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LETTER TO THE EDITOR

Macroscopic dynamics of systems with a small number of topological defects in equilibrium and non-equilibrium systems

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Abstract. We derive dynamic equations for one or a small number of topological defects which supplement the hydrodynamic equations (for systems close to local thermodynamic equilibrium) or phase equations (for systems far from equilibrium) for the slow variables of any ordered medium. Special cases are discussed and a generalisation of the Peach–Koehler force is presented.

The long-time behaviour of many systems in condensed matter physics is strongly influenced by the motion of a small number of topological defects. These systems fall into two classes: systems close to local thermodynamic equilibrium like liquid crystals (de Gennes 1982) or a rotating superfluid ^{4}He (Khalatnikov 1965) and non-equilibrium systems such as e.g. the Taylor instability (Swinney and Gollub 1981) which occurs when an isotropic liquid between two concentric cylinders is set into motion by rotation of the inner cylinder and the Bénard instability (Normand *et al* 1977) arising when a fluid layer between two plates is subjected to an external temperature gradient parallel to gravity.

In systems close to equilibrium the classical way of describing the long-time, low-frequency behaviour without defects is to derive nonlinear hydrodynamic equations (Landau and Lifschitz 1959, Martin *et al* 1972, Brand and Pleiner 1980) for the conserved quantities like density, entropy density, density of linear momentum etc and for the variables characterising spontaneously broken continuous symmetries like for example the deviations from a preferred direction in nematic liquid crystals. Recently (Pomeau and Manneville 1979, Brand and Cross 1983, Brand 1984) it has been proposed that an approach is used which is similar in spirit to the description of large aspect ratio systems in non-equilibrium phenomena like the Taylor or Bénard instability; the phase dynamics. As in hydrodynamics, one extracts the quantities which vary slowly in time and space. It turns out that this is the variation of the wavevector transverse to the rolls in Rayleigh–Bénard systems (Pomeau and Manneville 1979) and in the Taylor vortex state (Brand and Cross 1983), where one has an array of vortices parallel to the cylinder axis. In the Taylor wavy mode state, the second spatially periodic structure in the Taylor system, one has in addition a propagating wave in the azimuthal direction and it is possible (Brand and Cross 1983) to associate a slowly varying quantity with this motion as well. The coefficients in these phase equations have to be determined from microscopic theory as in hydrodynamics and one frequently uses

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amplitude equations (Newell 1974, Siggia and Zippelius 1981, Brand and Cross 1983, Pomeau *et al* 1983, Kuramoto 1984) to get explicit expressions for the phenomenological equations.

Here we focus on the question of how these sets of equations (hydrodynamic and phase dynamics) have to be generalised in order to incorporate the macroscopic motion of one or a small number of topological defects. In particular one would like to retain the form of the macroscopic equations, i.e. one wants to avoid in the final equations the appearance of amplitude equations. To avoid this we will present what one could call a far-field approximation, i.e. we will be mainly concerned with the influence of the defect on the hydrodynamic or phase equations and about the motion of the defect (as an extended object) in the background described by the hydrodynamic or phase equations. Without defects we have in general a set of macroscopic equations for the variables $\{\varphi_i\}$

$$\dot{\varphi}_i = g_i(\{\varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_m\varphi_k, \ldots\}) \tag{1}$$

valid far from any defect.

In the vicinity of the core region of a defect—denoted as Ω hereafter—one has to supplement (1) by a set of dynamic equations incorporating temporal and spatial variations of the order parameter profile $\{S_i\}$ close to the core of the defects as well as cross couplings to the set of variables $\{\varphi_i\}$

$$\dot{S}_i = h_i(\{S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \ldots\}) + l_i(\{S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, \ldots\}). \tag{2}$$

In a similar way one has to modify (1) by incorporating cross couplings to variations of the set $\{S_i\}$

$$\dot{\varphi}_i = g_i(\{\varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, \ldots\}) + m_i(\{\varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \ldots\}). \tag{3}$$

To be specific, we consider in the following one defect situated at location $\boldsymbol{R}(t)$ on a two-dimensional manifold. Then we have as infinitesimal virtual changes

$$\delta S_i = -\delta\boldsymbol{R}\cdot\nabla S_i. \tag{4a}$$

Similarly we find for the phase variation in the core region Ω, i.e. the region around $\boldsymbol{R}$ where S_i differ from their far-field values

$$\delta\varphi_i = -\delta\boldsymbol{R}\cdot\nabla\bar{\varphi}_i \tag{4b}$$

with $\bar{\varphi}_i$ being the phases associated with an isolated defect at $\boldsymbol{R}$. Here variations of S_i, δS_i and variations of $\bar{\varphi}_i$ (i.e. φ_i inside Ω), $\delta\varphi_i$ are rigidly coupled to $\delta\boldsymbol{R}$, whereas outside the volume Ω where $\{S_i\}$ are constants, there is no coupling to $\{\delta\varphi\}$.

If we rewrite (2) and (3) for a given set of variables φ_i and S_i, respectively, and make use of (4) we obtain, focussing on the slow motion of the defect, i.e. $\dot{\boldsymbol{R}}$

$$-\dot{\boldsymbol{R}}\cdot\nabla S_i = h_i(\{S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \ldots\}) + l_i(\{S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, \ldots\}) \tag{5}$$

$$-\dot{\boldsymbol{R}}\cdot\nabla\varphi_i = g_i(\{\varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, \ldots\}) + m_i(\{\varphi_k, \nabla_j\varphi_k, \nabla_j\nabla_l\varphi_k, S_k, \nabla_jS_k, \nabla_j\nabla_lS_k, \ldots\}). \tag{6}$$

Taking the inner product, i.e. multiplying (5) and (6) by the adjoint zero eigenvector of the operator that occurs on the RHS of (5) and (6) linearised about the isolated defect configuration and integrating over Ω we obtain†

$$\boldsymbol{R}\cdot\mathbf{D}=-\int_{\Omega}(j_s\nabla S+j_\varphi\nabla\bar{\varphi}) \tag{7}$$

with

$$\mathbf{D}=\int_{\Omega}(\nabla S\nabla S+S^2\nabla\bar{\varphi}\nabla\bar{\varphi}) \tag{8a}$$

and

$$j_s=h+l, \qquad j_\varphi=(g+m)S^2. \tag{8b}$$

To arrive at (7) and (8) we have not assumed any analyticity properties for the functional dependence of h, l, g and m which will be, in general, nonlinear functions of all the arguments. The generalisations of (7) to the case of a small number of defects which are well separated is straightforward. One just has to repeat the procedure outlined above for every defect separately.

Equations (7) and (8) *combined* with (1) constitute the main result of the present paper; (7) gives a dynamic equation for the defect as a macroscopic, extended object and (6) are the hydrodynamic or phase equations well outside the 'defect volume' Ω. In the past similar results for phase dynamics (Brand and Cross 1983) or hydrodynamics on the one hand and defect dynamics (Kawasaki 1984b) on the other have been derived *separately.*

Thus we propose that a condensed matter system containing a small number of topological defects can be described by supplementing the hydrodynamic or phase dynamic equations with an additional effective equation of motion for each defect‡. This latter equation is of a different type to the hydrodynamic or phase dynamic equation in the sense that it does not correspond to a conservation law or to a broken symmetry of the usual type. It is similar to a hydrodynamic equation because it also characterises the macroscopic properties of the system, namely the slow motion of the topological defect which determines the state over a large surrounding spatial region without having to specify details of the core structure. We emphasise that our approach is completely independent of the fact of whether or not a Liapunov functional for (2) and (3) exists.

If one assumes that (7) allows for a static solution one has

$$\int_{\Omega}[j_S(S,\bar{\varphi})\nabla S+j_\varphi(S,\bar{\varphi})\nabla\bar{\varphi}]=0. \tag{9}$$

To make (7) and (8) more explicit for special cases we assume for a first example that j_S and j_φ have a gradient expansion, e.g.

$$m=m_{ij}\nabla_i S\nabla_j\varphi+\tilde{m}_{ij}\nabla_i\nabla_j\varphi+\ldots \tag{10}$$

where m_{ij} are functions of S and ... indicates terms containing higher-order derivatives,

† In order not to overburden the notation we restrict ourselves to one pair of variables S and φ in the following. The generalisation to more variables is straightforward but requires the introduction of additional matrices. Since we concentrate here on the principles of the approach, we avoid these complications which reduce the transparency of the method.

‡ In retrospect, one might say that for incommensurate systems equations of a similar type have been given before (Kawasaki 1984a), although the generality of the approach was not recognised.

higher nonlinearities etc. Inserting (10) and a similar expansion for $l = l_{ij}\nabla_i\tilde{\varphi}\nabla_j\tilde{\varphi}+\dots$ into (5) and (6) we obtain, after taking (9) into account

$$\mathbf{D}\cdot\dot{\boldsymbol{R}} = \boldsymbol{\Pi}\cdot\nabla\tilde{\varphi}+\dots \tag{11}$$

with

$$\boldsymbol{\Pi} = -\int_\Omega (\nabla\tilde{\varphi}\nabla S\cdot\mathbf{m}+\nabla S\cdot\nabla\tilde{\varphi}\cdot\mathbf{l}) \tag{12}$$

where ... contains higher-order derivatives and higher nonlinearities and where we have introduced $\tilde{\phi} = \phi - \bar{\phi}$, the part of the phase which is slowly varying and is not related to the particular defect under consideration. $\mathbf{m}$ and $\mathbf{l}$ stand for the second-rank tensors with components m_{ij} and l_{ij}, respectively.

Here we have kept only the terms which give finite contributions to the RHS of (11) as Ω shrinks to zero. This can be seen by power counting since ∇S and $\nabla\bar{\varphi}$ are both of the order r_0^{-1}, r_0 being the characteristic length associated with Ω. The terms which give divergent contributions as $r_0\to 0$ have been excluded on physical grounds and those terms which vanish in the limit $r_0\to 0$ have been neglected†.

The RHS of (2) can be interpreted as a generalised Peach–Koehler force $\boldsymbol{X}$ (Peach and Koehler 1950) with $\mathbf{l}$, $\mathbf{m}$ linear in $\nabla\bar{\varphi}$. We note that in deriving (12) we have not assumed that we deal with a Hamiltonian system; if this is the case, however, the generalised Peach–Koehler force $\boldsymbol{X}$ can be obtained simply by variation from the potential, i.e. no explicit consideration of the amplitude dependence is necessary in this case (Kawasaki and Brand 1984). The general structure of the generalised Peach-Koehler force can be inferred by symmetry considerations. For example, for a dislocation in the roll structure of convection with wavevector $\boldsymbol{k}$ perpendicular to the rolls $\boldsymbol{\Pi}$ takes the following general form

$$\boldsymbol{\Pi} = b_1\hat{\boldsymbol{\nu}}\hat{\boldsymbol{k}} + b_2\hat{\boldsymbol{k}}\hat{\boldsymbol{\nu}} + b_3\hat{\boldsymbol{k}}\hat{\boldsymbol{k}} + b_4\hat{\boldsymbol{\nu}}\hat{\boldsymbol{\nu}} \tag{13}$$

where $\hat{\boldsymbol{\nu}}$ is the unit vector orthogonal to $\hat{\boldsymbol{k}}$ in the plane and the b's are coefficients which can be expressed as certain integrals over Ω. Thus we obtain

$$\mathbf{D}\cdot\dot{\boldsymbol{R}} = \boldsymbol{X} = b_1\hat{\boldsymbol{\nu}}(\hat{\boldsymbol{k}}\cdot\nabla\tilde{\varphi}) + b_2\hat{\boldsymbol{k}}(\hat{\boldsymbol{\nu}}\cdot\nabla\tilde{\varphi}) + b_3\hat{\boldsymbol{k}}(\hat{\boldsymbol{k}}\cdot\nabla\tilde{\varphi}) + b_4\hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}}\cdot\nabla\tilde{\varphi}). \tag{14}$$

We mention in passing that glide and climb in convective roll structures will enter (14) through parts of b_2, b_3 (glide) and b_1, b_4 (climb) provided $\mathbf{D}$ does not contain νk and $k\nu$ components. Equation (14) is to be supplemented with the phase dynamic equation (1) where φ is multivalued in the presence of a defect. Sometimes it is useful to express this equation in terms of a single valued phase φ by replacing $\nabla\varphi$ by $\nabla\varphi - 2\pi\Theta(\eta)\delta(\zeta)\nabla\zeta$ where $\Theta(\eta)$ is the step function and $\delta(\zeta)$ is the non-vanishing delta function on the surface (line) of discontinuity $\zeta=0$ with phase jump 2π that emerges from the defect and $\eta(r)$ = positive constant defines a family of smooth curves which intersect orthogonally the line of discontinuity such that the value of the constant becomes negative if the curve no longer intersects the line of discontinuity. Thus we find that, e.g. the simple diffusive phase dynamic equation is replaced by

$$\partial_t\varphi = D[\nabla^2\varphi - 2\pi\nabla\cdot\Theta(\eta)\delta(\zeta)\nabla\zeta] \tag{15}$$

with a single-valued phase φ. We stress that the domain of validity of (15) is the same as for a multivalued φ i.e. only outside Ω.

† It is presupposed that the defect volume is not excessively anisotropic, otherwise, power counting can be different.

In deriving the dynamic equations for the motions of the defects we had to include at intermediate steps equations which contained explicitly the moduli S_i and their gradients. The final equations, however, do not have this explicit dependence but only the phenomenological coefficients in our equations, e.g. the b's in (14) do, of course, depend on these values. To evaluate the phenomenological parameters one has to go back to a more microscopic description in pretty much the same spirit as one can calculate coefficients like the kinematic viscosity in the Navier–Stokes equation from a Boltzmann equation approach. Therefore, changing order parameter profiles near defects will change the algebraic numbers for the coefficients but not the symmetries of the basic equations.

Finally we consider a simple example; a defect in the convective structure of a high Prandtl number fluid (e.g. silicon oil, cf Bergé and Dubois 1982) for which so-called mean flow terms in the phase equation (which come predominantly from vertical vorticity effects) are believed to be unimportant (Cross 1983).

For the nonlinear phase equation far away from any defect we have (assuming a gradient expansion to be valid)

$$\dot{\varphi} = D_1\varphi_{xx} + D_2\varphi_{yy} + \tilde{D}_1\varphi_{xxxx} + \tilde{D}_2\varphi_{yyyy} + F_1\varphi_y\varphi_{yy} + F_2\varphi_x\varphi_{xx} + \ldots \tag{16}$$

where we have assumed the symmetry $\varphi \to -\varphi$ under $x \to -x$ and $y \to -y$ separately.

Close to the defect core we have two equations—one for the phase and one for the modulus

$$\dot{\varphi} = D_1\varphi_{xx} + D_2\varphi_{yy} + \tilde{D}_1\varphi_{xxxx} + \tilde{D}_2\varphi_{yyyy} + F_1\varphi_y\varphi_{yy} + F_2\varphi_x\varphi_{xx} + N_1S_x\varphi_x + N_2S_y\varphi_y + \ldots \tag{17}$$

$$\dot{S} = E_1S_{xx} + E_2S_{yy} + \tilde{N}_3\varphi_x^2 + \tilde{N}_4\varphi_y^2 + \alpha S_x^2 + \beta S_y^2 + \ldots. \tag{18}$$

From (17) and (18) we can now proceed as outlined above in (3)–(11) to get a dynamic equation for the defect as a macroscopic object.

$$\mathbf{D} \cdot \dot{\boldsymbol{R}} = \int_\Omega (\nabla\bar{\varphi} \cdot \mathbf{N} \cdot \nabla S \nabla\tilde{\varphi} + \nabla S \cdot \mathbf{N} \cdot \nabla\tilde{\varphi}\nabla\bar{\varphi}) \tag{19}$$

and for the generalised Peach–Koehler force we have

$$\boldsymbol{X} = b_1\hat{\boldsymbol{\nu}}\hat{\boldsymbol{k}} + b_2\hat{\boldsymbol{k}}\hat{\boldsymbol{\nu}} + b_3\hat{\boldsymbol{k}}\hat{\boldsymbol{k}} + b_4\hat{\boldsymbol{\nu}}\hat{\boldsymbol{\nu}}. \tag{20}$$

Further algebraic details and generalisations of the approach presented here will be found in Kawasaki (1985). Applications to other systems like nematics (as an example for a hydrodynamic system) and the wavy vortex state of the Taylor instability in which the defect triggers the onset of turbulence (King and Swinney 1983) will be given in separate publications. We mention in closing that so-called mean flow effects in the phase equations which are important in low Prandtl number fluids (Cross 1983) are naturally included in our basic equations (1). The vertical vorticity, e.g., which is believed to be of crucial importance in this connection can be just interpreted as an additional 'phase' equation. Using the approach given here it should also become possible to give a qualitative analytic discussion of the skewed varicose instability (Busse and Clever 1979) for which only numerical calculations are available up to now.

To sum up we have presented a novel approach of how the macroscopic motion of a small number of topological defects can be incorporated into the macroscopic description of condensed matter systems. The concept given above can be equally well applied to equilibrium and non-equilibrium systems and is independent of the existence of a Liapunov functional, the basic ingredient being the assumption that the defect (as an extended object) can be described as an entity which evolves dynamically on a time scale comparable to the time scales of the other macroscopic variables.

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