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NUMERICAL APPROXIMATIONS IN VARIATIONAL PROBLEMS WITH POTENTIAL WELLS*

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Abstract. In this paper, some numerical aspects of variational problems which fail to be convex are studied. It is well known that for such a problem, in general, the infimum of the energy (the functional that has to be minimized) fails to be attained. Instead, minimizing sequences develop oscillations which allow them to decrease the energy.

It is shown that there exists a minimizer for an approximation of the problem and the oscillations in the minimizing sequence are analyzed. It is also shown that these minimizing sequences choose their gradients in the vicinity of the wells with a probability which tends to be constant. An estimate of the approximate deformation as it approximates a measure and some numerical results are also given.

Key words. finite element method, variational problem, Young measure

AMS(MOS) subject classifications. 65N15, 65N30, 35J20, 35J70, 73C60

1. Introduction.

In this paper we study some numerical aspects of variational problems which fail to be convex. It is well known that for such a problem, in general, the infimum of the energy (the functional that has to be minimized) fails to be attained. Instead, minimizing sequences develop oscillations which allow them to decrease the energy.

Such oscillations are observed in the context of hyperelasticity for ordered materials such as crystals (see [3], [4], [6], [8], [16]–[24], [27], [30]). Indeed, in order to lower its energy such a material makes full use of its special structure. This structure is recorded in different models where generally it is assumed that the energy functional experiences several potential wells (see for instance [3], [23], [24], [27]). From the physical point of view it means that some linear deformations (related to the material under consideration) are of very low cost in energy. Thus, the strategy for the material to obtain a minimum energy configuration consists of using these low cost deformations on a finer and finer scale. This, of course, can be observed both experimentally and computationally [3], [4], [9], [11]–[14], [30].

Assume that we have an energy density $\phi : \mathbb{R}^n \to \mathbb{R}$ supported on k potential wells. That is, there are k vectors $w_i \in \mathbb{R}^n$, with $k \geq 2$, such that $\phi(w_i) = 0$ for $i = 1, \cdots, k$ and $\phi(\xi) > 0$ for $\xi \neq w_i$. Let $a \in \mathbb{R}^n$ be in the convex hull of the wells, but not equal to a well; that is, there is a vector $\alpha = (\alpha_1, \cdots, \alpha_k)$ such that

$$(1.1) \qquad \sum_{i=1}^{k} \alpha_i w_i = a \quad \text{with } 0 \leq \alpha_i < 1 \quad \text{and} \quad \sum_{i=1}^{k} \alpha_i = 1.$$

In addition, let $\psi : \mathbb{R} \to \mathbb{R}$ be a continuous nonnegative function such that

$$(1.2) \qquad \psi(0) = 0 \quad \text{and } \psi(t) > 0 \quad \text{for } t \neq 0.$$

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For instance $\psi(t) = |t|^q$, $q > 0$ would be suitable for our purpose. For a given polygonal domain $\Omega \subset \mathbb{R}^n$ with $\partial\Omega = \Gamma_0 \cup \Gamma_1$, let

$$V_a = \{v : \Omega \to \mathbb{R} \mid v \text{ is piecewise affine and } v(x) = a \cdot x \text{ for } x \in \Gamma_0\}. \tag{1.3}$$

By piecewise affine we mean that the function is continuous and affine on simplices covering Ω. We consider the minimization problem:

$$\text{Find } u \in V_a \quad \text{such that } E(u) = \inf_{v \in V_a} E(v) \tag{1.4}$$

where $E(v)$ is the total energy:

$$E(v) = \int_\Omega \phi(\nabla v(x)) + \psi(v(x) - a \cdot x)\, dx. \tag{1.5}$$

We could introduce some other spaces but the infinum of the energy is the same for any space containing V_a so we have restricted ourselves to this case. Energies such as (1.5) were introduced in [5]. If we set $u(x) = v(x) - a \cdot x$ then

$$\int_\Omega \phi(\nabla v) + \psi(v - a \cdot x)\, dx = \int_\Omega \phi(\nabla u + a) + \psi(u)\, dx.$$

So minimizing the integral on the left over $v \in V_a$ is equivalent to minimizing the integral on the right over $u \in V_0$. So, from now on we will assume that $a = 0$ and that zero is in the convex hull of the wells.

For the minimization problem (1.4), we will consider three cases: $\Gamma_0 = \partial\Omega$, $\Gamma_0 = \emptyset$, and $\emptyset \subsetneq \Gamma_0 \subsetneq \partial\Omega$. It follows from a later result that the infinum in each case is zero. However, for a function to have zero energy it must satisfy $\phi(\nabla v) = 0$ and $\psi(v(x)) = 0$ which would imply that $\nabla v = w_i$ almost everywhere and $v \equiv 0$ which is impossible, unless $w_i = 0$ for some i, but this is prohibited by (1.1). Thus, we cannot obtain minimizers of (1.5) directly and so we consider minimizing sequences. It is reasonable to expect that such a minimizing sequence will have a gradient which oscillates between the wells in order to reach the lower levels of energy. This is indeed what happens but, as we will show, these oscillations are done in an organized manner, provided that the number of wells is limited to $n+1$ and that the wells are chosen such that the vectors $w_i - w_1$ for $i = 2, \cdots, k$ are linearly independent. The mathematical explanation of the controlled oscillations of the minimizing sequences in this case lies in the fact that the Young measure (see [2], [8], [15], [25], [26], [28], [32]) associated to the problem is unique (see §4).

This paper is organized as follows. In §2 we prove an existence result for the minimizers of an approximation of the problem. In §3 we show, through an energy estimate, that the infinum of (1.4) is indeed equal to zero and we give different rates of convergence of this energy towards zero. Section 4 is devoted to the analysis of the oscillations of the minimizing sequences of (1.4). In particular we show that these minimizing sequences choose their gradients in the vicinity of the wells with a probability which tends to be constant (of course we assume we are in the case where the Young measure associated to the problem is unique). Moreover, since the problem at stake is the approximation of a measure, we give an estimate in this sense (Theorem 6). Finally we comment in §5 on some numerical experiments. Our results expand on the results obtained in one dimension by Collins, Kinderlehrer, and Luskin [10] and Collins and Luskin [14].

2. An existence result. Our first concern is to establish the existence of a solution of an approximation of the problem (1.4). We restrict ourselves to one example where such an existence can be proved, and we refer the reader to [7] for another case.

Recall that we are assuming $a = 0$ so that in all that follows

$$E(v) = \int_\Omega \phi(\nabla v(x)) + \psi(v(x))\, dx.$$

Let τ_h be a triangulation with mesh size h of the domain Ω and let V_h^0 be the approximation of V_0 corresponding to τ_h, i.e., V_h^0 is the space of continuous functions vanishing on Γ_0 and affine on each simplex of τ_h.

THEOREM 1 (existence). *If ϕ and ψ are continuous and* $\lim_{|t|\to+\infty} \psi(t) = +\infty$ *then there exists a $u_h \in V_h^0$ such that*

$$E(u_h) = \inf_{v \in V_h^0} E(v). \tag{2.1}$$

Proof. Every element of V_h^0 is completely determined by its value on the nodes of τ_h, so finding the minimum reduces to finding a vector $X = (u_h(n_1), \cdots, u_h(n_p))$ where the n_i's are the nodes of τ_h not on Γ_0, which minimizes $E(u_h)$. As ϕ and ψ are continuous, $E(u_h)$ is continuous in X.

Let $|X| \to +\infty$, then at least one component of X goes to infinity, so assume that $X_i = u_h(n_i) \to +\infty$. Now let $T \in \tau_h$ such that n_i is one of the vertices of T. Then we have

$$\int_\Omega \phi(\nabla u_h(x)) + \psi(u_h(x))\, dx$$
$$\geq \int_T \psi(u_h(x))\, dx \geq \inf_{|u| \geq \frac{1}{2}|u_h(n_i)|} \psi(u) \cdot \text{meas} \left\{ x \in T \mid |u_h(x)| \geq \frac{1}{2}|u_h(n_i)| \right\} \tag{2.2}$$

where $\text{meas}\, S$ denotes the Lebesgue measure of the set S. Assume that we have proved that

$$\text{meas}\, \{x \in T \mid |u_h(x)| \geq |u_h(n_i)|/2\} \geq \left(\tfrac{1}{3}\right)^n \text{meas}\, T, \tag{2.3}$$

then (2.2) reads

$$\int_\Omega \phi(\nabla u_h(x)) + \psi(u_h(x))\, dx \geq \left(\frac{1}{3}\right)^n \text{meas}\, T \inf_{|u| \geq \frac{1}{2}|u_h(n_i)|} \psi(u) \to +\infty$$

when $u_h(n_i) \to +\infty$, by our assumption on ψ. Thus $E(u_h) \to +\infty$ and the existence of u_h follows by an easy compactness argument. More precisely, choose $\bar{u} \in V_h^0$ such that $E(\bar{u}) < \infty$ and let $U = \{u \in V_h^0 \mid E(u) \leq E(\bar{u})\}$. Then by the above argument and the continuity of E, U is a compact set and as E is continuous there must exist a $u_h \in U \subset V_h^0$ such that $E(u_h) = \inf_{v \in U} E(v) = \inf_{v \in V_h^0} E(v)$.

To prove (2.3) note first that without loss of generality we can assume that $n_i = 0$ so that if we set $b = u_h(n_i)$ then

$$u_h(x) = a \cdot x + b.$$

Then we show that

$$\text{meas}\, \{x \in T \mid |a \cdot x + b| \geq \tfrac{1}{2}|b|\} \geq \left(\tfrac{1}{3}\right)^n \text{meas}\, T. \tag{2.4}$$

By changing u_h to $-u_h$ we see there is no loss of generality in assuming $b > 0$, so that (2.4) can be written as

$$\text{meas}\,\{x \in T \mid |\tfrac{a}{b} \cdot x + 1| \geq \tfrac{1}{2}\} \geq \left(\tfrac{1}{3}\right)^n \text{meas}\, T. \tag{2.5}$$

Consider the one-dimensional case first, i.e., $a/b = \alpha \in \mathbb{R}$ and $T = (0, T)$. Then if $\alpha \geq 0$ we clearly have

$$\text{meas}\,\{x \in T \mid |\alpha x + 1| \geq \tfrac{1}{2}\} = \text{meas}\, T;$$

hence (2.5) holds. If $\alpha < 0$ then $|\alpha x + 1| \geq \frac{1}{2}$ implies that

$$x \leq -\frac{1}{2\alpha} \quad \text{or} \quad x \geq -\frac{3}{2\alpha}.$$

When $-3/2\alpha \geq T$ we have $-1/2\alpha \geq T/3$ and

$$\left\{x \in T \mid |\alpha x + 1| \geq \frac{1}{2}\right\} = \left(0, -\frac{1}{2\alpha}\right)$$

and thus (2.5) holds. When $-3/2\alpha < T$ we have $1/\alpha > -2T/3$ and

$$\left\{x \in T \mid |\alpha x + 1| \geq \frac{1}{2}\right\} = \left(0, -\frac{1}{2\alpha}\right) \cup \left(-\frac{3}{2\alpha}, T\right)$$

and thus

$$\text{meas}\left\{x \in T \mid |\alpha x + 1| \geq \frac{1}{2}\right\} = -\frac{1}{2\alpha} + T + \frac{3}{2\alpha} = T + \frac{1}{\alpha} \geq \frac{1}{3} T;$$

hence (2.5) holds. Knowing now that (2.5) holds for the one-dimensional case, we use polar coordinates and write for $x = r\omega$, with ω a unit vector in $\mathbb{R}^n$,

$$\begin{aligned} \text{meas}\left\{x \in T \mid \left|\frac{a}{b} \cdot x + 1\right| \geq \frac{1}{2}\right\} &= \int_{\{x \in T \mid |\frac{a}{b} \cdot x + 1| \geq \frac{1}{2}\}} dx \\ &= \int_{\{r\omega \in T \,:\, |\frac{a}{b} \cdot r\omega + 1| \geq \frac{1}{2}\}} r^{n-1}\, d\omega\, dr. \end{aligned} \tag{2.6}$$

For fixed ω we have to integrate over the set

$$\{r \mid \left|\tfrac{a}{b} \cdot \omega r + 1\right| \geq \tfrac{1}{2}\}$$

and the measure of this set is certainly larger than $r(\omega)/3$ where $r(\omega)$ is the largest r such that $r\omega \in T$. Hence for fixed ω

$$\int_{\{r \mid |\frac{a}{b} \cdot \omega r + 1| \geq \frac{1}{2}\}} r^{n-1}\, dr \geq \int_{(0, r(\omega)/3)} r^{n-1}\, dr$$

and (2.6) becomes

$$\text{meas}\left\{x \in T \mid \left|\frac{a}{b} x + 1\right| \geq \frac{1}{2}\right\} \geq \int_{|\omega|=1} \int_{(0, r(\omega)/3)} r^{n-1}\, dr\, d\omega = \left(\frac{1}{3}\right)^n \text{meas}\, T$$

which completes the proof. □

3. Energy estimate. In what follows we will assume the the triangulation of the domain is regular.

THEOREM 2 (energy estimate). *Assume that for some constants m and $q > 0$*

$$\psi(t) \leq m|t|^q; \tag{3.1}$$

then if ϕ is bounded on bounded sets

$$E_h = \inf_{v \in V_h^0} E(v) \leq Ch^\gamma,$$

where $\gamma = \frac{1}{2}$ for $q \geq 1$ and $\Gamma_0 \neq \emptyset$, and $\gamma = q/(q+1)$ for $q < 1$ and $\Gamma_0 \neq \emptyset$ or $\Gamma_0 = \emptyset$.

Proof. Clearly since $a = 0$ belongs to the convex hull of the w_i's, we can find w_i's—that for simplicity we will still label by $w_1, \cdots, w_k$—such that (1.1) holds and the vectors $w_i - w_1$ for $i = 2, \cdots, k$ are linearly independent.

It is easy to see (cf. §4) that the vector α satisfying (1.1) is unique. Let p be the number of $\alpha_i \neq 0$ and renumber the wells so that $\alpha_i > 0$ for $i = 1, \cdots, p$. Let

$$w_h(x) = \min_{1 \leq i \leq p} w_i \cdot x + h^\beta \tag{3.2}$$

where $\beta \in (0, 1)$. First we note that

$$w_h(x) \leq h^\beta \quad \forall x. \tag{3.3}$$

If not, then we have for some x, $w_i \cdot x > 0$ for $i = 1, \cdots, p$ and $\sum_{i=1}^k \alpha_i w_i \cdot x > 0$ contradicting (1.1). Second, all the wells for which $\alpha_i \neq 0$ participate in w_h; otherwise, there is an j such that $w_j \cdot x + h^\beta \geq w_i \cdot x + h^\beta$ for $i = 1, \cdots, p$ and for all x. Thus

$$w_j \cdot x = \sum_{i=1}^k \alpha_i w_j \cdot x \geq \sum_{i=1}^k \alpha_i w_i \cdot x = 0 \quad \forall x,$$

and so $w_j \cdot x \geq 0$ for all x which is possible only if $w_j = 0$, a contradiction of (1.1).

The set

$$S_h = \{x \in \mathbb{R}^n \mid w_h(x) \geq 0\}$$

is the intersection of p half spaces and thus is a convex domain having p edges. Let W be the subspace of $\mathbb{R}^n$ spanned by $\{w_i\}_{i=1}^p$. Then $S_h \cap W$ is a $p-1$-simplex with vertices $v_0, v_1, \cdots v_{p-1}$. Note that the functions $w_i \cdot x$ are constant on any subspace orthogonal to W so we just need to define our function on W. For any $z \in \mathbb{Z}^{p-1}$ set

$$w_{h,z}(x) = w_h\left(x - \sum_{i=1}^{p-1} z_i(v_i - v_0)\right). \tag{3.4}$$

Clearly $w_{h,z}$ is a piecewise affine function, nonnegative on the set

$$S_{h,z} = S_h + \sum_{i=1}^{p-1} z_i(v_i - v_0). \tag{3.5}$$

Note that these subsets are disjoint. Let

$$u_h(x) = \sup_{z \in \mathbb{Z}^{p-1}} w_{h,z}(x). \tag{3.6}$$

Then u_h is a piecewise affine function equal to $w_{h,z}$ on $S_{h,z}$. Also note that for a given x, the supremum in (3.6) is taken only over a finite number of z such that $S_{h,z}$ neighbors x. It is clear that

$$|u_h(x)| \leq Ch^\beta \tag{3.7}$$

for some constant C. Moreover we have that

$$\nabla u_h = w_i \tag{3.8}$$

except on the edges of the function u_h where ∇u_h switches from one well to another. To match the boundary condition, we introduce the function η_h where

$$\eta_h(x) = \min(\operatorname{dist}(x, \Gamma_0), h^\beta)/h^\beta. \tag{3.9}$$

We have that $|\eta_h| \leq 1$ and $|\nabla \eta_h| \leq h^{-\beta}$. If $\Gamma_0 = \emptyset$ we take $\eta_h \equiv 1$. We modify u_h by replacing it by $\eta_h u_h$, which we still denote by u_h. If $|\Gamma_0|$ denotes the $(n-1)$-dimensional area of Γ_0 then this modification changes the value of u_h on a domain of volume less than

$$C|\Gamma_0|h^\beta. \tag{3.10}$$

On this domain $\nabla(\eta_h u_h)$ is bounded by $|\nabla \eta_h||u_h| + |\nabla u_h|$, which is bounded by some constant independent of h. To make $u_h \in V_h^0$ we next modify u_h on the simplices where u_h has an edge which intersects the simplex. On this simplex we replace u_h by the affine function which agrees with u_h on the vertices of the simplex. Now the volume of the simplices where this modification occurs is no more than

$$C|\Gamma_0|h^\beta + h \cdot \big((n-1)\text{-dimensional area of the edge of } u_h \text{ due to (3.6)}\big) \tag{3.11}$$

as the edge of u_h cuts one simplex at a time, and any dimension of a simplex is bounded by h. Let $N(h^\beta)$ be the number of $S_{h,z}$ covering Ω. By a scaling argument we have

(3.12)

$$\begin{aligned}(n-1)\text{-dimensional area of the edge of } u_h \text{ due to (3.6)} &\leq CN(h^\beta)(h^\beta)^{p-2} \\ &\leq CN(1)(h^\beta)^{p-2}/(h^\beta)^{p-1} \\ &\leq Ch^{-\beta}.\end{aligned}$$

Hence, by (3.10)–(3.12), we have obtained a function $u_h \in V_h^0$ such that (3.8) holds except on a set S of volume less than

$$Ch^{1-\beta} + C|\Gamma_0|h^\beta \tag{3.13}$$

where, of course, the gradient of u_h is bounded. We also have that (3.7) holds everywhere, and thus

$$\begin{aligned}E(u_h) &= \int_\Omega \phi(\nabla u_h) + \psi(u_h)\,dx \\ &= \int_{\Omega\setminus S} \phi(\nabla u_h) + \int_S \phi(\nabla u_h) + \int_\Omega \psi(u_h) \\ &\leq C(h^{1-\beta} + |\Gamma_0|h^\beta + h^{q\beta}).\end{aligned}$$

So if $|\Gamma_0| > 0$ and $q \geq 1$ we have, if h is assumed to be less than 1,

$$E_h \leq Ch^{\min(1-\beta,\beta)}$$

which has maximum order for $\beta = \frac{1}{2}$ and gives

$$E_h \leq Ch^{\frac{1}{2}}.$$

If $|\Gamma_0| > 0$ and $q < 1$ or $|\Gamma_0| = 0$ then we have

$$E_h \leq Ch^{\min(1-\beta,q\beta)}$$

which has maximum order for $\beta = 1/(q+1)$ and gives

$$E_h \leq Ch^{q/(q+1)}.$$

□

Remark 1. We do not know whether or not these estimates are sharp. For particular results in this direction see [7] and [14].

4. Analysis of oscillations. In what follows we assume that $2 \leq k \leq n+1$ and that the vectors

$$w_i - w_1 \quad \text{are linearly independent.} \tag{4.1}$$

Then we can prove the following theorem.

THEOREM 3 (unique Young measure). *If the vectors $w_i - w_1$ for $i = 2, \cdots, k$ are linearly independent then the vector α which satisfies* (1.1) *is unique. Also, for any minimizing sequence of* (1.4) *bounded in $W^{1,\infty}(\Omega)$ the corresponding Young measure is unique and equals*

$$\nu_x \equiv \nu = \sum_{i=1}^{k} \alpha_i \delta_{w_i},$$

where δ_{w_i} is the Dirac mass at w_i.

Proof. The first part of this theorem is of course well known; however, we give a proof of it for use in later results. If we consider the wells w_i and α to be column vectors, then condition (1.1) can be written as

$$\begin{pmatrix} w_1 & w_2 & \cdots & w_k \\ 1 & 1 & \cdots & 1 \end{pmatrix} \alpha = e_{n+1}, \tag{4.2}$$

where e_{n+1} is the usual $(n+1)$th basis vector in $\mathbb{R}^{n+1}$. Let M be the $n+1 \times k$ matrix on the left-hand side of (4.2). Subtracting the first column of M from the other columns, we get

$$\begin{pmatrix} w_1 & w_2 - w_1 & \cdots & w_k - w_1 \\ 1 & 0 & \cdots & 0 \end{pmatrix}$$

and we see that this matrix has rank k since the vectors $w_i - w_1$ are linearly independent. Thus M has rank k and $M^T M$ is invertible. We can then rewrite (4.2) as $M^T M\alpha = M^T e_{n+1}$ and then solve for α to get

$$\alpha = Ae_{n+1}, \tag{4.3}$$

where $A = (M^TM)^{-1}M^T$. This proves the first part of the theorem.

For the second part, let $\{u_k\}$ be a sequence, as in the proof of Theorem 2, such that

$$|u_k|,\ |\nabla u_k| \le C \quad \text{and} \quad E(u_k) \to 0. \tag{4.4}$$

It is well known (see [2], [8], [15], [25], [26], [28], [31], [32]) that there exists a Young measure ν_x corresponding to this sequence such that

$$\int_\Omega F(x, \nabla u_k(x))\, dx \to \int_\Omega \int_{\mathbb{R}^n} F(x,\lambda)\, d\nu_x(\lambda)\, dx \tag{4.5}$$

for any Carathédory function F. In particular, if we take $F(x,\xi) = \phi(\xi)$ then we have that

$$0 = \lim_{k\to\infty} \int_\Omega \phi(\nabla u_k)\, dx = \int_\Omega \int_{\mathbb{R}^n} \phi(\lambda)\, d\nu_x(\lambda)\, dx.$$

Thus ν_x is supported only on the wells, and we can write

$$\nu_x = \sum_{i=1}^k \beta_i(x)\delta_{w_i}, \tag{4.6}$$

with

$$0 \le \beta_i(x) \le 1 \quad \text{and} \quad \sum_{i=1}^k \beta_i(x) = 1, \tag{4.7}$$

since ν_x is a probability measure. Now from (4.4) we can extract a subsequence, still denoted by u_k, such that

$$u_k \to u \quad \text{uniformly in } \Omega. \tag{4.8}$$

On the other hand, from $E(u_k) \to 0$, and again up to an extracted subsequence, we deduce that

$$\psi(u_k) \to 0 \quad \text{a.e. in } \Omega.$$

Hence, from (4.8) and the continuity of ψ

$$\psi(u) = 0 \quad \text{a.e. in } \Omega$$

and $u = 0$ by (1.2). Then from (4.4) we deduce now that up to an extracted subsequence

$$u_k \rightharpoonup 0 \quad \text{in } W^{1,\infty}(\Omega) \text{ weak-}*$$

and in particular

$$\nabla u_k \rightharpoonup 0 \quad \text{in } L^\infty(\Omega) \text{ weak-}*.$$

So, using (4.5) with $F(x,\xi) = \chi(x)\xi$ where χ is the characteristic function of a measurable set $\omega \subset \Omega$, we obtain

$$\begin{aligned} 0 &= \lim_{k\to\infty} \int_\omega \nabla u_k\, dx \\ &= \int_\omega \int_{\mathbb{R}^n} \lambda\, d\nu_x(\lambda)\, dx = \sum_{i=1}^k w_i \int_\omega \beta_i(x)\, dx. \end{aligned} \tag{4.9}$$

From (4.7) and (4.9) we see that the vector $\{1/|\omega| \int_\omega \beta_i(x)\,dx\}$ satisfies the same conditions as α does in (1.1), but since α is unique, we must have that $\alpha_i = 1/|\omega| \int_\omega \beta_i(x)\,dx$. Since this holds for all ω, we must have $\beta_i(x) = \alpha_i$ almost everywhere by the Lebesgue differentiation theorem. So the Young measure is unique. □

In order to obtain further estimates, the behavior of ϕ near the wells is important. To control it we introduce the function Π defined by

$$\Pi(\xi) = w_i, \quad \text{where } w_i \text{ is the well of smallest index } i \text{ such that} \quad |\xi - w_i| = \min_j |\xi - w_j|. \tag{4.10}$$

The function Π takes only a finite number of values, i.e., the w_i's. Moreover, it is clearly a Borel function so that if $\xi(x)$ is any measurable function, $\Pi(\xi(x))$ will be measurable as well.

From now on we will assume that there are constants λ_1, $\lambda_2 > 0$ and $p > 1$, and $q > 1$ such that

$$\phi(\xi) \geq \lambda_1 |\xi - \Pi\xi|^p = \lambda_1 \min_i |\xi - w_i|^p \quad \forall\, \xi \in \mathbb{R}^n, \tag{4.11}$$

$$\psi(t) \geq \lambda_2 |t|^q \quad \forall\, t \in \mathbb{R}. \tag{4.12}$$

We next prove three lemmas which we use in the rest of the analysis.

LEMMA 1. *For any $B \subset \Omega$ and $r \leq p$, there exists a constant $C = C(B, r, p, \lambda_1)$ such that*

$$\int_B |\nabla v - \Pi \nabla v|^r\, dx \leq C E(v)^{r/p}$$

for all $v \in V_0$.

Proof. Applying Hölder's inequality and (4.11) we have

$$\int_B |\nabla v - \Pi\nabla v|^r\, dx \leq |B|^{(p-r)/p} \left(\int_B |\nabla v - \Pi \nabla v|^p\, dx \right)^{r/p} \leq |B|^{(p-r)/p} \left(\frac{E(v)}{\lambda_1} \right)^{r/p}. \qquad \square$$

LEMMA 2. *If $B \subset \Omega$ is a Lipschitz domain and $r, s > 1$ then there exists a constant $C = C(B, r, s)$ such that for all $v \in V_0$*

$$\int_{\partial B} |v|^r\, ds \leq C \left(\int_B |v|^{(r-1)s'}\, dx \right)^{1/s'} ||v||_{1,s,B},$$

where s' is the conjugate exponent for s (i.e., $1/s + 1/s' = 1$) and

$$||v||_{1,s,B} = \left(\int_B |\nabla v|^s + |v|^s\, dx \right)^{1/s}. \tag{4.13}$$

Proof. By the trace theorem for $W^{1,1}(B)$ (see [1]), there exists a constant C such that

$$\int_{\partial B} |u|\, ds \leq C \int_B |u| + |\nabla u|\, dx.$$

Applying this result to $u = |v|^r$, we have

$$\int_{\partial B} |v|^r\, ds \le C \int_B |v||v|^{r-1} + r|v|^{r-1}|\nabla v|\, dx.$$

Hence by Hölder's inequality we have

$$\int_{\partial B} |v|^r\, ds \le C \left(\int_B |v|^{(r-1)s'}\, dx \right)^{1/s'} ||v||_{1,s,B}. \qquad \square$$

LEMMA 3. *If $B \subset \Omega$ is a Lipschitz domain and $s = \min(p, q)$, then there exists a constant $C = C(B, w_i, \lambda_i, p, q)$ such that*

(4.14)

$$\left| \int_B \Pi \nabla v(x)\, dx \right| \le C \left\{ E(v)^{1/p} + E(v)^{1/(q+s')} \left(1 + E(v)^{s'/q(q+s')} + E(v)^{s'/p(q+s')} \right) \right\}$$

for all $v \in V_0$. (s' is the conjugate of s.)

Proof. First we have that

$$\begin{aligned} \left| \int_B \Pi \nabla v(x)\, dx \right| &\le \int_B |\Pi \nabla v - \nabla v|\, dx + \left| \int_B \nabla v\, dx \right| \\ &\le CE(v)^{1/p} + \left| \int_B \nabla v\, dx \right| \end{aligned} \tag{4.15}$$

by Lemma 1.

Next we use the divergence theorem to get

$$\left| \int_B \nabla v\, dx \right| = \left| \int_{\partial B} vn\, ds \right| \le |\partial B|^{1/r'} \left(\int_{\partial B} |v|^r\, ds \right)^{1/r},$$

where n is the outward normal on ∂B and $|\partial B|$ is the $(n-1)$-dimensional Hausdorff measure of ∂B. Applying Lemma 2 to the last term, we have for any $r > 1$ and $s = \min(p, q)$,

$$\left| \int_B \nabla v\, dx \right| \le |\partial B|^{1/r'} \left(\int_B |v|^{(r-1)s'}\, dx \right)^{1/rs'} ||v||_{1,s,B}^{1/r}. \tag{4.16}$$

Next we choose r such that $(r-1)s' = q$, i.e., $r = (q + s')/s'$, and we obtain

$$\begin{aligned} \left| \int_B \nabla v\, dx \right| &\le C \left(\int_B |v|^q\, dx \right)^{1/(q+s')} ||v||_{1,s,B}^{s'/(q+s')} \\ &\le CE(v)^{1/(q+s')} ||v||_{1,s,B}^{s'/(q+s')}. \end{aligned} \tag{4.17}$$

Moreover, by Hölder's inequality we have

$$\begin{aligned} \int_B |v|^s\, dx &\le |B|^{1-s/q} \left(\int_B |v(x)|^q\, dx \right)^{s/q} \\ &\le CE(v)^{s/q} \end{aligned} \tag{4.18}$$

by (4.12) and

$$\int_B |\nabla v|^s \,dx \le \int_B |\nabla v - \Pi\nabla v|^s \,dx + \int_B |\Pi\nabla v|^s \,dx$$
$$(4.19) \qquad \le C\left(\int_B |\nabla v - \Pi\nabla v|^p \,dx\right)^{s/p} + C$$
$$\le CE(v)^{s/p} + C$$

by (4.11). Combining (4.18) and (4.19) we obtain

$$||v||^s_{1,s,B} \le C\left(E(v)^{s/q} + E(v)^{s/p} + 1\right);$$

hence,

$$(4.20) \qquad ||v||^{s'/(q+s')}_{1,s,B} \le C\left(E(v)^{s'/q(q+s')} + E(v)^{s'/p(q+s')} + 1\right).$$

Then (4.14) follows from (4.15), (4.17), and (4.20). □

Remark 2. In the case of $\Gamma_0 \neq \emptyset$ and where the number of wells is less than $n+1$, Poincaré type inequalities can be used to improve our estimates (see [7]). However, the estimates presented here have the advantage of holding for all cases.

THEOREM 4 (Young measure estimate). *For* $0 < R < \frac{1}{2}\min_{i\neq j}|w_i - w_j|$ *and any Lipschitz domain* $B \subset \Omega$ *let*

$$B^R_i = \{x \in B \mid \nabla v(x) \in B(w_i, R)\}$$
$$B^R_e = B - \bigcup_{i=1}^k B^R_i.$$

If (4.11) *and* (4.12) *hold then there exists a constant* C *with* $C = C(R, B, w_i, \lambda_i, p, q)$ *such that if* $s = \min(p,q)$ *and* $s' = s/(s-1)$ *then*

(4.21)

$$\left||B^R_i| - \alpha_i|B|\right| \le C\left\{E(v)^{1/p} + E(v)^{1/(q+s')}\left(E(v)^{s'/q(q+s')} + E(v)^{s'/p(q+s')} + 1\right)\right\}$$

for $i = 1, \cdots, k$ *and for all* $v \in V_0$.

Proof. First note that

$$B^R_e = \{x \in B : |\nabla v(x) - \Pi\nabla v(x)| \ge R\};$$

thus by the Chebyshev inequality [33] and by Lemma 1 we have

$$(4.22) \qquad |B^R_e| \le \frac{1}{R}\int_B |\nabla v - \Pi\nabla v| \,dx \le CE(v)^{1/p}.$$

By the choice of R, we have $B^R_i \cap B^R_j = \emptyset$ for $i \neq j$ and so

$$(4.23) \qquad \sum_{i=1}^k |B^R_i| = |B| - |B^R_e|.$$

Also we have

$$\sum_{i=1}^{k} w_i|B_i^R| = \sum_{i=1}^{k} \int_{B_i^R} w_i\,dx = \int_{B-B_e^R} \Pi\nabla v\,dx. \tag{4.24}$$

Let

$$\epsilon = \begin{pmatrix} \int_{B-B_e^R} \Pi\nabla v\,dx \\ -|B_e^R| \end{pmatrix}.$$

We see that (4.23) and (4.24) form a set of equations similar to those for α in (1.1) and so using the same matrix as in (4.2), we can write

$$\begin{pmatrix} w_1 & w_2 & \cdots & w_k \\ 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} |B_1^R| \\ \vdots \\ |B_k^R| \end{pmatrix} = |B|e_{n+1} + \epsilon.$$

Thus

$$\begin{pmatrix} |B_1^R| \\ \vdots \\ |B_k^R| \end{pmatrix} = |B|Ae_{n+1} + A\epsilon$$
$$= |B|\alpha + A\epsilon$$

with A as in (4.3) and so

$$\big||B_i^R| - \alpha_i|B|\big| \leq ||A||\,|\epsilon|.$$

The value of $||A||$ depends only on the wells and using Lemma 3 and (4.22) we can estimate $|\epsilon|$ to obtain (4.21). □

Remark 3. The estimate (4.22) can be improved when $E(v)$ is small; indeed by the Chebyshev inequality we have

$$\begin{aligned} |B_e^R| &\leq \frac{1}{R^p} \int_B |\nabla v - \Pi\nabla v|^p\,dx \\ &\leq \frac{1}{\lambda_1 R^p} E(v). \end{aligned} \tag{4.25}$$

We next apply the result of Theorem 4 to a solution u_h of (2.1).

THEOREM 5. *If* (3.1), (4.11), *and* (4.12) *hold then for* $0 < R < \frac{1}{2}\min_{i\neq j}|w_i - w_j|$ *and any Lipschitz domain* $B \subset \Omega$ *let*

$$B_i^R = \{x \in B \mid \nabla u_h(x) \in B(w_i, R)\}$$
$$B_e^R = B - \bigcup_{i=1}^{k} B_i^R.$$

Then if $s = \min(p, q)$ *and* $s' = s/(s-1)$ *there exists a constant* C *such that for* $h < 1$

(4.26) $$\left||B_i^R| - \alpha_i|B|\right| \le Ch^{1/2\min\left(1/p,1/(q+s')\right)} \quad \text{if } \Gamma_0 \ne \emptyset$$

(4.27) $$\left||B_i^R| - \alpha_i|B|\right| \le Ch^{q/(q+1)\min\left(1/p,1/(q+s')\right)} \quad \text{if } \Gamma_0 = \emptyset.$$

Moreover,

(4.28) $$|B_e^R| \le Ch^{1/2} \quad \text{if } \Gamma_0 \ne \emptyset$$

(4.29) $$|B_e^R| \le Ch^{q/(q+1)} \quad \text{if } \Gamma_0 = \emptyset.$$

Proof. From (4.21) and Theorem 2 we deduce that

$$\left||B_i^R| - \alpha_i|B|\right| \le Ch^{\gamma\min\left(1/p,1/(q+s')\right)}$$

and (4.26), (4.27) follow. Equations (4.28) and (4.29) are easy consequences of (4.25) and Theorem 2. □

This gives an estimate for the rate of convergence of the probability for u_h to have its gradient in $B(w_i, R)$ towards α_i. We now estimate at what rate ∇u_h is getting close to the Young measure defined in Theorem 3. For this we evaluate ∇u_h and ν_x against some function $F(x,\xi)$. More precisely, we have the following theorem.

THEOREM 6 (error estimate). *Let $F(x,w) : \Omega \times \mathbb{R}^n \to \mathbb{R}$ be a function satisfying*

(4.30) $$|F(x,\xi) - F(x,\Pi\xi)| \le \rho|\xi - \Pi\xi| \quad \text{for all } \xi \in \mathbb{R}^n.$$

If A is the matrix defined in (4.3), *define the function $G(x)$ by*

(4.31) $$G_i(x) = \sum_{j=1}^{k} A_{ji} F(x, w_j) \quad \text{for } i = 1, \cdots, n$$

and

(4.32) $$\operatorname{err}(v,F) = \left|\int_\Omega \left[F(x,\nabla v(x)) - \sum_{i=1}^{k} \alpha_i F(x,w_i)\right] dx\right|.$$

If $G \in L^{p'}(\Omega)$, $\nabla \cdot G \in L^{q'}(\Omega)$ and $G \in L^{(q+s')/q}(\Gamma_1)$ then there exists a constant C depending on G, such that

(4.33) $$\begin{aligned}\operatorname{err}(v,F) \le C\Big\{ & E(v)^{1/p} + E(v)^{1/q} \\ & + E(v)^{1/(q+s')}\left(E(v)^{s'/q(q+s')} + E(v)^{s'/p(q+s')} + 1\right)\Big\}\end{aligned}$$

where $s = \min(p,q)$ and s' is the conjugate of s as before.

Proof. First we write

(4.34) $$\begin{aligned}\operatorname{err}(v,F) \le & \left|\int_\Omega [F(x,\nabla v(x)) - F(x,\Pi\nabla v(x))]\, dx\right| \\ & + \left|\int_\Omega \left[F(x,\Pi\nabla v(x)) - \sum_{i=1}^{k}\alpha_i F(x,w_i)\right] dx\right| \\ = & \, I_1 + I_2.\end{aligned}$$

Then by (4.30) and Lemma 1 we have

$$\begin{aligned} I_1 &\le \rho \int_\Omega |\nabla v(x) - \Pi\nabla v(x)|\,dx \\ &\le C\rho E(v)^{1/p}. \end{aligned} \tag{4.35}$$

Next for any scalar valued function g we have that

$$\begin{aligned} \int_\Omega (\Pi\nabla v(x)) g(x)\,dx &= \sum_{i=1}^k w_i \int_{\Omega_i} g(x)\,dx \\ \int_\Omega g(x)\,dx &= \sum_{i=1}^k \int_{\Omega_i} g(x)\,dx \end{aligned} \tag{4.36}$$

where $\Omega_i = \{x \in \Omega : \Pi\nabla v(x) = w_i\}$. Let $\beta_i = \int_{\Omega_i} g(x)\,dx$ and then we have that (4.36) is a set of equations for β similar to (1.1), and thus we can write

$$\begin{pmatrix} w_1 & w_2 & \cdots & w_k \\ 1 & 1 & \cdots & 1 \end{pmatrix} \beta = \begin{pmatrix} \int_\Omega (\Pi\nabla v(x)) g(x)\,dx \\ \int_\Omega g(x)\,dx \end{pmatrix}.$$

Using (4.3) we get

$$\begin{aligned} \beta &= A \begin{pmatrix} \int_\Omega (\Pi\nabla v(x)) g(x)\,dx \\ \int_\Omega g(x)\,dx \end{pmatrix} \\ &= \left(\int_\Omega g(x)\,dx\right) \alpha + A \begin{pmatrix} \int_\Omega (\Pi\nabla v(x)) g(x)\,dx \\ 0 \end{pmatrix}. \end{aligned}$$

Writing this component by component we have

$$\beta_i - \alpha_i \int_\Omega g(x)\,dx = \sum_{j=1}^n \int_\Omega A_{ij} (\Pi\nabla v(x))_j g(x)\,dx. \tag{4.37}$$

We use (4.37) with $g(x) = F(x, w_i)$ and note that

$$\beta_i = \int_{\Omega_i} F(x, w_i)\,dx = \int_{\Omega_i} F(x, \Pi\nabla v(x))\,dx.$$

Now we sum the resulting equations from $i = 1$ to k and get

$$\sum_{i=1}^k \beta_i - \sum_{i=1}^k \alpha_i \int_\Omega F(x, w_i)\,dx = \sum_{i=1}^k \sum_{j=1}^n \int_\Omega A_{ij} (\Pi\nabla v(x))_j F(x, w_i)\,dx$$

or, equivalently,

$$\int_\Omega \left[F(x, \Pi\nabla v(x)) - \sum_{i=1}^k \alpha_i F(x, w_i) \right] dx = \int_\Omega (\Pi\nabla v(x)) \cdot G(x)\,dx.$$

Then we have

$$\begin{aligned} I_2 &= \left| \int_\Omega (\Pi\nabla v(x)) \cdot G(x)\,dx \right| \\ &\le \left| \int_\Omega (\Pi\nabla v(x) - \nabla v(x)) \cdot G(x)\,dx \right| + \left| \int_\Omega \nabla v(x) \cdot G(x)\,dx \right| \\ &= I_3 + I_4. \end{aligned} \tag{4.38}$$

Next we estimate I_3 using Hölder's inequality and Lemma 1 to get

$$(4.39)\qquad \begin{aligned} I_3 &\leq ||G||_{L^{p'}} \left(\int_\Omega |\nabla v(x) - \Pi \nabla v(x)|^p \, dx \right)^{1/p} \\ &\leq C||G||_{L^{p'}} E(v)^{1/p}, \end{aligned}$$

where $||G||_{L^{p'}}$ is the $L^{p'}$ norm of the Euclidean norm of G over Ω. Using the divergence theorem we have for any $r > 1$,

$$(4.40)\qquad \begin{aligned} I_4 &= \left| \int_{\Gamma_1} v(s) G(s) \cdot n \, ds - \int_\Omega v(x) \nabla \cdot G(x) \, dx \right| \\ &\leq \int_{\Gamma_1} |v(s) G(s)| \, ds + C||\nabla \cdot G||_{L^{q'}} E(v)^{1/q} \\ &\leq C||G||_{r',\Gamma_1} |v|_{r,\Gamma_1} + C||\nabla \cdot G||_{L^{q'}} E(v)^{1/q}. \end{aligned}$$

(In the derivation of the above inequality we just used Hölder's inequality and (4.12). $||G||_{r',\Gamma_1}$ denotes the $L^{r'}(\Gamma_1)$ norm of G, which is guaranteed to exist.) Using (4.16), (4.17), and Lemma 2 we see that

$$(4.41)\qquad I_4 \leq C||G||_{r',\Gamma_1} \left(\int_\Omega |v(x)|^{(r-1)s'} \, dx \right)^{1/rs'} ||v||_{1,s,\Omega}^{1/r} + ||\nabla \cdot G||_{L^{q'}} E(v)^{1/q}.$$

Arguing as in Lemma 3, (4.17)–(4.20) with $r = (q + s')/s'$ and $r' = (q + s')/q$ we get

$$(4.42)\qquad I_4 \leq C||G||_{r',\Gamma_1} E(v)^{1/(q+s')} \left\{ 1 + E(v)^{s'/q(q+s')} + E(v)^{s'/p(q+s')} \right\} + ||\nabla \cdot G||_{L^{q'}} E(v)^{1/q}.$$

Combining (4.34), (4.35), and (4.37)–(4.42) the result follows. □

THEOREM 7 (convergence estimate). *Assume that* (3.1), (4.11), *and* (4.12) *hold and that the assumptions of the previous theorem hold. Let* u_h *be a solution of* (2.1); *then there exists a constant* C *such that for* $h < 1$

$$(4.43)\qquad \operatorname{err}(u_h, F) \leq C h^{\frac{1}{2} \min(1/p, 1/q)} \qquad \textit{if } \Gamma_0 = \partial\Omega$$

$$(4.44)\qquad \operatorname{err}(u_h, F) \leq C h^{\frac{1}{2} \min\left(1/p, 1/(q+s')\right)} \qquad \textit{if } \emptyset \subsetneq \Gamma_0 \subsetneq \partial\Omega$$

$$(4.45)\qquad \operatorname{err}(u_h, F) \leq C h^{q/(q+1) \min\left(1/p, 1/(q+s')\right)} \qquad \textit{if } \Gamma_0 = \emptyset.$$

Proof. When $\Gamma_0 = \partial\Omega$ we have $\Gamma_1 = \emptyset$ and so in (4.42) the terms involving Γ_1 are zero. Thus, we have

$$(4.46)\qquad \operatorname{err}(v, F) \leq C \left\{ E(v)^{1/p} + E(v)^{1/q} \right\},$$

and the error estimate (4.43) follows from Theorem 2. Next we consider the cases when $\Gamma_0 \neq \partial\Omega$. From (4.33) we deduce that

$$\operatorname{err}(u_h, F) \leq C E(u_h)^{\gamma \min\left(1/p, 1/(q+s')\right)}$$

and (4.44), (4.45) follow from Theorem 2. □

5. Numerical example. For a numerical example we let the energy be

$$E(u) = \int_{\Omega} \phi(\nabla u(x)) + u(x)^2 \, dx$$

where

$$\Omega = [0,1]^2$$

and

$$\phi(\xi) = |\xi - w_1|^2 |\xi - w_2|^2$$

with $w_1 = (-1, 1)$ and $w_2 = (1, -1)$.

For the numerical calculation we use a uniform mesh of triangles on Ω of size $h = 1/N$ formed by dividing Ω into uniform squares of size $h \times h$ and dividing each square into two triangles by cutting along the $(1, -1)$ direction. We start with a random initial guess near $u = 0$ and then use an iterative method to update the value of u to decrease the energy (see [9]). Figure 1 shows the resulting approximations for meshes of size $h = 1/30$ and $h = 1/50$. For other calculations of this type see [9], [11]–[13], [30].

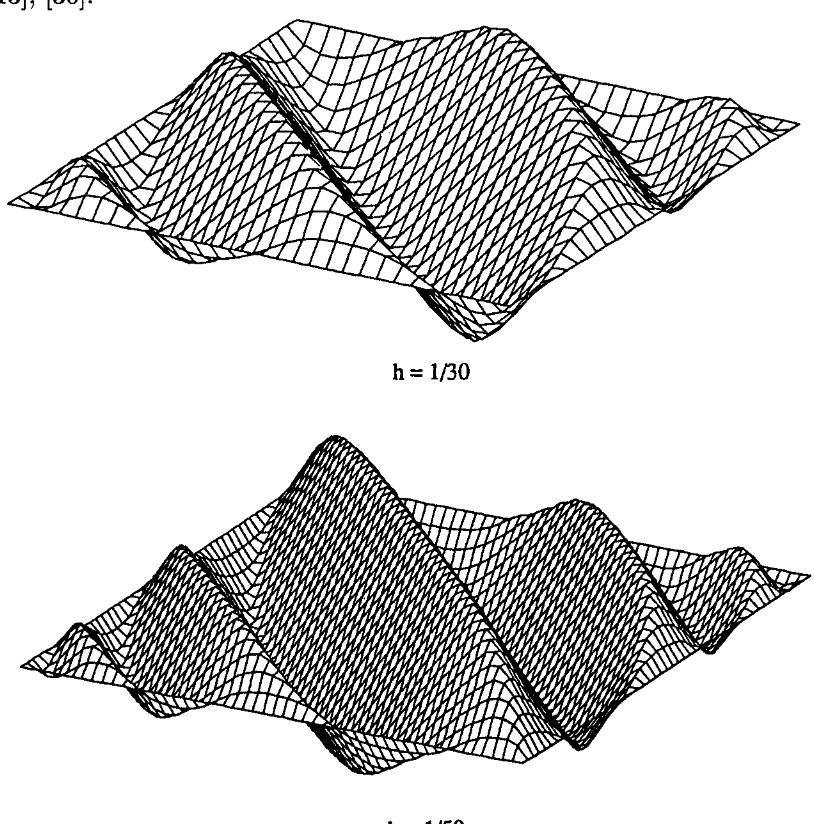

FIG. 1. *Computational results for $h = 1/30$ and $h = 1/50$.*

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