Manifold self-localization in a deformable medium

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Directed manifolds (domain walls, interfaces, vortex lines) in a deformable medium can exist in a correlated state in which the manifold is self-localized by its own strain field. Depending on the temperature, manifold/medium dimensionalities, and the strength of the coupling with the medium, the degree of localization of the ground state can vary both continuously and discontinuously; there can be phase transitions from self-localized to free-manifold state.

The concept of a manifold is a central paradigm in condensed matter physics, covering the cases of domain walls in ferroelectric and ferromagnetic materials, flux lines in type-II superconductors, interfaces, and many more. Manifolds exist in symmetry-broken states of various systems, and occur as translationally-invariant topological solutions of the corresponding field theories.

In this work we show that the deformability of a real system can bring the manifold into a new correlated self-localized state (SL) which forms through the following scenario: a deformable continuum responds to the presence of the manifold by a strain field decaying away from the manifold; this field interacts with the manifold, suppressing its displacements and as a result the manifold can be bound to the strain field. Self-localization takes place only if the overall free energy of the system with the SL manifold is less than that of the free manifold in the strain-free medium.

We start from two examples demonstrating the physics of self-localization.

1. A domain wall in a two dimensional elastic medium.

The position of the wall relative to axes x and t can be represented by the function $x = h(t)$. The interactions of the domain wall with the elastic medium can then be modeled by a Hamiltonian in which the wall is represented as an elastic string of stiffness coefficient m:

$$H = \frac{1}{2}m \int dt (\partial h/\partial t)^2 - V \int dt [\partial u/\partial x(x = h)]$$

$$+ \frac{1}{2} \int dx dt [A(\partial u/\partial t)^2 + B(\partial u/\partial x)^2]$$

(1)

The deformations of the medium give rise to the last term; for simplicity these have been described by a scalar displacement field u, with A and B being elastic constants. The second term provides the coupling between the deformation and the wall, in terms of the strain evaluated at the wall position $x = h$. Since $-\partial u/\partial x$ is proportional to the local density change, phenomenologically the coupling $-V(\partial u/\partial h)$ is the lowest order term in the expansion of the interaction in powers of the variable part of the medium density. The coupling constant V is independent of the elastic properties of the medium, and can be estimated in terms of the bulk phase transition temperature $T_c$ and lattice spacing $a$ as $|V|a \approx T_c$. In writing the coupling in the form $-V(\partial u/\partial h)$ it was assumed that we are not too close to the bulk critical point so that the range of the interaction between the wall and an individual atom is of order $a$, which is invisibly small in the long-wavelength theory we are using and thus does not appear; however the scale $a$ will provide a short-distance cutoff implicitly present in Eq. (1).

Placing the wall at the origin $h = 0$, and minimizing Eq. (1), we find $\partial u/\partial x = (V/B)\delta(x)$ and $u(x) = (V/2B)\text{sign}(x)$, which means that at $T = 0$ the strain field is localized at the domain wall (the true range of the delta-function is the lattice spacing $a$). The magnitude of the maximal strain can be estimated as $|V|/Ba = |V|a/Ba^2 \approx T_c/Ba^2$: it is small compared to unity, since $T_c$ is much smaller than the binding energy per atom $Ba^2$; this justifies the use of linear elasticity theory.

At a finite temperature T, the wall and the medium degrees of freedom each fluctuate strongly - for the uncoupled system ($V = 0$) the mean-square fluctuations diverge with the system size $L$ as $< h^2 > \approx TL/m$, and $< u^2 > \approx [T/\sqrt{AB}]\ln(L/a)$, respectively. To understand the system at finite temperature, below we develop a variational theory valid to zero order in $< u^2 > / < h^2 >$ (i.e. ignoring medium fluctuations), and having the spirit of Flory-type theories of polymer physics.

Assume that the magnitude of the medium deformation is of order $u_0$ in a region of size $L$ perpendicular to the wall and negligible elsewhere. The corresponding strain field creates a localizing potential for the wall [second term of Eq. (1)]. Both the localizing potential and the wall itself fluctuate; however, for a macroscopic system the medium fluctuations are much weaker than those of the free wall, and so for a first approximation we can ignore medium fluctuations altogether, and consider the domain wall to be fluctuating in a fixed average self-consistent potential due to the strain in the medium. The localizing potential confines the domain wall within a region of typical size $L$. This diminishes the available number of wall configurations, thus decreasing the entropy and increasing the free energy. The corresponding confinement free energy is given by $T^2/mL^2$, so that the total variational free energy (per unit length in the $t$ direction) is estimated as...
where the second term is the free energy gain of localization (corresponding to the second term of Eq. (1), while the last term is the increase in the elastic energy due to the creation of the strained region near the wall [the last term of Eq. (1)]. The variational parameters $L$ and $u_0$ can be found by minimizing Eq.(2). The minimum over $u_0$ is given by $u_0 = V/B$, and then Eq.(2) becomes

$$F(L, u_0 = V/B) \cong \frac{T^2}{mL^2} - \frac{V^2}{2BL}$$

This expression (shown schematically in Figure 1a) has a minimum for finite $L$ and $F_{\text{min}} < 0$, which implies that despite strong thermal fluctuations an elastic strain always accompanies the domain wall; the strain is localized within an equilibrium localization length given by

$$L_{\text{eq}} \cong \frac{T^2B}{mV^2}$$

We will call the domain wall (plus the accompanying strain field) self-localized because the wall is "attached" to the strain field it generates - the probability of finding the wall a distance $x$ away from the strain peak is significant for $|x| \leq L_{\text{eq}}$, negligible elsewhere, and goes to zero as $|x| \to \infty$. Note that self-localization does not imply any breaking of translational symmetry: both the wall and the strain field can be shifted simultaneously without energy cost. Fluctuations of the SL wall will necessarily involve the degrees of freedom of the medium; therefore the SL wall possesses a larger stiffness than the same free wall in an undeformable medium.

The continuum result (4) is valid whenever the localization length $L_{\text{eq}}$ is much bigger than the lattice spacing $a$. Correspondingly we will distinguish between the cases $L_{\text{eq}} \gg a$ (the macroscopically SL state) and $L_{\text{eq}} \cong a$ (microscopically SL). These meet at the crossover temperature $T^* \cong \sqrt{|V/ma/B|} \ll T_c$. For $T \leq T^*$ we have $L_{\text{eq}} \cong a$. Since the domain wall is an anisotropic object, it is also localized in the $t$ direction over a different length scale $L_t$, which can be estimated from $L_{t,\text{eq}} \cong TL_t/a$. At the crossover temperature $T^*$, we find $L_{t,\text{eq}} \cong ma^2/T^* \cong (T_c/T^*)a \gg a$. On length scales smaller than $L_t$ the domain wall is essentially decoupled from the continuum, and so the fluctuations of the medium at that scale can be estimated as $<u^2> \cong |T/\sqrt{AB}| \ln(L_t/a)$. Our theory will be valid whenever $<u^2>$, evaluated at the smallest allowed scale $L_{t,\text{eq}}$, is much smaller than $a^2$. This gives rise to the inequality

$$\frac{T^*}{a^2\sqrt{AB}} \ln(ma/T^*) \ll 1$$

For most practical purposes ($A \cong B$) the condition (5) is satisfied exceptionally well, because $T^* \ll T_c \ll Ba^2$. Only when there are special reasons for $A$ to be very small (a quasi-one-dimensional medium, for example), do we have to start worrying about the role of the medium fluctuations. For every case consider below the neglect of the medium fluctuations can be justified on similar grounds.

The consequences of manifold self-localization depend on the dimensionalities of the manifold and the continuum as demonstrated by the next example.

2. A flux line (directed polymer) of stiffness $m$ in a three-dimensional crystal. We will assume that the strains are localized within a region of size $L$ around the vortex. The energy cost of the elastic distortion (the last term in Eq.(2)), is now estimated as $BL^2(u_0/L)^2 = B^2u_0^2$, where $B$ is some combination of the elastic constants of the crystal. As a result, the total variational free energy per unit length will have the form

$$F(L, u_0 = V/B) \cong \frac{T^2}{mL^2} - \frac{V^2}{2BL^2}$$

The minimum value with respect to $u_0$ is

$$F(L, u_0 = V/L) \cong \frac{T^2}{mL^2} - \frac{V^2}{2BL^2}$$

In contrast with Eq. (3), both terms have the same scaling dependence on $L$, and the outcome depends on the relative size of the coefficients. The two terms are of similar size at the critical temperature

$$T_{\text{loc}} \cong \sqrt{mV^2/B};$$

for $T > T_{\text{loc}}$ the free energy (7) is minimized for the free vortex ($L = \infty$) in the strain-free medium ($u_0 = 0$), while for $T < T_{\text{loc}}$ the free energy is minimized as $L \to 0$. Since the strain (which is of order $u_0/L \cong V/BL^2$) diverges as $L \to 0$, this indicates that the linear elasticity theory used to estimate the last term of Eq.(6) fails below the localization temperature (8). There are several equivalent ways to cure this problem.

First, we can add anharmonic terms to the right-hand side of Eq.(6) which will guarantee that the equilibrium $L$ cannot fall below some microscopic scale for $T < T_{\text{loc}}$. Alternatively we can introduce a short-length cutoff $a$ and continue to use Eqs.(6) and (7), but restrict the minimization to the region $L \geq a$. Neither of these procedures provides a quantitative picture for $T < T_{\text{loc}}$ but for the purposes of illustration we note that using the cutoff (we adopt it hereafter) predicts that for $T \leq T_{\text{loc}}$ the free energy density is given by

$$F \cong (T^2 - T_{\text{loc}}^2)/ma^2$$

In contrast to the case of a domain wall in two dimensions, a flux line in a three-dimensional crystal can exist either in the high-temperature free state or in the low-temperature microscopically SL phase. The theory developed here is valid only for temperatures well below the superconductive temperature $T_c$; since $T_c \ll Ba^2$, one can deduce from (8) that $T_{\text{loc}} \ll T_c$. 


The nature of these results – having the same $1/L^2$ dependence of both the "localizing" and "delocalizing" terms of the free energy (7), plus the fact that the expression for the phase transition temperature (8) is cutoff-independent – shows that three dimensions is the lower critical dimensionality (the self-localization problem).

The critical behavior (9) predicted by our variational theory is only an estimate, and a more detailed theory is needed to reveal the essential singularities that are expected to occur at the critical point in a marginal case. The long-ranged nature of bulk elasticity is clearly important here: the equilibrium medium displacement away from the vortex depends on the variational localization of the displacement field well-localized; in all other cases it is long-ranged. The case $2D/(2 - D) < d - D$ and $D < 2$ is the practically most important case of a domain wall in a three-dimensional crystal. The free energy per unit area will now have the form

$$F(L, u_0 = V/B) \equiv (T/a^2)e^{-mL^2}/T - V^2/BL$$

which generalizes Eq.(4). At the minimum one has $F_{\text{min}} < 0$, which implies that the manifold is in a macroscopically SL state as long as $L_{eq} > a$. Should the localization length $L_{eq}$ decrease (due to some change in the system parameters), the system continuously crosses over into a microscopically SL state characterized by $L_{eq} \cong a$.

The case $2D/(2 - D) = d - D$ and $D < 2$, similar to the previously analyzed problem of a flux line, is marginal. Here the manifold can exist either in a high-temperature free state or in a low-temperature microscopically SL phase separated by a continuous phase transition.

For $2D/(2 - D) < d - D$ and $D < 2$ the right-hand side of (11) (shown schematically in Figure 1b) has a maximum at a scale $L_{\text{max}}$ [actually given by (12)], approaches zero from above as $L \to \infty$, vanishes at a scale $L_0 < L_{\text{max}}$ up to a scale factor $L_0$ is still given by the right-hand side of (12), and goes to minus infinity as $L \to 0$. Here the outcome depends on the relationship between the cutoff $a$, and the scales $L_0$ and $L_{\text{max}}$.

For $a > L_{\text{max}}$ (the high-temperature limit) the free-energy density (with the cutoff) has a single minimum at $L = \infty$: the manifold is in a free state.

For $L_0 < a < L_{\text{max}}$ (intermediate temperatures) the free energy density has a global minimum at $L = \infty$, and a local minimum at $L \cong a$. The ground state is still a free manifold, but now a microscopically SL state can be metastable because of the barrier separating it from the free state.

For $a < L_0$ (a low-temperature limit) the free energy density has a global minimum at $L \cong a$, and a local minimum at $L = \infty$. The ground state is a microscopically SL manifold but a free manifold can be metastable due to the free energy barrier separating it from the SL state.

The condition $a = L_0$ determines a first-order phase transition point between the microscopically SL phase and a free manifold.

4. For the marginal case $D = 2$ we will consider only the practically most important case of a domain wall in a three-dimensional crystal. The free energy per unit area will now have the form

$$F(L, u_0 = V/B) \equiv (T/a^2)e^{-mL^2}/T - V^2/BL$$

where the first term is the free energy of confinement which for $D = 2$ replaces the first terms of Eqs.(10-11).

To simplify the analysis it is convenient to introduce the dimensionless coupling constant $\gamma = (V^2a^2/B)(m/T^3)^{1/2}$. For $D = 2$ the parameter $V$ is estimated as $|V|a^2 \cong T_c \cong ma^2$, and the corresponding coupling constant is $\gamma \cong (T_c/Ba^2)(T_c/T)^{3/2}$, thus implying that for $T < T_c$ the parameter $\gamma$ can vary from a very small value of order $T_c/Ba^2 \ll 1$ (for a temperature close to $T_c$) to infinity (the zero-temperature limit).

In the low-temperature limit ($\gamma \gg 1$) the function (13) is monotonic increasing which means that the ground state is a microscopically SL domain wall. In
the high temperature limit ($\gamma \ll 1$) the right-hand side of (13) (shown schematically in Figure 1c) has a maximum at some $L_{\text{max}}$, and a minimum at some $L_{\text{min}} > L_{\text{max}}$. The transition between the two behaviors occurs at $\gamma \approx 1$ which corresponds to the temperature $T_1 \approx T_c(T_c/Ba^3)^{2/3} < T_c$ and $L_1 = L_{\text{max}} = L_{\text{min}} \approx (T_1/m)^{1/2}$. Since the scale $L_1 \approx (T_1/m)^{1/2} \approx a(T_1/T_c)^{1/2}$ is much smaller than the cutoff $a$ we conclude that the domain wall will be in a microscopically SL state $L_{eq} \approx a$ both for $T < T_1$ and in some temperature range above $T_1$ until the cutoff $a$ coincides for the first time with $L_{\text{min}}$ ($L_{\text{min}}$ increases with the temperature). This will happen at some $\gamma \ll 1$, and in this limit $L_{\text{min}}$ can be estimated as $L_{\text{min}} \approx (T/m)^{1/2} \ln^{1/2}(1/\gamma)$. The condition $L_{\text{min}} = a$ determines a crossover temperature $T^*$ as a solution to the equation $\ln^{1/2}(1/\gamma) \approx a(m/T)^{1/2}$. Remembering that $\gamma = (V^2a^2/B)(m/T)^{1/2} \approx (T_c/Ba^3)(T_c/T)^{3/2}$, we can solve the equation with logarithmic accuracy, $\ln(Ba^3/T_c) \gg 1$, to find $T^* \approx T_c/\ln(Ba^3/T_c)$.

The physical significance of the crossover temperature $T^*$ is that for $T < T^*$ the free energy density has a single minimum at $L_{eq} \approx a$, and the domain wall is in a microscopically SL state. At the same time for $T > T^*$ the free energy density has a minimum at

$$L_{eq}^2 \approx (T/m) \ln(Ba^3/mV^4a^4)$$

The ground state is still self-localized but its localization length (14) is bigger than $a$ and grows with temperature. The bulk phase transition temperature $T_c$ sets a natural upper bound to $L_{eq}$, which can be estimated as $L_{eq} \leq a \ln^{1/2}(Ba^3/T_c)$. In reality the dependence (14) is only reliable for $T^* < T < T_c$ excluding the temperature range of bulk critical fluctuations.

Because thermal fluctuations are only marginally relevant for a domain wall in a three-dimensional crystal, experimental verification of the law (14) (for example, by measuring the strain profile induced by the wall) may not be easy unless $\ln(Ba^3/T_c) \gg 1$, and the bulk critical region is narrow.

It is known experimentally and well-understood theoretically how topological defects and other inhomogeneities deform the embedding medium at zero temperature. In our language this corresponds to the microscopically SL manifold. As we have shown, thermal fluctuations can change this picture drastically leading to the possibility of macroscopically SL states or even strain-free states. The fact that the manifold is in a SL state should be especially important when the accompanied strain field is long-ranged (this excludes domain walls), and when there are many manifolds present. We speculate that the SL transition predicted for a single flux line will manifest itself in a structural transition of a dilute system of vortices. The present theory implies that there is a similar phenomenon for any $D = 1$ manifold in a deformable medium in three dimensions.

The problems analyzed above involve directed manifolds placed in a deformable medium. For the special case of line manifolds ($D = 1$) they are connected to quantum-mechanical phenomena at $T = 0$ through the Feynman formulation of quantum mechanics. The relationship goes through the correspondence temperature $\rightarrow$ Planck’s constant, line configuration $\rightarrow$ particle world line, position along the line $\rightarrow$ imaginary time, and line stiffness $\rightarrow$ particle mass. Then line self-localization phenomena are formally related to the polaron effect in quantum physics - an electron placed in an elastic continuum might get self-trapped by its own strain field. More precisely, the Hamiltonian Eq. (1) can be viewed as an imaginary-time Action for the polaron problem in one dimension, while the expression for the localization length (4) can be related to the size of a large polaron in the adiabatic limit. This implies that the SL manifold has a well-localized probability distribution function which depends only on transverse coordinates. This is qualitatively different from the free manifold, which has a Gaussian probability distribution function that depends on all coordinates.

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