm 3,\ldots$, into a function $v(x,t)$, $x \in \mathbb{R}$, $t \ge 0$,

$$v(x,t) = u(x,t) \text{ for } |x| \le L; \quad v(R_{nL}(x),t) = v(x,t),\ n = \pm 1, \pm 3, \ldots \text{ for all } x, \tag{1.3}$$

which solves $v_t = f(v) = -\dfrac{1}{\beta} \operatorname{arctanh} v + J * v$. The same occurs to the local version of (1.1), i.e. the Allen-Cahn equation $u_t = u_{xx} + \phi(u)$ with the Laplacian defined with Neumann boundary conditions. Thus, if $u(x,t)$ solves the Allen-Cahn equation in $[-L,L]$ with Neumann boundary conditions, $v(x,t)$ defined by (1.3) solves the Allen-Cahn equation on the whole line. This is why we have denoted by J^{neum} the kernel in (1.2).

The choice of Neumann boundary conditions simplifies the analysis. For instance the stationary, spatially homogeneous solutions of (1.1) turn out to be independent of L. In particular we are interested in the two solutions $m^{(\pm)}(x), |x| \le L$, $m^{(\pm)}(x) \equiv \pm m_\beta$ with $m_\beta > 0$ solving the mean field equation $m_\beta = \tanh\{\beta m_\beta\}$, $\beta > 1$, which are stationary solutions of (1.1), for any value of L (we are not making here explicit the dependence on L). It can also be seen that $m^{(\pm)}$ are locally stable, namely that there are neighborhoods (in the L^2 or in the L^∞ norms) of $m^{(\pm)}$ which are attracted by $m^{(\pm)}$ under the evolution generated by (1.1).

$m^{(\pm)}$ play here the role of pure phases and the tunnelling events which occur within a time $\tau > 0$ are then represented by the set of orbits

$$\begin{aligned} \mathcal{U}_\tau[m^{(-)}, m^{(+)}] = \Big\{ & u \in C^\infty\big((-L,L) \times (0,\tau); (-1,1)\big) : \\ & \lim_{t \to 0^+} u(\cdot,t) = m^{(-)},\ \lim_{t \to \tau^-} u(\cdot,t) = m^{(+)} \Big\}. \end{aligned} \tag{1.4}$$

Due to the stationarity of $m^{(\pm)}$ no element in $\mathcal{U}_\tau$ can satisfy (1.1) and therefore other forces must enter into the game. Their choice can be related to a Lagrangian action in the following way. Call $b = b(x,t)$, $|x| \le L$, $0 \le t \le \tau$, an "external force", and consider the corresponding evolution equation

$$u_t = f_L(u) + b. \tag{1.5}$$

We are of course only interested in forces b able to produce orbits in $\mathcal{U}_\tau[m^{(-)}, m^{(+)}]$. To select among them we introduce an action functional

$$I_\tau(u) = \frac{1}{4}\int_0^\tau \int_{-L}^{L} b^2 \, dx \, dt \equiv \frac{1}{4}\int_0^\tau \int_{-L}^{L} \big(u_t - f_L(u)\big)^2 \, dx \, dt, \tag{1.6}$$

which is interpreted as "the cost" of the force field b which produces the orbit u. In other words $I_\tau(u)$ is the penalty assigned to the orbit u if one thinks of b as an electric field, (1.6) is the dissipation due to a constant resistivity, the value of which in (1.6) is set equal to 4.

In the above setting it looks natural to ascribe the actual tunnelling event to the force field which has the minimal cost. This leads to the variational problem

$$P_{[m^{(-)},m^{(+)}]} := \inf_{\tau>0} \inf_{u \in \mathcal{U}_\tau[m^{(-)},m^{(+)}]} I_\tau(u). \tag{1.7}$$

Observe that the inf in the formulation (1.7) automatically lifts the "unnatural constraint" in (1.4) where functions are restricted to the C^∞ class. Actually the relevant space is the one for which I_τ is finite and this selects the space of L^2 functions the time derivative of which is also in L^2.

The variational problem with $\tau > 0$ fixed is exactly the Euler-Lagrange variational problem with Lagrangian $\mathcal{L}(u, u_t) = (u_t - f_L(u))^2/4$. The corresponding Euler-Lagrange equation is

$$b_t = -b f_L'(u), \tag{1.8}$$

which we may regard as an equation for b with u determined by b through equation (1.5). Equation (1.8) is then the equation for the optimal force needed for tunnelling and places the whole problem in the light of an "engineering design of forces".

We next introduce some physical considerations in order to relate the waiting time for tunnelling to the penalty $P_{[m^{(-)},m^{(+)}]}$. In statistical mechanics the forces b are random and their probability is a datum of the problem. Thus one knows, in principle, the probability of any possible force field b in (1.5) and in particular of those which give rise to a tunnelling. These probabilities are expected to be very small, exponentially small with an exponent proportional to $-\epsilon^{-d}$ (d the space dimension; here $d = 1$), $\epsilon > 0$ a small parameter which represents the ratio between microscopic and macroscopic lengths. The proportionality coefficient is called the "rate function of large deviation" and we interpret our $I_\tau(u)$ as such a rate function (which in the applications could have quite a different expression than our simple formula (1.6)). Thus we are supposing that the probability of observing u goes like $\exp\{-\epsilon^{-d} I_\tau(u)\}$ and, since the time to wait before observing an event is proportional to the inverse of its probability, the expected time T for tunnelling goes as $\exp\{\epsilon^{-d} P_{[m^{(-)},m^{(+)}]}\}$. Thus T is very long, as it scales like ϵ^{-d}, and the main interest in statistical mechanics is to estimate the proportionality coefficient $P_{[m^{(-)},m^{(+)}]}$, which, as we will see, can be done quite explicitly within our scheme. The next problem is to understand how the tunnelling proceeds once it starts and this is described by the minimizing sequences which realize $P_{[m^{(-)},m^{(+)}]}$. Even though the problem is much more complex than the mere computation of $P_{[m^{(-)},m^{(+)}]}$, nevertheless, in our context, it has a quite complete and detailed answer. We in fact see that all the minimizing sequences are very similar to each other, following (1.1) in some parts of the tunnelling orbit and its time reversal, in other parts.

The relation between variational problems and large deviations is well established, see the classical reference by Friedlin and Ventsel, [13]. The application of the theory to tunnelling in the spirit outlined above has been first and beautifully carried out by Faris and Jona-Lasinio, [12], in the context of the stochastic Allen-Cahn equation $u_t = u_{xx} + \phi(u) + \sqrt{\epsilon}b$ for a particular choice of force ϕ, with b a standard white noise in space-time and with Dirichlet boundary conditions at $\pm L$. The rate function in such cases has a structure similar to (1.6) and we in fact use many of the ideas contained in [12]. Their adaptation to (1.1) is from one side simpler because we only look at the variational problem and avoid all questions concerning probabilities, but, on the other side, it brings in new difficulties as we miss a characterization of the stationary solutions of the deterministic problem (i.e. without b) which are instead easy in the case $u_{xx} + \phi(u) = 0$, as is discussed in the beginning of Section 5 below.

We finally mention that our analysis heavily exploits that there is no restriction on the times τ in the inf in (1.7). We see that a good approximation to the inf can be obtained by taking times τ of the order of $e^{2\alpha L}$, $\alpha > 0$ (for L large). The question, which will be hopefully studied in a forthcoming paper, is to determine how the result changes if we restrict the inf to times τ much smaller than $e^{2\alpha L}$ or much larger. In the second case it is easy to see that $P_{[m^{(-)},m^{(+)}]}$ is not really affected, but in the former the penalty becomes larger and an interesting question is to design the right forces b which produce such a faster tunnelling.

In the next section we state a few properties of the model which are simple but fundamental for the whole analysis. Then in Section 3 we state the main results. In Section 4 and Section 5 we discuss upper and, respectively, lower bounds on $P_{[m^{(-)},m^{(+)}]}$. Section 6 contains some bibliographical remarks and the acknowledgments. Some of the proofs are only sketched for reasons of space. The reader may find the missing details in a companion paper, [1].

2 Work, energy, reversibility

We denote by $\mathcal{U}_\tau[m, m']$ the space of orbits which go from m to m' in a time τ and define the work done by the force f_L along the orbit $u \in \mathcal{U}_\tau[m, m']$ as

$$W_\tau(u) := \int_0^\tau \int_{-L}^{L} f_L(u) u_t \, dx \, dt.$$

We also call $I_\tau^{\mathrm{rev}}(u)$

$$I_\tau^{\mathrm{rev}}(u) := \frac{1}{4} \int_0^\tau \int_{-L}^{L} (u_t + f_L(u))^2 \, dx \, dt,$$

"rev" stands for reversed. Notice in fact that, if u solves (1.1), then the reversed orbit $v(x,t) := u(x, \tau - t)$ solves $v_t = -f_L(v)$. Thus $I_\tau^{\mathrm{rev}}(u)$ is the penalty for departures from reversed orbits. The following theorem and corollary are quite general and do not use the specific form of the force field f_L.

Theorem 1. *For any* τ *and* $u \in \mathcal{U}_\tau[m, m']$

$$I_\tau(u) = I_\tau^{\rm rev}(u) - W_\tau(u). \tag{2.1}$$

Proof. By expanding the square on the r.h.s. of (1.6),

$$\frac{1}{4}\big(u_t - f_L(u)\big)^2 = \frac{1}{4}\big(u_t + f_L(u)\big)^2 - u_t f_L(u),$$

(2.1) follows after space-time integration.

■

Corollary 1. *For any* τ *and* $u \in \mathcal{U}_\tau[m, m']$

$$I_\tau(u) \geq \sup_{0\leq t\leq\tau} -W_t(u). \tag{2.2}$$

If there is $v \in \mathcal{U}_\tau[m', m]$ *which solves* (1.1)*, then* $v^{\rm rev}(x, t) = v(x, \tau - t) \in \mathcal{U}_\tau[m, m']$ *and*

$$I_\tau(v^{\rm rev}) = W_\tau(v) = -W_\tau(v^{\rm rev}). \tag{2.3}$$

Proof. Since $I_t^{\rm rev}(u) \geq 0$, $0 \leq t \leq \tau$, (2.2) follows from (2.1); (2.3) also follows because $I_\tau^{\rm rev}(v^{\rm rev}) = 0$.

■

Note that, if v satisfies the reversed equation, i.e. $v_t = -f_L(v)$, then v solves (1.5) with $b = -2f_L(v)$. By direct inspection such a pair b and v solves the Euler-Lagrange equation (1.8) (with v in place of u), which seems to indicate that in the same context of (2.3)

$$\inf_{u\in\mathcal{U}_\tau[m,m']} I_\tau(u) = -W_\tau(v^{\rm rev}) = W_\tau(v). \tag{2.4}$$

Equation (2.4) and more generally a control of the work functional $W_\tau(u)$ are easy in "gradient systems" and fortunately (1.1) is "gradient".

Definition 1. We say that the force f_L is gradient if there exists a functional $\mathcal{F}_L$ defined on $L^\infty([-L, L]; [-1, 1])$ such that for any $\tau > 0$ the work $W_\tau(u)$ done by f_L along the orbit $u \in \mathcal{U}_\tau[m, m']$, satisfies

$$W_\tau(u) = \mathcal{F}_L(u(\cdot, 0)) - \mathcal{F}_L(u(\cdot, \tau)). \tag{2.5}$$

Theorem 2. *Equation* (2.5) *holds with*

$$\mathcal{F}_L(m) = \int_{-L}^{L} \phi_\beta(m)dx + \frac{1}{4}\int_{-L}^{L}\int_{-L}^{L} J^{\rm neum}(x, y)(m(x) - m(y))^2 dx\, dy, \tag{2.6}$$

where

$$\phi_\beta(m) = \tilde\phi_\beta(m) - \min_{|s|\leq 1}\tilde\phi_\beta(s), \qquad \tilde\phi_\beta(m) = -\frac{m^2}{2} - \frac{1}{\beta}\mathcal{S}(m), \qquad \beta > 1,$$

$$\mathcal{S}(m) = -\frac{1-m}{2}\log\frac{1-m}{2} - \frac{1+m}{2}\log\frac{1+m}{2}.$$

Proof. By direct inspection $f_L(m) = -\dfrac{\delta \mathcal{F}_L(m)}{\delta m}$, the functional derivative of $\mathcal{F}_L$, and (2.5) follows. Theorem 2 is proved.

■

Note that the work done by f_L on orbits u which solve (1.1) is always nonnegative so that the free energy $\mathcal{F}_L(u(\cdot,t))$ is a nonincreasing function of t.

With the help of Theorems 1 and 2 Corollary 1 becomes:

Theorem 3. *For any τ and $u \in \mathcal{U}_\tau[m,m']$,*

$$I_\tau(u) = I_\tau^{\mathrm{rev}}(u) + [\mathcal{F}_L(m') - \mathcal{F}_L(m)] \geq \sup_{0\leq t\leq\tau} \{\mathcal{F}_L(u(\cdot,t)) - \mathcal{F}_L(u(\cdot,0))\}.$$

If there is $v \in \mathcal{U}_\tau[m',m]$ which solves (1.1)*, then*

$$\inf_{u\in\mathcal{U}_\tau[m,m']} I_\tau(u) = \mathcal{F}_L(m') - \mathcal{F}_L(m).$$

The infimum on the l.h.s. is a minimum, the minimizer is unique and is given by the time reversal of v.

3 Main results

The optimal strategy for connecting $m^{(-)}$ to $m^{(+)}$ shows the emergence of spatial patterns. In fact for L large enough it costs too much to connect $m^{(-)}$ and $m^{(+)}$ using orbits $u(x,t)$ which are spatially constant ($u(x,t)$ independent of x). Indeed by continuity there is a time t_0 when $u(\cdot,t_0) = 0$ and by Theorem 3 $I_\tau(u) \geq \mathcal{F}_L(u(\cdot,t_0)) = 2L\phi_\beta(0)$. There are instead spatially dependent orbits the free energies of which are bounded independently of L. They are constructed using profiles which have values close to $-m_\beta$ and m_β except for an interpolating interval of fixed length. In such a class for L large enough there is a special profile $\hat{m}_L$ which is stationary, [8], [6], [2], and we see by following the strategy proposed in [12] for the Allen-Cahn case that the best way to connect $m^{(-)}$ with $m^{(+)}$ is by passing close to $\hat{m}_L$. These ideas are used to prove the following theorem:

Theorem 4. *For any L large enough*

$$P_{[m^{(-)},m^{(+)}]} = \mathcal{F}_L(\hat{m}_L). \tag{3.1}$$

$\hat{m}_L$ is called a finite volume "instanton". Instantons are defined as stationary solutions of the whole line version of (1.1) which have definite and opposite signs at $\pm\infty$. Existence of instantons has been established in [9], [10], [7], where it is proved that there is a solution of the equation

$$\bar{m}(x) = \tanh\{\beta J * \bar{m}(x)\}, \quad x \in \mathbb{R}, \tag{3.2}$$

which is increasing, antisymmetric and converges exponentially fast to $\pm m_\beta$ as $x \to \pm\infty$. Any other solution of (3.2), which is strictly positive definite [respectively negative] as $x \to \infty$ [respectively $x \to -\infty$], is a translate of $\bar{m}(x)$.

$n(x) := \bar{m}(x)\mathbf{1}_{|x|\leq L}$ is not a stationary solution of (1.1) because $f_L(n) \neq 0$ for some $|x| > L-1$. However, in a "small" neighborhood of n there is one (and only one) stationary solution. More precisely in [2] it is shown that given any $\epsilon > 0$ for all L large enough there is an antisymmetric function $\hat{m}_L(x)$ which solves

$$\hat{m}_L(x) = \tanh\left\{\beta J^{\text{neum}} * \hat{m}_L(x)\right\}, \quad |x| \le L, \tag{3.3}$$

and is such that

$$\|\hat{m}_L - \bar{m}\|_\infty \le \epsilon, \tag{3.4}$$

where $\|\cdot\|_\infty$ is the L^∞ norm in $[-L, L]$. Moreover $\hat{m}_L$ is the unique solution in the neighborhood (3.4). A stronger property is stated below. By an abuse of notation $\hat{m}_L$ is also called an instanton.

We conclude by remarking that the mere existence of an antisymmetric function $\hat{m}_L \neq m^{(0)}$ ($m^{(0)} \equiv 0$) is very easy to prove. Consider in fact the orbit of (1.1) which starts from $m_0(x) = \bar{m}(x)\mathbf{1}_{|x|\le L}$. Antisymmetry is preserved by the dynamics. Thus any limit point of the orbit is antisymmetric; the limit points solve (3.3) because $\mathcal{F}_L$ is strictly decreasing at points which are not solutions of (3.3). If L is large enough, $\mathcal{F}_L(m^{(0)}) > \mathcal{F}_L(m_0)$. Hence $m^{(0)}$ is not a limit point.

The proof of Theorem 4 shows that any minimizing sequence in (1.7) passes arbitrarily close to $\hat{m}_L$. A stronger characterization actually holds as we are going to see. In fact a much more refined analysis of (1.1) than the previous simple argument for the existence of an instanton shows that there are two invariant, one-dimensional manifolds, $v^{(\pm)}(\cdot, s)$, $s \in \mathbb{R}$, (dependence on L is not made explicit), which connect $\hat{m}_L$ to $m^{(-)}$ and, respectively, to $m^{(+)}$. Existence and properties of invariant manifolds have been proved in [2] for a dynamics closely related to the one we are considering, see (4.5) below. In a future paper we will extend the results to our dynamics (1.1) and prove that the manifolds $v^{(\pm)}(\cdot, s)$ satisfy the following two properties:

$$\lim_{s\to-\infty} \|v^{(\pm)}(\cdot, s) - \hat{m}_L\|_2 = 0, \quad \lim_{s\to\infty} \|v^{(\pm)}(\cdot, s) - m^{(\pm)}\|_2 = 0,$$

where $\|\cdot\|_2$ is the L^2 norm,

$$T_t(v^{(\pm)}(\cdot, s)) = v^{(\pm)}(\cdot, s+t), \quad \text{for all } s \in \mathbb{R} \text{ and all } t \ge 0$$

and we recall that $T_t(m)$ is the semigroup generated by (1.1). Again dependence on L is not made explicit. Moreover $\mathcal{F}_L(v^{(\pm)}(\cdot, s)) < \mathcal{F}_L(\hat{m}_L)$ for any $s \in \mathbb{R}$.

It is also proved that manifolds with such properties are unique, except of course for the trivial change $s \to s + a$ in the parametrization and space reversal, $x \to -x$. By symmetry it is easily seen that $v^{(-)}(x, s) = -v^{(+)}(-x, s)$.

Roughly speaking the next theorem says that the solution to (1.7) is given by an orbit which is made by patching together the time reversed of $v^{(-)}$ with $v^{(+)}$.

Theorem 5. *For all L large enough, if (τ_n, u_n) is a minimizing sequence for (1.7), then $\tau_n \to \infty$, and, given any $\epsilon > 0$ and $T > 0$, u_n (or its image under $x \to -x$) has the following property as soon as n is large enough. The interval $[0, \tau_n]$ divides into five, consecutive intervals, $I_1, .., I_5$. For $t \in I_1$, $\|u_n(\cdot, t) - m^{(-)}\|_2 \le \epsilon$; for $t \in I_3$, $\|u_n(\cdot, t) - \hat{m}_L\|_2 \le \epsilon$; for $t \in I_5$, $\|u_n(\cdot, t) - m^{(+)}\|_2 \le \epsilon$. Finally*

$$\|u_n(\cdot, t) - v^{(-)}(\cdot, T - (t - t'))\|_2 \le \epsilon, \qquad t \in I_2 = [t', t' + 2T],$$

while

$$\|u_n(\cdot,t) - v^{(+)}(\cdot, -T + (t - t''))\|_2 \le \epsilon, \qquad t \in I_4 = [t'', t'' + 2T].$$

Theorem 5 will be proved in a future paper. We have stated it here only for the sake of presentation just to give a more complete picture on the tunnelling phenomenon. Indeed Theorem 4 answers the first question about tunnelling, namely the time to wait for observation of the tunnelling (see the Introduction for a discussion on the relation between the latter and the penalty $P_{[m^{(-)},m^{(+)}]}$). Theorem 5 instead specifies also the way the tunnelling occurs. While it is well established that a minimizing sequence can be obtained by following the reversed flow on the invariant manifolds, see [12], our statement in Theorem 5 completes the picture by saying that "this is in fact the only possible way" as any other pattern would lead to a larger penalty.

The time for the tunnelling, once it starts, is dictated by the flow along the invariant manifolds except for the motion close to its endpoints, which can be reached only after an infinite time if motion is all the way along the invariant manifolds. To keep the time τ finite we then need to depart from the manifolds with "shortcuts" close to the endpoints.

The optimal force to add for tunnelling is then $b(x,t) = -2f_L(v^{(-)}(x,t))$ when the orbit follows in reversed time the manifold $v^{(-)}$ while $b = 0$ along $v^{(+)}$ as the motion is then classical. Then theorem 5 provides an answer also to the question raised in the Introduction about the optimal design of external forces to add to have a tunnelling.

4 Upper bound

We prove (3.1) by proving lower and upper bounds and start from the latter, namely we prove that

$$P_{[m^{(-)},m^{(+)}]} \le \mathcal{F}_L(\hat{m}_L) \tag{4.1}$$

by exhibiting a sequence (τ_n, u_n), $\tau_n \to \infty$, $u_n \in \mathcal{U}_{\tau_n}[m^{(-)}, m^{(+)}]$ such that

$$\lim_{n\to\infty} I_{\tau_n}(u_n) \le \mathcal{F}_L(\hat{m}_L).$$

Lemma 1. *Suppose that there are two sequences, $m_n^{\pm}$, such that $\|m_n^{\pm}\|_\infty \le c < 1$,*

$$\lim_{n\to\infty} \|m_n^{\pm} - \hat{m}_L\|_2 = 0, \qquad \lim_{t\to\infty} \|T_t(m_n^{\pm}) - m^{(\pm)}\|_2 = 0 \tag{4.2}$$

and $\mathcal{F}_L(m_n^{\pm}) \le \mathcal{F}_L(\hat{m}_L)$. Then (4.1) holds.

Proof. By (4.2) there is t_n such that

$$\|T_{t_n}(m_n^{\pm}) - m^{(\pm)}\|_2 \le \frac{1}{n}. \tag{4.3}$$

Set $\tau_n = 2t_n + 4$ and divide $[0,\tau_n]$ into 6 intervals. In the first one, $[0,1]$, we set

$$u_n(\cdot,t) = a(t)\, T_{t_n}(m_n^-) + [1 - a(t)]\, m^{(-)}, \quad t \in [0,1],$$

$a(t)$ being a smooth increasing function with $a(0) = 0$ and $a(1) = 1$. Let

$$u_n(\cdot, t) = T_{t_n+1-t}(m_n^-), \quad t \in [1, 1 + t_n],$$

while for $1 + t_n \le t \le t_n + 2$

$$u_n(\cdot, t) = a\big(t - (t_n + 1)\big)\, \hat{m}_L + [1 - a\big(t - (t_n + 1)\big)]\, m_n^-$$

with the reversed prescription and with $m^{(-)}$ replaced by $m^{(+)}$ in $[t_n + 2, 2t_n + 4]$.

$I_{\tau_n}(u_n)$ is then the sum of six terms, each one representing the contribution of the corresponding time interval. The time integral over $[0, 1]$ yields

$$\frac{1}{4}\int_0^1 \int_{-L}^{L} \Big(a_t\, [T_{t_n}(m_n^-) - m^{(-)}] - f_L(u_n)\Big)^2 dx\, dt. \tag{4.4}$$

By (4.3) $\lim_{n\to\infty} \|T_{t_n}(m_n^-) - m^{(-)}\|_2 = 0$. Moreover $u_n = m^{(-)} + a(t)\, [T_{t_n}(m_n^-) - m^{(-)}]$ so that, following the observation that $\|u_n\|_\infty$ is bounded away from 1, $\lim_{n\to\infty} \|f_L(u_n(\cdot, t))\|_2 = 0$. Hence (4.4) vanishes as $n \to \infty$.

By Theorem 3 the integral over t in $[1, 1 + t_n]$ is equal to $\mathcal{F}_L(m_n^-) - \mathcal{F}_L(T_{t_n}(m_n^-))$; $\mathcal{F}_L(\hat{m}_L) \ge \mathcal{F}_L(m_n^-)$ by assumption and $\mathcal{F}_L(T_{t_n}(m_n^-)) \ge 0$ so that

$$\mathcal{F}_L(m_n^-) - \mathcal{F}_L(T_{t_n}(m_n^-) \le \mathcal{F}_L(\hat{m}_L).$$

The integrals over t in $[t_n + 1, t_n + 2]$, $[t_n + 2, t_n + 3]$ and $[2t_n + 3, 2t_n + 4]$ vanish as $n \to \infty$. The proof is analogous to that in the first time interval and it is omitted. Finally in the fifth interval, $[t_n + 3, 2t_n + 3]$, $u_n(\cdot, t) = T_{t-(t_n+3)}\big(m_n^+\big)$ solves (1.1) and there is no penalty. Lemma 1 is proved. ■

By Lemma 1 (4.1) follows once we exhibit two sequences $m_n^\pm$ which satisfy (4.2). We start by quoting some results from [2] which refer to the flow $S_t(m)$ which is the solution of the equation

$$u_t = g_L(u) = -u + \tanh\{\beta J^{\text{neum}} * u\}, \qquad u(\cdot, 0) = m. \tag{4.5}$$

Like for $T_t(m)$, $\mathcal{F}_L(S_t(m))$ is also a nonincreasing function of t which strictly decreases unless m is stationary, i.e. $m = \tanh\{\beta J^{\text{neum}} * m\}$. Observe that m is stationary for (4.5) if and only if m is stationary for (1.1). In [2] it is proved that there exist two manifolds, $w^{(\pm)}(\cdot, s)$, $s \in \mathbb{R}$, analogous to the invariant manifolds $v^{(\pm)}(\cdot, s)$ introduced in Section 3, namely $\mathcal{F}_L(w^{(\pm)}(\cdot, s)) < \mathcal{F}_L(\hat{m}_L))$ for any $s \in \mathbb{R}$, and

$$S_t(w^{(\pm)}(\cdot, s)) = w^{(\pm)}(\cdot, s + t), \tag{4.6}$$

$w^{(\pm)}(\cdot, \cdot) \in (-m_\beta, m_\beta)$, and

$$\lim_{s\to-\infty} w^{(\pm)}(\cdot, s) = \hat{m}_L, \qquad \lim_{s\to\infty} w^{(\pm)}(\cdot, s) = m^{(\pm)} \tag{4.7}$$

(the limits in (4.7) can be taken both in L^∞ and in L^2). Finally, by symmetry under reflections and under change of sign of (4.5), for all $x \in [-L, L]$ and all $s \in \mathbb{R}$

$$w^{(+)}(x, s) = -w^{(-)}(-x, s). \tag{4.8}$$

Thus the choice $m_n^{(\pm)}(x) = w^{(\pm)}(x,-n)$ would satisfy the assumptions of Lemma 1 if (4.6) had T_t instead of S_t. So we need an extra argument. It is known, see for instance [10], that limit points of $T_t(w^{(+)}(\cdot,-n))$ as $t \to +\infty$ do exist and, if m^* is a limit point, then m^* is a stationary solution of (1.1). By monotonicity and lower semicontinuity of the free-energy functional, $\mathcal{F}_L(m^*) \le \mathcal{F}_L(\hat{m}_L)$ so that by Theorems 8 and 9 below m^* can either be equal to $m^{(+)}$ or to $m^{(-)}$. Since there is an open neighborhood of $m^{(+)}$ (respectively of $m^{(-)}$) which is attracted in L^2 by $m^{(+)}$ (respectively by $m^{(-)}$), it then follows that $T_t(w^{(+)}(\cdot,-n))$ converges to m^* as $t \to +\infty$ (and not only by subsequences).

By symmetry under change of sign $T_t(-m) = -T_t(m)$ for any m. Then

$$\lim_{t\to+\infty} T_t\big(w^{(+)}(\cdot,-n)\big) = m^{(\sigma)}, \qquad \lim_{t\to+\infty} T_t\big(-w^{(+)}(\cdot,-n)\big) = m^{(-\sigma)}, \tag{4.9}$$

where $\sigma \in \{\pm\}$. By (4.8),

$$\lim_{t\to+\infty} T_t\big(w^{(-)}(\cdot,-n)\big) = m^{(-\sigma)}. \tag{4.10}$$

We now call σ_n the value of σ for which $\lim_{t\to+\infty} T_t\big(w^{(\sigma_n)}(\cdot,-n)\big) = m^{(+)}$ and we set $m_n^{\pm} = w^{(\pm\sigma_n)}(\cdot,-n)$. Then by (4.9) and (4.10) $m_n^{\pm}$ satisfy the assumptions of Lemma 1.

5 Lower bound

To complete the proof of Theorem 4 it suffices to show that

$$P_{[m^{(-)},m^{(+)}]} \ge \mathcal{F}_L(\hat{m}_L), \tag{5.1}$$

which together with (4.1) proves that $P_{[m^{(-)},m^{(+)}]} = \mathcal{F}_L(\hat{m}_L)$ and thus Theorem 4. The main point in the proof of the lower bound is that the free energy of the first excited state is $\mathcal{F}_L(\hat{m}_L)$, namely:

Theorem 6. *For all L large enough there is $\epsilon > 0$ so that, if m is stationary and $\mathcal{F}_L(m) < \mathcal{F}_L(\hat{m}_L) + \epsilon$, then $m \in \{m^{(-)}, m^{(+)}, \hat{m}_L\}$.*

With the help of Theorem 6 the proof of the lower bound proceeds by observing that the basins of attraction of $m^{(-)}$ and $m^{(+)}$ (denoted by $\mathcal{B}^-$ and $\mathcal{B}^+$) are open sets in the L^2 topology. This follows from the continuity of $T_t(m)$ on m and from the already remarked fact that $m^{(-)}$ and $m^{(+)}$ are locally stable (namely there are open neighborhoods of $m^{(-)}$ and $m^{(+)}$ which are attracted by $m^{(-)}$ and $m^{(+)}$). Then given an orbit $u \in \mathcal{U}_\tau[m^{(-)}, m^{(+)}]$ there must be a time $t_0 \in (0,\tau)$ such that $u(\cdot,t_0) \notin \mathcal{B}^- \cup \mathcal{B}^+$. The proof of the lower bound is then be completed by showing that $\mathcal{F}_L(u(\cdot,t_0)) \ge \mathcal{F}_L(\hat{m}_L)$. Indeed, $\mathcal{F}_L(u(\cdot,t_0)) \ge \mathcal{F}_L(T_s(u(\cdot,t_0)))$, $s \ge 0$, and by the lower semicontinuity of $\mathcal{F}_L$, if $T_{s_n}(u(\cdot,t_0))) \to m^*$ as $s_n \to \infty$, then $\mathcal{F}_L(u(\cdot,t_0)) \ge \mathcal{F}_L(m^*)$. As was already observed, convergent subsequences do exist and their limit points are stationary. On the other hand m^* cannot be equal to $m^{(-)}$ or to $m^{(+)}$ because by construction $u(\cdot,t_0) \notin \mathcal{B}^- \cup \mathcal{B}^+$ so that by Theorem 6 $\mathcal{F}_L(u(\cdot,t_0)) \ge \mathcal{F}_L(\hat{m}_L)$ and the lower bound is proved.

It thus remains to prove Theorem 6. For Allen-Cahn (i.e. $u_t = u_{xx} + \phi(u)$ with Neumann conditions) the proof is easy. In fact the stationary solutions satisfy $u_{xx} = -\phi(u)$. If we interpret u as a position and x as a time, they are the orbits of a one-dimensional particle of mass 1 subject to the force field $-\phi(u)$, which have zero velocity at the times $-L$ and L. There is a full characterization of such orbits and Theorem 6 then follows.

We miss an analogous characterization of the stationary solutions of (1.1), but we have a fairly good knowledge of the energy landscape in a "small" open set U which is the union of suitable neighborhoods of $m^{(\pm)}$ and of translated instantons. The main feature (related to the one-dimensional nature of the model) is that the sublevel $\{m \in L^\infty([-L,L]) : \mathcal{F}_L(m) < \mathcal{F}_L(\hat{m}_L) + \epsilon\}$, $\epsilon > 0$ small enough, is contained in U so that the proof of Theorem 6 requires only an analysis of U. Roughly speaking the open set U is made of profiles m which are either everywhere close to m_β (or to $-m_\beta$) or else they are close to a "shifted instanton". To define "closeness" we use averages. Given $\ell > 0$ we denote by $\mathcal{D}^{(\ell)}$ the partition of $\mathbb{R}$ into the intervals $[n\ell,(n+1)\ell)$, $n \in \mathbb{Z}$, and define

$$m^{(\ell)}(x) := \fint_{I_x^{(\ell)}} m(y)\,dy, \quad \fint_\Lambda m(y)\,dy := \frac{1}{|\Lambda|}\int_\Lambda m(y)\,dy, \tag{5.2}$$

where $I_x^{(\ell)}$ is the interval in $\mathcal{D}^{(\ell)}$, which contains the point x. Given an "accuracy parameter" $\zeta > 0$ we then introduce

$$\eta^{(\zeta,\ell)}(m;x) = \begin{cases} \pm 1 & \text{if } |m^{(\ell)}(x) \mp m_\beta| \le \zeta, \\ 0 & \text{otherwise.} \end{cases} \tag{5.3}$$

Calling ℓ_- and ℓ_+ two values of the parameter ℓ, with ℓ_+ an integer multiple of ℓ_- we define a "phase indicator"

$$\Theta^{(\zeta,\ell_-,\ell_+)}(m;x) = \begin{cases} \pm 1 & \text{if } \eta^{(\zeta,\ell_-)}(m;\cdot) = \pm 1 \text{ in } [-L,L] \cap \left(I_{x-\ell_+}^{(\ell_+)} \cup I_x^{(\ell_+)} \cup I_{x+\ell_+}^{(\ell_+)}\right), \\ 0 & \text{otherwise,} \end{cases}$$

and call contours of m the connected components of the set $\{x : \Theta^{(\zeta,\ell_-,\ell_+)}(m;x) = 0\}$. $\Gamma = [x_-, x_+)$ is a plus contour if $\eta^{(\zeta,\ell_-)}(m;x_\pm) = 1$ and a minus contour if $\eta^{(\zeta,\ell_-)}(m;x_\pm) = -1$. Otherwise it is called mixed.

The parameters (ζ,ℓ_-,ℓ_+,L) are called compatible with $(\zeta_0,c_1,\kappa) \in \mathbb{R}_+^3$ if $\zeta \in (0,\zeta_0)$, $\ell_- \le \kappa\zeta$, $\ell_+ \ge 1/\ell_-$; L is a multiple integer of ℓ_+ and ℓ_+ a multiple integer of ℓ_-. In [1] we prove the following theorem, which adapts results already known in the literature.

Theorem 7. *There are positive constants ζ_0, c_1, κ, c_2 and ω such that, if (ζ,ℓ_-,ℓ_+,L) is compatible with (ζ_0,c_1,κ), then*

$$\mathcal{F}_L(m) \ge \sum_{\Gamma \text{ contour of } m} w_{\zeta,\ell_-,\ell_+}(\Gamma) \qquad \forall m \in L^\infty([-L,L];[-1,1]), \tag{5.4}$$

where

$$w_{\zeta,\ell_-,\ell_+}(\Gamma) = c_1\zeta^2\frac{\ell_-}{\ell_+}|\Gamma| \text{ if } \Gamma \text{ is a plus or a minus contour;}$$

$w_{\zeta,\ell_-,\ell_+}(\Gamma) = \max\left\{c_1\zeta^2\frac{\ell_-}{\ell_+}|\Gamma| \,;\, \mathcal{F}(\bar{m}) - c_2 e^{-\omega\ell_+}\right\}$ *if Γ is a mixed contour and $\mathcal{F}(m)$, $m \in L^\infty(\mathbb{R};[-1,1])$, is defined as in (2.6) with $L = \infty$ and with J in place of J^{neum}.*

"Good choice of parameters". In the sequel we take $\zeta \le \zeta_0$ suitably small, $L > \zeta^{-8}$ and $\ell_\pm$ determined by L and ζ as follows. ℓ_+ is the smallest number $\ge \zeta^{-4}$ such that $L = n\ell_+$, $n \in \mathbb{N}$; ℓ_- is the largest number $\le \zeta^2$ such that $\ell_+ = p\ell_-$, $p \in \mathbb{N}$, $p > 1$.

Definition 2. We write $\bar{m}_\xi(x) = \bar{m}(x-\xi)$, $\xi \in \mathbb{R}$ and given $k \in \mathbb{N}$ and $(\zeta, \ell_-, \ell_+, L)$ as above and calling $\Theta = \Theta^{(\zeta,\ell_-,\ell_+)}$ we define

$U_- = \big\{m \in L^\infty([-L,L];[-1,1]) : \Theta(m,\cdot) < 1,\ |\{\Theta(m,\cdot) = 0\}| \le k\ell_+\big\}$;

$U_+ = \big\{m : -m \in U_-\big\}$;

$U_{-,+} = \big\{m \in L^\infty([-L,L];[-1,1]) : m$ has a unique mixed contour Γ, $|\Gamma| \le k\ell_+$, and there exists $\xi \in \Gamma$ such that $\mathrm{dist}(\xi, [-L,L]\setminus\Gamma) \ge \ell_+/2$, and $|m^{(\ell_-)} - \bar{m}_\xi^{(\ell_-)}| \le 2\zeta$ on $[-L,L]\big\}$;

$U_{+,-} = \{m : -m \in U_{-,+}\}$.

We also define

$$U = U_- \cup U_{-,+} \cup U_{+,-} \cup U_+,$$

namely U_- and U_+ are the sets of those m which are in the minus, respectively plus, phase, except for the "small region" $\{x : \Theta(m,x) = 0\}$. $U_{-,+} \cup U_{+,-}$ instead describes the intermediate times in a tunnelling orbit, when the minus and the plus phases coexist in a same m. $U_{-,+} \cup U_{+,-}$ is made by profiles m which are either close to an instanton $\bar{m}_\xi$ or to $-\bar{m}_\xi$. The region $\{x : \Theta(m,x) = 0\}$, $m \in U_{-,+} \cup U_{+,-}$, which separates the two phases both present in m, is then "the interface".

As a corollary of Theorem 7 we have:

Theorem 8. *If $\zeta > 0$ is small enough, there is $k \in \mathbb{N}$ such that for L large enough*

$$\big\{m \in L^\infty([-L,L];[-1,1]) : \mathcal{F}_L(m) < \mathcal{F}_L(\hat{m}_L) + \zeta^{100}\big\} \subset U$$

(recall that U depends on k and on ζ).

Details of the proof of Theorem 8 are reported in [1]. Given $r \in (0,1)$ we call

$$V_r^\pm = \Big\{m \in U : |\{\Theta(m,\cdot) = \pm 1\}| \ge 2L - rL\Big\}, \qquad V_r^0 = U \setminus (V_r^+ \cup V_r^-),$$

and Theorem 6 follows directly from

Theorem 9. *Let ζ, k and L be as in Theorem 8. Suppose that m is stationary for equation (4.5) and $\mathcal{F}_L(m) < \mathcal{F}_L(\hat{m}_L) + \zeta^{100}$. If $m \in V_r^+$, then $m = m^{(+)}$; if $m \in V_r^-$, then $m = m^{(-)}$; if $m \in V_r^0$, then $m = \hat{m}_L$.*

If m is stationary, m is differentiable and $|m_x| \le \beta\|J_x\|_\infty$ as follows by differention w.r.t. x of the equation $m = \tanh\{\beta J^{\mathrm{neum}} * m\}$. Then, if $m \in V_r^0$, $\|m - \bar{m}_\xi\|_\infty \le 2\zeta + \beta\|J_x\|_\infty\ell_-$ for some $|\xi| \le (1-r)L$. If ζ is sufficiently small and L correspondingly large, $\|m - \bar{m}_\xi\|_\infty \le \epsilon$, with ϵ the same small parameter introduced in [2], where it is shown that in such a case $m = \hat{m}_L$. The statements about $m \in V_r^\pm$ do not follow (at least directly) from the literature and need a proof. We report it in [1], where in order to exploit results already known in the literature we study the flow $S_t(m)$ which solves (4.5) and prove that $S_t(m) \to m^{(\pm)}$ for any regular $m \in V_r^\pm$. This concludes the proof of Theorem 9 because we have already noticed that, if m is stationary, it is regular and because the stationary points of (4.5) and of (1.1) are the same.

The proof of Theorem 9 is reported in [1].

6 Bibliographical remarks

Quantum tunnelling has been studied as a large deviation problem via the Feynman-Kac formula, see [15].

Metastability in the Ising model has been extensively studied, see [18] and references therein. Metastability in the stochastic Allen-Cahn equation with additive small random noise has been studied in $d = 1$ dimensions in [12] and in [5]; there is also an analysis in the $d = 2$ case in [16].

Tunnelling between pure phases (i.e. the problem discussed here) has been studied for the Ising model in [17].

The existence and stability properties of the invariant manifolds $v^{(\pm)}$ in the $d = 1$, deterministic Allen-Cahn equation are studied in [3], [4], [14] and [11].

Existence of the finite volume instanton for the nonlocal equation considered here is proved in [8] and in [6] while the analysis of the invariant manifolds for the equation (4.5) is proved in [2]. The mountain pass lemma and variational techniques have been used in [6] to study the finite volume instanton.

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