Research description

The analysis of the structure and evolution of singularities in partial differential equations (PDE) problems, such as in Ginzburg-Landau models, has led to a wealth of new mathematical tools, results and questions over the past 15 years. In these problems, there is typically an "order parameter" (a vector-valued function φ) representing the different phases of the system and a free energy functional for φ,

$$E_\varepsilon(\varphi) = \int_\Omega \left[\frac{\varepsilon^2}{2} |\nabla \varphi|^2 + W(\varphi) \right] dx \tag{1}$$

with a small parameter ε. The choice of the order parameter and of the potential depend on the problem being considered: some examples include formation and evolution of vortices in superconductors or of phase boundaries in conserved or non-conserved Allen-Cahn or Cahn-Hilliard systems. I am interested in gradient flows associated to E_ε and its stationary equilibria, in the limit as $\varepsilon \to 0$. To study these singularly perturbed problems, many new methods are being introduced, involving sharp variational methods for isolating vortices and transition layers, viscosity solutions, and spectral analysis for rigorous multi-scale asymptotics. I am mostly concerned with the qualitative information one obtains for the related vortex or multi-phase boundaries, when studying analytically the convergence of these singularly perturbed systems as $\varepsilon \to 0$. Often these problemes lead to challenging analytical questions as well as nice geometrical results for the singularities thus obtained.

I. Structure of "vortices"

The simplest model for superconductors that has been extensively studied by mathematicians over the past 10 years is given by the above Ginzburg-Landau energy (1) for a complex-valued order parameter. Here the potential W vanishes on the unit circle in $\mathbb{C}$ and the Euler–Lagrange equations are an elliptic system which regularizes the classical problem of harmonic maps to the circle. Vortices are points of concentration of the energy, and corresponds to zeros of the order parameter. By incorporating an appropriate vector field (the magnetic potential), one obtains a gauge-invariant functional which is the classical Ginzburg-Landau model of superconductivity.

A. Lawrence Doniach model: a semi-discrete Ginzburg-Landau functional.

High-temperature superconductors are layered materials and the Lawrence–Doniach system is a variational model commonly used by physicists in which the material is described by a coupled array of superconducting planes rather than as a three-dimensional solid. As such it can be thought of as a semi-discrete Ginzburg-Landau functional. In recent results with S. Alama and J. Berlinsly, and in ongoing projects with S. Alama, and E. Sandier, we are studying the structure of vortices and of the vortex lattice in the Lawrence-Doniach model in parallel magnetic fields.

In [1,3] we study the structure of low-energy critical points of the Lawrence–Doniach functional in a "weak-coupling" limit. We study two different cases: when the domain is bounded and of rectangular cross-section, and with a doubly-periodic ansatz. In the periodic case we have developed a new functional setting for the variational problem in order to eliminate the infinite-dimensional degeneracy due to gauge invariance. We classify all low energy solutions in the finite cross-section case; in the periodic case, energy minimization selects a *unique* period lattice from all possible geometries. This periodic lattice is not the usual "Abrikosov" vortex lattice observed in classical superconductors. In particular, we obtain its shape by direct minimization techniques, rather than by numerical approximation as in the classical case. Finally, (following a suggestion of A. Barhi,) we combine *a priori* estimates on solutions and a novel argument based on the implicit function theorem to determine the range of validity of our perturbation approach in terms of various parameters in the model. In particular, this analysis indicates that the results are appropriate for *large applied fields.*

In our recent preprint ([22]) with S. Alama and E. Sandier, we study the structure of *isolated* vortices in the Lawrence–Doniach model. The isolated vortex cannot be radial due to the half-discrete, half-continuous nature of the model and so the problem is fully two-dimensional. Also, due again to the discrete nature of the problem, vortices are not the classical "Abrikosov" vortices which are defined as zeros of the order parameter. Nevertheless we can extend the energy methods of Sandier (see also Jerrard) for the classical G–L models, to locate the singularities and then obtain uniform estimates strong enough to pass to the continuum limit. In particular, we prove that the core structure of Lawrence–Doniach vortices is different from what physicists had predicted.

We are now studying the case of sparsely distributed vortices (when applied fields are small) in order to characterize when the continuum limit described above is more appropiate than the "weak coupling" limit in our previous papers.

B. A Ginzburg-Landau model with spin and its fractional degree vortices.

In a new class of Ru-based superconductors, ferromagnetism is observed at or near the onset of superconductivity at the critical temperature T_C, which has led physicists to hypothesize that it is the same physical mechanism responsible for both types of ordering.

In the simpler setting where one does not include the magnetic field, the functional takes the form:

$$E(\Psi) = \int_\Omega \left\{ |\nabla\Psi|^2 + \frac{1}{2\varepsilon^2}(|\Psi|^2 - 1)^2 + \gamma|\psi_1^2 + \psi_2^2|^2 \right\} dx.$$

In the case that $-1 < \gamma < 0$, we recently discovered a new type of vortices which have *half-integer* degrees. Their occurence is due to the fact that the singular limit of the energy is a harmonic map problem on a 2-torus, and hence the minimizers will prefer to have two fractional degrees rather than integer ones. This contrasts with the classical Ginzburg-Landau functional, where the corresponding harmonic map problem is S^1-valued and hence has classical integer degrees. To prove our result, we obtain in our paper [25] a precise asymptotic expansion of the functional, in the same spirit as the expansion done by Bethuel, Brezis, and Hélein [BBH] for the classical Ginzburg-Landau functional. Recently, with Petru Mironescu, we are in the process of understanding the shape of the "core" of the vortices. Indeed, there are now two ways to resolve the singularity at the center of a half-degree vortex Ψ. One is that Ψ vanishes at the center of the vortex, as for classical G-L vortices. However, for the fractional degree vortex, it turn out that Ψ will rotate along S^2 so that instead of vanishing, it will choose to have a non-zero spin.

In our preprints [23] and [24], we study the effect of the coupling of the superconductor parameter $\Psi : \Omega \to \mathbb{C}^2$, $\Omega \subset \mathbb{R}^2$, with the spin $S = \Re\Psi \times \Im\Psi$ due to the ferromagnetism. In particular, we study its effect on the first and second cricital field when, respectively, vortices enter the superconductor and when the superconductor reverts to normal material. We show that (in appropriate regimes,) there can be no first critical field so that there is a "spontaneous vortex state", while in [24], we show that the second critical field increases with spin coupling, and can be infinite (i.e. the normal state is never minimizing.)

C. Symmetric isolated vortices.

In joint works with S. Alama and T. Giorgi, we have studied isolated, radially symmetric vortices for the classical gauge-invariant Ginzburg–Landau model and for S. C. Zhang's $SO(5)$-model of high-temperature superconductivity. Zhang's model was introduced in 1997 and is one of the new competing models in the physics literature for describing high-temperature cuprate superconductors. It includes an antiferromagnetic phase which has been observed in such superconductors.

In [4], [6], we consider a single isolated, symmetric vortex within the Zhang's $SO(5)$ model. We introduce an appropriate analytical setting for this Ginzburg-Landau functional and show that a new type of vortices with *antiferromagnetic* cores are present in the $SO(5)$ model. We then show that when the chemical potential parameter goes below a certain critical value, the vortices with "normal" cores bifurcates to vortices with antiferromagnetic cores. In the small ϵ ("high-κ") limit we can show that the solutions which bifurcate from the normal core solution are always nondegenerate local minimizers of the energy, and hence are *unique.* In particular we can show that the bifurcation is continuous and hence the transition is *second order* rather than first order, as was believed in the physics literature (by Arovas, Berlinsky, Kallin, & Zhang.)

An open problem in classical Ginzburg-Landau vortices. The ideas developed in [4] are used in [7] to partially resolve an open problem in the classical Ginzburg-Landau model of superconductivity, namely that (radial) vortices are indeed *unique*, at least when $\varepsilon^2 \leq 1/2d^2$, where d is the degree of the vortex. The restriction on ϵ is technical and is necessary to obtain the nondegeneracy of the local minimizers of the (radial) Ginzburg-Landau functional. Our result combined with the recent uniqueness results of Pacard & Rivière proves that an entire degree-one solution of G–L must be unique (for $\epsilon \leq \frac{1}{\sqrt{2}}$.)

We are currently studying symmetric vortices in other gauge field models and multi-vortex configurations in the $SO(5)$ model. In particular, we want to see what mixed phases are present when we vary the imposed magnetic field and chemical potential. For these questions the model must be refined to include the magnetization as an additional order parameter. Also, we plan to study how the dynamics of the vortices is affected by their antiferromagnetic cores.

II. Dynamics of interfaces

Most of the models that I will discuss in this section can be viewed as gradient flows for the Ginzburg-Landau energy (1) when the potential W vanishes along isolated points rather than the unit circle.

Viscosity solutions Method: The notion of viscosity solutions is a notion of weak solutions to PDE's which was introduced in the mid-eighties by Crandall and Lions and further developped by them and also by Evans, Ishii and many others. This method had a very big success in the phase transition litterature when Evans-Soner-Souganidis proved the convergence of the Allen-Cahn equation to the mean curvature flow for the limiting interface, even past singularities. In [18], we had used this method to handle the case that the potential W has unequal wells (when the interface evolves with constant speed.) Recently, with S.-A. Shim (a post-doc at McMaster who is at Seoul Univ as of this September,) we have extended the viscosity method to handle the case of a competition-diffusion system in population biology for which comparison methods are available. We use this extension to obtain the convergence to an interface problem evolving by mean curvature. This convergence was previously done by Ei and Yanagida in the case of smooth curves. We use our weak viscosity solution approach to obtain long-time behavior for the system, even past singularities.

In addition, with A.-M. Matei (a post-doc at McMaster, who started this September at Loyola Univ.), we are currently extending the viscosity method to handle operators which are more complicated than the laplacian, for example which involve the p-laplacian. These PDE are interesting in themselves and many new and beautiful results have been obtained recently for the stationary case by Kawohl, among others.

Energy Methods: Another powerful approach to prove rigorously the convergence of diffuse interface models is the Energy Method, whereby we use the energy functional as a Lyuapunov function for the dynamics. With B. Stoth we have been able to solve a variety of different problems, usually in radial settings, using the Energy Method. Our method does not rely on maximum principle arguments, and hence is useful in handling vector-valued systems. Although radiality is a strong assumption, I know of no other method which has been used for rigorous analysis of singularly perturbed systems for which there are no comparison principles available. Here are some problems which we have solved using this method:

(1) An alternative to the standard Cahn-Hilliard equation is a non-local Allen-Cahn system, introduced in the scalar case by Rubinstein and Sternberg. This equation takes the form $u_t - \varepsilon\Delta u + \frac{1}{\varepsilon}W'(u) - \frac{1}{\varepsilon|\Omega|}\int_\Omega W'(u)\,dx = 0$, and the mass constraint is felt through the (nonlocal) Lagrange multiplier. In [12], we prove convergence to a volume preserving mean curvature flow in the radial case in $\mathbf{R}^n$. Moreover, we compare the limiting dynamics for this nonlocal flow with the Mullins-Sekerka evolution, which gives the expected limiting behavior for the (scalar-valued) Cahn-Hilliard flow (as derived by Pego, Stoth, Alikakos-Bates-Chen).

(2) In [9], we extend this method to the vector valued Allen-Cahn equation, where W now vanishes on a manifold M (with one or more components.) This choice of potential W has been introduced by Rubinstein-Sternberg-Keller to model reversible chemical reactions. Here φ is a vector of concentrations of the reactants, and the manifold M represents the possible equilibrium states. For M with two components, formal asymptotics by Rubinstein-Sternberg-Keller suggest the formation of interfaces as $\varepsilon \to 0$, which move by mean curvature. In each bulk region φ takes its values in some connected component of M, and evolves according to a harmonic map flow with values in M. Consider the case $W(\varphi) = (b - |\varphi|)^2(|\varphi| - a)^2$, vanishing on concentric circles of radii $b > a > 0$, with $\varphi \in \mathbf{R}^2$. In [9] we find that there must also be a jump condition linking the harmonic map flows across the interfaces. This jump condition is obtained as a by-product of our rigorous proof of the formally derived results of Rubinstein-Sternberg-Keller in the radial case.

(3) Recently much attention has centered around superconductors, for which $W(\varphi) = (1 - |\varphi|^2)^2$, $\varphi \in \mathbf{R}^2$ and the energy must be modified to include the effects of the magnetic field. In [10], we use a new method which combines energy estimates with maximum principle arguments to study rigorously the asymptotic behavior of a time–dependent Ginzburg–Landau model for type I superconductors. The expected asymptotic behavior (for small penetration depth λ) depends strongly on the value of the Ginzburg–Landau parameter κ. When $\kappa < 1/\sqrt{2}$ ("type I") vortices are not observed; rather, when the strength of the applied magnetic field exceeds some critical

value H_c, normally conducting and superconducting regions may coexist in the material, creating interfaces. In [10], we prove that as $\lambda \to 0$, the interface separating the superconducting and normal phases evolves according to a classical one–phase Stefan problem (without surface tension) for H. We do this for in an infinite wire with circular cross section with constant external applied field parallel to the wire and radial initial data.

(4) The Energy Method may also be combined with local analysis and spectral estimates in order to treat some nonradial problems. In collaboration with N. Alikakos and G. Fusco [11] we describe some aspects of the dynamics of the Cahn-Hilliard and nonlocal Allen-Cahn equations. In particular we consider the dynamics of almost spherical interfaces and establish that almost spherical interfaces either persist forever inside the region or eventually reach the boundary, a phenomenon which happens superslowly as was predicted by asymptotics of Ward. This result is similar to results of Alikakos-Fusco, but our approach is simpler since it combines spectral estimates with energy methods.

The method should be extended in two different directions. First, in ongoing projects with N. Andre and I. Shafrir, and with C. Liu, we consider potentials vanishing on other manifolds. The difficulty is to find the appropriate parameters which separate the interface and bulk flows, in the same way as v_ε, f_ε do for circular M. Across the interfaces we expect φ to resemble an ODE heteroclinic solution with minimal energy connecting the appropriate points lying on different components of M. In the situation where $M \subset \mathbf{R}^2$ has two components, one lying inside the other, Sternberg has shown that these optimal heteroclinics do indeed exist. We conjecture that the jump condition derived in [9] is only needed in case of degeneracy, that is when minimizing heteroclinics form a continuum (as in the case of concentric circles.) In addition, the case where the potential is the same as in (2) (i.e. vanishing on two circles,) but in higher dimensions (i.e. when the number of reactants $N > 2$) is still open because new difficulties of a geometrical nature are present since the harmonic map flow in higher dimensions is more complicated.

Triple Junctions. To model physical systems with three (or more) conserved phases, we introduced in collaboration with Garcke and Stoth [8], a vector-valued Cahn–Hilliard equation which conserves mass:

$$\varphi_t = \Delta(-\varepsilon\Delta\varphi + \frac{1}{\varepsilon}\nabla_\varphi W(\varphi)), \tag{2}$$

where $N \geq 3, n = 3$ and $W \geq 0$ has three (or more) isolated global minima. In the limit as $\epsilon \to 0$ we showed formally that the domain separates into regions where the solution approaches one of the three global minima of W. The interfaces separating the regions should evolve according to a limiting "sharp interface" model with conservation which is a generalization of the Mullins–Sekerka problem. In particular they should meet three-at-a-time at *triple junctions*, where Young's law determines their meeting angle. More precisely this limiting interface model includes equilibrium equations in bulk, the Gibbs–Thomson relation on the interfaces, Young's law at triple junctions together with a dynamic law of Stefan type. Following the variational approach of Luckhaus, we propose a notion of weak solutions for this sharp interface model based on integration by parts on manifolds together with measure theoretical tools. Through an implicit time discretization we construct approximate solutions by stepwise minimization. Under the assumption that there is no loss of area as the time step tends to zero, we show the existence of a weak solution. This implicit time discretization approach should prove useful in a numerical simulation of this Mullins–Sekerka system.

The rigorous convergence of the vector-valued "diffuse interface" models to the limiting "sharp interface" models is a challenging problem and it is still open for the simpler vector-valued Allen–Cahn equation introduced in [17]. One of the difficulties in these problems is that the limiting flows usually develop singularities in finite time. Specifically, initial configurations with many grains (and hence many triple junctions) will develop singularities when triple junctions coalesce. These topological catastrophes are inevitable, as can be seen by the von Neumann–Mullins law for the area A of a grain with s sides, $\frac{dA}{dt} = \frac{\pi}{3}(s-6)$, and numerical simulations done in collaboration with B. Wetton [16]. In [17], F. Reitich and myself proved the local in time existence for the limiting geometric flow and this result was recently extended by D. Kinderlehrer when the initial data is close to a stationnary solution. In addition, there has been an extensive study of the numerical methods for the simulations of grain growth by D. Kinderlherer and many collaborators. In [16] we found that there are many physically reasonable ways of extending the flow past a singularity, and so the later flow is not uniquely determined by the past evolution. This nonuniqueness is also present in curvature motion without angle conditions (as was pointed out by Evans and Spruck.) The weak formulation for grain boundary motion should ideally resolve this nonuniqueness.

In passing from the Ginzburg-Landau systems described above to a weakly formulated limiting flow, one is also confronted with the possible existence of high multiplicity interfaces: several distinct layers for $\varepsilon > 0$ which collapse to a single interface in the limit $\varepsilon \to 0$. Indeed, in passing to the limit in the diffuse model the energy "remembers" multiplicities, even though they are not visible in the sharp interface flow. (See [12], as well as the papers of Ilmanen and Soner.) In [15], we used methods from [20,21] to prove that radial solutions of the Allen-Cahn equation may indeed exhibit interfaces with arbitrarily high multiplicity. The existence of multiple interfaces for other Ginzburg-Landau systems is as yet unknown.

Stationary Wave Solutions. An important step in proving convergence to the limiting flow in these problems is the approximation of the solution by its first-order term in the expansion. In the vector-valued Allen-Cahn equation, the first term in the asymptotic expansion at a triple junction is a stationary wave solution in $\mathbf{R}^2$ with "triple layer structure": at infinity it approaches the three minima of W along cones, and across the interfaces it approaches one of the three (one-dimensional) stationary wave solutions connecting pairwise the three global minima of W. The existence of such a solution is essential to any proof of convergence to the sharp interface model, and with Gui and Schatzman [14] we have shown that such a solution exists when W has the symmetries of the equilateral triangle. In [13] we improve [14] to handle stationary waves and saddle solutions with rectangular geometry. Our result demonstrates an unexpected difference between the scalar and vector valued Allen–Cahn equations, namely that in the vectorial case the transition profiles may vary tangentially along the interface. In particular, de Giorgi's conjecture's proved by Ghoussoub-Gui and Cabre, cannot be true in the vectorial case. Recently M. Schatzman has extended our result in [14] to handle the case that the potential W is not symmetric.

References *to my previous work are listed on my Curriculum Vitae.*

Suggested letters of references: The following is a list of distinguished mathematicians who are well acquainted with my research, and could provide letters of reference.

Prof. Haïm Brezis, Université de Paris VI and Rutgers University.
Prof. D. Kinderlehrer, Carnegie Mellon University.
Prof. Wei-Ming Ni, University of Minnesota.
Prof. P. Sternberg, Indiana University.
Prof. L.C. Evans, University of California at Berkeley.