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OF A VARIATIONAL PROBLEM
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NUMERICAL APPROXIMATION OF THE SOLUTION OF A VARIATIONAL PROBLEM WITH A DOUBLE WELL POTENTIAL*

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Abstract. Variational problems with a double well potential are not lower semicontinuous and can fail to attain a minimum value. Rather, minimizing sequences can have oscillations and converge only in the weak topology.

Such functionals arise in the description of equilibria of crystals or other ordered materials. Stable configurations for solid crystals which have symmetry-related (martensitic) energy wells have a fine-scale microstructure which can be related to the oscillations which energy minimizing sequences for the bulk energy exhibit. We give an analysis of approximation methods for variational problems with a double well potential to give a rigorous justification for the use of such numerical methods to model the behavior of this class of solid crystals.

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

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

1. Introduction. Variational problems which are not convex can fail to attain a minimum value. For such problems, the minimizing sequences can have oscillations which converge weakly, but which do not converge strongly enough to evaluate the limit functional.

Such functionals arise in the description of equilibria of crystals or other ordered states. The free energy density for a solid crystal which has symmetry-related (martensitic) variants or exhibits a solid-solid phase transition will have multiple, distinct energy wells [1], [2], [7]–[15]. Such materials often have a fine-scale microstructure [4] which has recently been related to the oscillations which energy minimizing sequences for the bulk energy exhibit [1], [2], [5], [13]–[15]. Even though this microstructure may average to a smooth deformation, the smooth deformation is generally not in equilibrium.

The functionals used to model these materials are not weakly lower semicontinuous, and therefore a deformation attaining minimum energy does not exist for many prescribed boundary displacements. However, a description of the solution can be obtained by using the concept of the Young measure or parametrized measure, which is more general than the averaged deformation, to capture the information in minimizing sequences of deformations [1], [2], [5], [13]–[15].

Recent numerical experiments for two and three dimensional solids have exhibited microstructure on the scale of the grid [6], [7], [17]. In this paper, we present the analysis of the numerical approximation for a one-dimensional model.

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2. Definitions and Statement of Main Results. For Lebesgue measurable sets $\Gamma \subset (0, 1)$, we denote by $|\Gamma|$ the Lebesgue measure of Γ . We denote by L^2 with norm $|g|_{L^2}$ the usual space of Lebesgue measurable functions on $(0, 1)$ such that

$$|g|_{L^2} \equiv \left[\int_0^1 g(x)^2 dx \right]^{1/2} < \infty.$$

We consider the functional

$$(2.1) \quad \mathcal{E}(v) = \int_0^1 [\phi(v'(y)) + (v(y) - f(y))^2] dy,$$

where $\phi(s)$ is a real-valued continuous function of one variable such that for $s_L < \bar{s} < s_U$, $0 < \bar{\alpha} < (s_U - s_L)/2$, and $\lambda_1, \lambda_2 > 0$ we have

$$(2.2) \quad \begin{aligned} \phi(s) &> \phi(s_L) = \phi(s_U) = 0, & \text{for } s \neq s_L, s_U, \\ \phi(s) &\geq \lambda_1(s - s_L)^2, & \text{for } |s - s_L| \leq \bar{\alpha}, \\ \phi(s) &\geq \lambda_1(s - s_U)^2, & \text{for } |s - s_U| \leq \bar{\alpha}, \\ \phi(s) &\geq \lambda_1 \bar{\alpha}^2, & \text{for } s_L + \bar{\alpha} < s < s_U - \bar{\alpha}, \\ \phi(s) &\geq \lambda_2(s - \bar{s})^2, & \text{for } s < s_L - \bar{\alpha} \text{ or } s > s_U + \bar{\alpha}, \end{aligned}$$

and where

$$f(y) = \bar{s}y + b.$$

The functional $\mathcal{E}$ is well-defined for $v \in H^1$ where

$$H^1 = \{v \in L^2 : v' \in L^2\}.$$

We shall give results for the minimization of the functional $\mathcal{E}$ over finite element spaces $\mathcal{M}_h$. To define $\mathcal{M}_h$, let $h = 1/M$ for some $M \in \mathbb{N}$, $x_i = ih$ for $i = 0, \dots, M$ and $I_i = (x_{i-1}, x_i)$ for $i = 1, \dots, M$. Let $\mathcal{M}_h$ be the space of piecewise linear, continuous functions or

$$\mathcal{M}_h \equiv \{v \in C(0, 1) : v|_{I_i} \text{ is linear for } i = 1, \dots, M\}.$$

Let $u_h \in \mathcal{M}_h$ satisfy

$$\mathcal{E}(u_h) = \min_{v_h \in \mathcal{M}_h} \mathcal{E}(v_h) \equiv E_h.$$

We shall show in section 3 that $E_h \rightarrow 0$ as $h \rightarrow 0$. However, we note that there does not exist $u \in H^1$ such that $\mathcal{E}(u) = 0$. (If $\mathcal{E}(u) = 0$, then $u(x) = f(x)$ a.e. However, $\phi(f') = \phi(\bar{s}) > 0$.) Further, $u'_h(x)$ does not converge as $h \rightarrow 0$ in any L^p space. Rather, we shall show that $u'_h(x)$ and nonlinear functions of $u'_h(x)$ converge weakly. We show below that the topology of this convergence is metrizable since it is convergence in the weak-*

topology of a suitable Banach space [16], and we give an error estimate for this convergence in an appropriate metric.

We define a family of parametrized measures on the Borel sets A of $\mathbb{R}$ by

$$m_{x,\epsilon,h}(A) = \frac{|\{y \in B_\epsilon(x) : u'_h(y) \in A\}|}{|B_\epsilon(x)|},$$

where $0 < \epsilon < 1$ and $B_\epsilon(x) = (x - \epsilon, x + \epsilon) \cap (0, 1)$. For $0 < \alpha \leq \bar{\alpha}$ we define the open sets

$$\Omega^{L,\alpha} = (s_L - \alpha, s_L + \alpha), \quad \Omega^{U,\alpha} = (s_U - \alpha, s_U + \alpha), \quad \Omega^{C,\alpha} = \mathbb{R} - \Omega^{L,\alpha} - \Omega^{U,\alpha}.$$

In what follows, c_i for $i = 1, 2, \dots$ will denote positive constants which are independent of x, ϵ, h , and α ; and θ_i for $i = 1, 2, \dots$ will denote constants which are independent of x, ϵ, h , and α and such that $-1 \leq \theta_i \leq 1$.

In the jargon of the calculus of variations, the measure

$$\nu_x \equiv \gamma \delta_{s_L} + (1 - \gamma) \delta_{s_U}, \quad 0 < x < 1,$$

where $\gamma = (s_U - \bar{s}) / (s_U - s_L)$ and $\delta_{\hat{s}}$ is the Dirac delta function with unit mass concentrated at $\hat{s}$ for $\hat{s} = s_L, s_U$, is the unique Young measure associated with minimizing (2.1). The approximate solutions $u'_h(x)$ oscillate between the energy wells at $s = s_L$ and $s = s_U$. Our first theorem gives a rate of convergence for the convergence of the measure $m_{x,\epsilon,h}$ to the measure $\nu_x \equiv \gamma \delta_{s_L} + (1 - \gamma) \delta_{s_U}$.

THEOREM 1. *For $h^{1/2} \leq \alpha \leq \bar{\alpha}$ there exists a positive constant, c_1 , such that*

$$(2.3) \quad \begin{aligned} |m_{x,\epsilon,h}(\Omega^{L,\alpha}) - \gamma| &\leq \frac{c_1 h^{1/2}}{\epsilon}, \\ |m_{x,\epsilon,h}(\Omega^{U,\alpha}) - (1 - \gamma)| &\leq \frac{c_1 h^{1/2}}{\epsilon}, \\ |m_{x,\epsilon,h}(\Omega^{C,\alpha})| &\leq \frac{c_1 h^2}{\alpha^2 \epsilon}. \end{aligned}$$

Our next result gives a rate of convergence for weak limits of nonlinear functions of $u'_h(x)$.

THEOREM 2. *Assume that for $F(y, s) : (0, 1) \times \mathbb{R} \rightarrow \mathbb{R}$ there exists $\rho > 0$ such that*

$$(2.4) \quad |F(y, s) - F(y, s_L)| \leq \rho |s - s_L| \quad \text{for } |s - s_L| \leq \bar{\alpha}, \quad y \in (0, 1),$$

$$(2.5) \quad |F(y, s) - F(y, s_U)| \leq \rho |s - s_U| \quad \text{for } |s - s_U| \leq \bar{\alpha}, \quad y \in (0, 1).$$

Further, assume that

$$(2.6) \quad |F(y, s)| \leq c_2 \quad \text{for } s_L - \bar{\alpha} \leq s \leq s_U + \bar{\alpha}, \quad y \in (0, 1),$$

$$(2.7) \quad |F(y, s)| \leq c_3 \phi(s) \quad \text{for } s \leq s_L - \bar{\alpha} \quad \text{or} \quad s \geq s_U + \bar{\alpha}, \quad y \in (0, 1),$$

and

$$(2.8) \quad \left| \frac{\partial F}{\partial y}(y, s) \right| \leq c_4 \quad \text{for } s \in \mathbb{R}, \quad y \in (0, 1).$$

Then there exists a positive constant c_5 such that

$$(2.9) \quad \left| \int_0^1 F(x, u'_h(x)) dx - \int_0^1 [\gamma F(x, s_L) + (1 - \gamma) F(x, s_U)] dx \right| \leq c_5(1 + c_4 + \rho)h^{1/4}.$$

It follows from Lemma 4 that $u'_h(x) \in \Omega^{L, \bar{\alpha}} \cap \Omega^{U, \bar{\alpha}}$ for h sufficiently small. Thus, $F(y, s)$ need only be defined for s in the interval $[s_L - \bar{\alpha}, s_U + \bar{\alpha}]$ and the hypothesis (2.7) can be eliminated. However, since our argument to obtain uniform bounds for $u'_h(x)$ in Lemma 4 does not generalize to three space dimensions, we have retained hypothesis (2.7) in Theorem 2 and we have not utilized the uniform bounds for $u'_h(x)$ in the proof of Theorem 2. Further, condition (2.8) in Theorem 2 can be weakened to allow a finite number of discontinuities in y for $F(y, s)$ by a straightforward modification of our proof.

We can define a metric for the weak-* topology on compact subsets of the dual of $C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])$, $C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])^*$, by, for example [16]

$$(2.10) \quad d(L_1, L_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{|\langle L_1 - L_2, F_{m,n} \rangle|}{(m+1)(n+1)2^m 2^n}$$

for $L_1, L_2 \in C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])^*$ where

$$F_{m,n}(x, s) = \cos(m\pi x) \cos(n\pi \mathcal{S}(s)) \in C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])$$

and

$$\mathcal{S}(s) = (s_L - \bar{\alpha}) + (s_U - s_L + 2\bar{\alpha})s.$$

We identify (for h sufficiently small) with $u'_h(x)$ the functional $L_{u'_h(x)} \in C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])^*$ where

$$\langle L_{u'_h(x)}, F \rangle \equiv \int_0^1 F(x, u'_h(x)) dx$$

and we identify with $\nu_x \equiv \gamma \delta_{s_L} + (1 - \gamma) \delta_{s_U}$ the functional $L_{\nu_x} \in C([0, 1] \times [s_L - \bar{\alpha}, s_U + \bar{\alpha}])^*$ where

$$\langle L_{\nu_x}, F \rangle \equiv \int_0^1 [\gamma F(x, s_L) + (1 - \gamma) F(x, s_U)] dx.$$

We can prove the following error estimate for the convergence of $u'_h(x)$ to ν_x .

THEOREM 3. We have for h sufficiently small that

$$(2.11) \quad d(L_{u'_h(x)}, L_{\nu_x}) \leq 4c_5[1 + \pi(1 + s_U - s_L + 2\bar{\alpha})]h^{1/4}.$$

Proof of Theorem 3. It follows from Theorem 3 that

$$\begin{aligned} d(L_{u'_h(x)}, L_{\nu_x}) &\leq c_5 \left[\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{1 + m\pi + n\pi(s_U - s_L + 2\bar{\alpha})}{(m+1)(n+1)2^m 2^n} \right] h^{1/4} \\ &\leq 4c_5[1 + \pi + \pi(s_U - s_L + 2\bar{\alpha})]h^{1/4}. \end{aligned}$$

□

Our true interest, based on the mechanical problem of deforming a crystal, lies in minimizing the functional

$$\int_0^1 \phi(v') dy$$

subject to the Dirichlet boundary conditions

$$v(0) = f(0) \text{ and } v(1) = f(1).$$

Whenever $f(x)$ is an affine function with $s_L \leq s \leq s_U$, it turns out that [3]

$$\inf_{v \in \mathcal{V}} \int_0^1 \phi(v') dy = \inf_{v \in H^1} \mathcal{E}(v)$$

where

$$\mathcal{V} \equiv \{v \in H^1 : v(0) = f(0) \text{ and } v(1) = f(1)\}.$$

Now the variational principal

$$(2.12) \quad \inf_{v \in \mathcal{V}} \int_0^1 \phi(v') dy$$

may have many solutions, both in the sense that the limit of a minimizing sequence need not be unique and in the sense that the possible Young measure need not be unique. However, the simplest limit deformation in this case is affine and the unconstrained problem

$$(2.13) \quad \inf_{v \in H^1} \mathcal{E}(v)$$

has this as its unique limit deformation. Moreover, in our present situation, the Young measure so generated is also unique. Since the corresponding multi-dimensional Dirichlet

problem gives a unique Young measure for appropriate affine boundary conditions [2], we utilize the term

$$\int_0^1 (v(y) - f(y))^2 dy$$

in the definition of $\mathcal{E}(v)$ to select a unique Young measure analogous to the selection of a unique Young measure for multi-dimensional problems by appropriate Dirichlet boundary conditions. Thus, we consider (2.1) in place of the more traditional variational integral.

Our results remain valid when the wells of $\phi(s)$ are at different heights and when we consider the Dirichlet problem to minimize $\mathcal{E}(v)$ over $\mathcal{V}$. If $\hat{\phi}(s) = \phi(s) + l(s)$ where $l(s)$ is an affine function and

$$\hat{\mathcal{E}}(v) = \int_0^1 [\hat{\phi}(v'(y)) + (v(y) - f(y))^2] dy,$$

then for $v \in \mathcal{V}$,

$$(2.14) \quad \hat{\mathcal{E}}(v) = \mathcal{E}(v) + l(v(1) - v(0)) = \mathcal{E}(v) + l(f(1) - f(0)).$$

We are interested in choosing the affine function $l(s)$ to render equal the heights of the wells of $\hat{\phi}(s)$. The numerical approximation for the Dirichlet problem is to determine $u_h \in \mathcal{M}_h \cap \mathcal{V}$ so that

$$(2.15) \quad \mathcal{E}(u_h) = \min_{v_h \in \mathcal{M}_h \cap \mathcal{V}} \mathcal{E}(v_h) \equiv \hat{E}_h.$$

By (2.14), we have that u_h also satisfies

$$(2.16) \quad \hat{\mathcal{E}}(u_h) = \min_{v_h \in \mathcal{M}_h \cap \mathcal{V}} \hat{\mathcal{E}}(v_h),$$

for any affine function $l(s)$. Our techniques will allow us to prove the following theorem for the Dirichlet problem.

THEOREM 4. *Suppose that $\phi(s) + l(s)$ has two minimum energy wells of equal height and satisfies the conditions (2.2) for an affine function $l(s)$. Then the estimates (2.3), (2.9), and (2.11) of Theorems 1–3 hold for the Dirichlet approximation (2.15).*

3. Proofs of the Theorems. We note that $v_h(x) + f(x) \in \mathcal{M}_h$ if $v_h \in \mathcal{M}_h$ and that

$$\mathcal{E}(v + f) = \int_0^1 [\phi(v'(y) + \bar{s}) + v(y)^2] dy.$$

Further, $\phi(s + \bar{s})$ satisfies (2.2) if $\phi(s)$ satisfies (2.2). Thus, we may assume in the following without loss of generality that $f(y) \equiv 0$, so $\bar{s} = 0$. Hence,

$$s_L \leq 0 \leq s_U$$

and

$$\gamma s_L + (1 - \gamma) s_U = 0.$$

LEMMA 1. *There exists a positive constant, c_6 , such that*

$$(3.1) \quad E_h \leq c_6 h^2.$$

Proof. Define $v_h(x) \in \mathcal{M}_h$ by $v_h(0) = 0$ and for $k = 0, \dots, M-1$,

$$v_h(x_{k+1}) = \begin{cases} v_h(x_k) + h s_L & \text{if } |v_h(x_k) + h s_L| \leq |v_h(x_k) + h s_U|, \\ v_h(x_k) + h s_U & \text{if } |v_h(x_k) + h s_L| > |v_h(x_k) + h s_U|. \end{cases}$$

It follows that $\phi(v'_h(x)) \equiv 0$.

We shall show that

$$v_h(x) \leq (s_U - s_L)h/2 \quad \text{for } x \in (0, 1).$$

Let N be a positive integer such that

$$v_h(x_N) \geq v_h(x_k) \quad \text{for } k = 0, \dots, M.$$

If $x_N = 0$, then $v_h(x) \leq 0$ for all $x \in (0, 1)$. So, we may assume that $x_N > 0$. Now

$$|v_h(x_{N-1}) + h s_L| > |v_h(x_{N-1}) + h s_U|$$

and

$$v_h(x_N) = v_h(x_{N-1}) + s_U h.$$

There are now two cases. First, if $v_h(x_N) \leq 0$, then $v_h(x_N) \leq (s_U - s_L)h/2$ since $(s_U - s_L)h/2 \geq 0$. Second, if $v_h(x_N) > 0$, then $v_h(x_{N-1}) + h s_L \leq 0$ and

$$v_h(x_{N-1}) + s_U h < -v_h(x_{N-1}) - s_L h.$$

So, in this case $v_h(x_{N-1}) < (-s_L - s_U)h/2$, and $v_h(x_N) < (s_U - s_L)h/2$. Thus,

$$v_h(x) \leq (s_U - s_L)h/2 \quad \text{for } x \in (0, 1).$$

The proof that

$$-v_h(x) \leq (s_U - s_L)h/2 \quad \text{for } x \in (0, 1)$$

is similar. Thus, we have shown that

$$(3.2) \quad |v_h(x)| \leq (s_U - s_L)h/2 \quad \text{for } x \in (0, 1).$$

Hence, it follows that

$$E_h \leq \mathcal{E}(v_h) \leq \max |v_h|^2 \leq \frac{(s_U - s_L)^2 h^2}{4}. \quad \square$$

For the Dirichlet problem, it is necessary to estimate

$$\min_{v_h \in \mathcal{M}_h \cap \mathcal{V}} \mathcal{E}(v_h) \equiv \hat{E}_h.$$

We have in this case the following lemma.

LEMMA 2. Assume that there exists $\lambda_3 \geq \lambda_1 > 0$ such that

$$(3.3) \quad \begin{aligned} \phi(s_L + \alpha) &\leq \lambda_3 \alpha^2, \\ \phi(s_U + \alpha) &\leq \lambda_3 \alpha^2, \end{aligned}$$

for $|\alpha| \leq \bar{\alpha}$. Then there exists a positive constant, c_7 , such that

$$\min_{v_h \in \mathcal{M}_h \cap \mathcal{V}} \mathcal{E}(v_h) \leq c_7 h^2.$$

Proof. We define $w_h \in \mathcal{M}_h \cap \mathcal{V}$ by

$$w_h(x) = v_h(x) - v_h(1)x$$

where $v_h(x) \in \mathcal{M}_h$ is the function defined in Lemma 1. Now by (3.2),

$$\begin{aligned} \int_0^1 w_h(x)^2 dx &\leq 2 \int_0^1 [v_h(x)^2 + (v_h(x) - w_h(x))^2] dx \\ &\leq (s_U - s_L)^2 h^2. \end{aligned}$$

Further,

$$\begin{aligned} \phi(w_h'(x)) &\leq \lambda_3 v_h(1)^2 \\ &\leq \frac{\lambda_3}{4} (s_U - s_L)^2 h^2, \quad x \in (0, 1). \end{aligned}$$

Thus,

$$\min_{v_h \in \mathcal{M}_h \cap \mathcal{V}} \mathcal{E}(v_h) \leq \left(\frac{\lambda_3}{4} + 1\right) (s_U - s_L)^2 h^2. \quad \square$$

It follows from the Sobolev inequalities that $u_h \rightarrow 0$ uniformly. To see this, note that from (2.2)

$$s^2 \leq \lambda_2^{-1} \phi(s) + (s_L - \bar{\alpha})^2 + (s_U + \bar{\alpha})^2.$$

So,

$$\int_0^1 u_h'(x)^2 dx \leq \lambda_2^{-1} E_h + (s_L - \bar{\alpha})^2 + (s_U + \bar{\alpha})^2.$$

Thus, there exists c_8 such that

$$|u_h'|_{L^2} \leq c_8.$$

LEMMA 3. There exists a positive constant, c_9 , such that

$$(3.4) \quad \delta_h \equiv \sup_{x \in (0,1)} |u_h(x)| \leq c_9 h^{1/2}.$$

Proof. By the Cauchy-Schwarz inequality, for $x, y \in (0, 1)$,

$$\begin{aligned} u_h(x)^2 &= u_h(y)^2 + 2 \int_y^x u_h(w) u'_h(w) dw \\ &\leq u_h(y)^2 + 2 |u_h|_{L^2} |u'_h|_{L^2} \\ &\leq u_h(y)^2 + 2c_8 |u_h|_{L^2}. \end{aligned}$$

Next, we integrate with respect to y to obtain

$$\begin{aligned} u_h(x)^2 &\leq |u_h|_{L^2}^2 + 2c_8 |u_h|_{L^2} \\ &\leq E_h + 2c_8 E_h^{1/2}. \end{aligned}$$

The result now follows from Lemma 1. $\square$

The following lemma gives bounds for $u'_h(x)$.

LEMMA 4. *We have the bound*

$$\min(s_L - \sqrt{\frac{c_6}{\lambda_1}} h^{1/2}, -\sqrt{\frac{c_6}{\lambda_2}} h^{1/2}) \leq u'_h(x) \leq \max(s_U + \sqrt{\frac{c_6}{\lambda_1}} h^{1/2}, \sqrt{\frac{c_6}{\lambda_2}} h^{1/2}),$$

for $x \in (0, 1)$. Further, we have that

$$u'_h(x) \in \Omega^{L, \alpha} \cap \Omega^{U, \alpha}, \quad x \in (0, 1), \quad \alpha \leq \bar{\alpha},$$

for $h < \min(\alpha^2 \lambda_1 c_6^{-1}, (s_L - \bar{\alpha})^2 \lambda_2 c_6^{-1}, (s_U + \bar{\alpha})^2 \lambda_2 c_6^{-1})$.

Proof. For $v_h \in \mathcal{M}_h$, we can write

$$\begin{aligned} \mathcal{E}(v_h) &= \int_0^1 \phi(v'_h) + v_h^2 dx \\ &= \sum_{k=1}^M \int_{x_{k-1}}^{x_k} \phi(v'_h) dx + \sum_{k=1}^M \int_{x_{k-1}}^{x_k} v_h^2 dx. \end{aligned}$$

The quantities in the sum are positive and from Lemma 1 we know that for the minimizing u_h , $\mathcal{E}(u_h) \leq c_6 h^2$, so we have $h\phi(u'_h|_{I_k}) \leq c_6 h^2$. Let $s_k = u'_h|_{I_k}$. From (2.2) there are four cases for s_k :

- (A) $|s_k - s_L| \leq \bar{\alpha} \implies \phi(s_k) \geq \lambda_1 |s_k - s_L|^2 \implies \lambda_1 |s_k - s_L|^2 h \leq c_6 h^2,$
- (B) $|s_k - s_U| \leq \bar{\alpha} \implies \phi(s_k) \geq \lambda_1 |s_k - s_U|^2 \implies \lambda_1 |s_k - s_U|^2 h \leq c_6 h^2,$
- (C) $s_L + \bar{\alpha} < s_k < s_U - \bar{\alpha} \implies \phi(s_k) \geq \lambda_1 \bar{\alpha}^2 \implies \lambda_1 \bar{\alpha}^2 h \leq c_6 h^2,$
- (D) $s_k < s_L - \bar{\alpha} \text{ or } s_k > s_U + \bar{\alpha} \implies \phi(s_k) \geq \lambda_2 s_k^2 \implies \lambda_2 s_k^2 h \leq c_6 h^2.$

The first part of Lemma 4 now follows from (A), (B), and (D), and the second part of Lemma 4 follows from (A), (B), (C), and (D). $\square$

We now turn to estimates for the parametrized measure, $m_{x,\epsilon,h}$.

Proof of Theorem 1. For $0 < \alpha \leq \bar{\alpha}$, let

$$\Gamma_h^\alpha = \{y \in (0, 1) : u'_h(y) \in \Omega^{C,\alpha}\}.$$

Then by (2.2),

$$(3.5) \quad \lambda_1 |\Gamma_h^\alpha| \alpha^2 \leq E_h.$$

For $0 < \alpha \leq \bar{\alpha}$, let

$$\begin{aligned} \Lambda_{x,\epsilon,h}^{L,\alpha} &= \{y \in B_\epsilon(x) : u'_h(y) \in \Omega^{L,\alpha}\}, \\ \Lambda_{x,\epsilon,h}^{U,\alpha} &= \{y \in B_\epsilon(x) : u'_h(y) \in \Omega^{U,\alpha}\}, \\ \Lambda_{x,\epsilon,h}^{C,\alpha} &= \{y \in B_\epsilon(x) : u'_h(y) \in \Omega^{C,\alpha}\}. \end{aligned}$$

Also, let $x_-(\epsilon) = \max(0, x - \epsilon)$ and $x_+(\epsilon) = \min(1, x + \epsilon)$. Then

$$\begin{aligned} 2\delta_h &\geq |u_h(x_+(\epsilon)) - u_h(x_-(\epsilon))| \\ &= \left| \int_{x_-(\epsilon)}^{x_+(\epsilon)} u'_h(y) dy \right| \\ &= \left| \int_{\Lambda_{x,\epsilon,h}^{L,\alpha}} u'_h(y) dy + \int_{\Lambda_{x,\epsilon,h}^{U,\alpha}} u'_h(y) dy + \int_{\Lambda_{x,\epsilon,h}^{C,\alpha}} u'_h(y) dy \right|. \end{aligned}$$

Now

$$\begin{aligned} \left| \int_{\Lambda_{x,\epsilon,h}^{L,\alpha}} u'_h(y) dy - s_L |\Lambda_{x,\epsilon,h}^{L,\alpha}| \right| &\leq \alpha |\Lambda_{x,\epsilon,h}^{L,\alpha}|, \\ \left| \int_{\Lambda_{x,\epsilon,h}^{U,\alpha}} u'_h(y) dy - s_U |\Lambda_{x,\epsilon,h}^{U,\alpha}| \right| &\leq \alpha |\Lambda_{x,\epsilon,h}^{U,\alpha}|, \\ \left| \int_{\Lambda_{x,\epsilon,h}^{C,\alpha}} u'_h(y) dy \right| &\leq |\Lambda_{x,\epsilon,h}^{C,\alpha}|^{1/2} |u'_h|_{L^2}. \end{aligned}$$

So,

$$\begin{aligned} &\left| s_U |\Lambda_{x,\epsilon,h}^{U,\alpha}| + s_L |\Lambda_{x,\epsilon,h}^{L,\alpha}| \right| \\ &\leq 2\delta_h + \alpha (|\Lambda_{x,\epsilon,h}^{U,\alpha}| + |\Lambda_{x,\epsilon,h}^{L,\alpha}|) + c_8 |\Lambda_{x,\epsilon,h}^{C,\alpha}|^{1/2}. \end{aligned}$$

Also, $\Lambda_{x,\epsilon,h}^{C,\alpha} \subset \Gamma_h^\alpha$, so by (3.5)

$$|\Lambda_{x,\epsilon,h}^{C,\alpha}| \leq E_h/(\alpha^2 \lambda_1).$$

Thus,

$$(3.6) \quad \begin{aligned} |s_L m_{x,\epsilon,h}(\Omega^{L,\alpha}) + s_U m_{x,\epsilon,h}(\Omega^{U,\alpha})| &\leq \frac{2\delta_h}{\epsilon} + \alpha + \frac{E_h^{1/2} c_8}{\alpha \lambda_1^{1/2} \epsilon}, \\ m_{x,\epsilon,h}(\Omega^{L,\alpha}) + m_{x,\epsilon,h}(\Omega^{U,\alpha}) + m_{x,\epsilon,h}(\Omega^{C,\alpha}) &= 1, \\ |m_{x,\epsilon,h}(\Omega^{C,\alpha})| &\leq \frac{E_h}{\alpha^2 \lambda_1 \epsilon}. \end{aligned}$$

Hence, for $\gamma = s_U/(s_U - s_L)$,

$$|m_{x,\epsilon,h}(\Omega^{U,\alpha}) - (1 - \gamma)| \leq \frac{1}{s_U - s_L} \left[\frac{2\delta_h}{\epsilon} + \alpha + \frac{E_h^{1/2} c_8}{\alpha \lambda_1^{1/2} \epsilon} \right] + \frac{(1 - \gamma)E_h}{\alpha^2 \lambda_1 \epsilon}.$$

Now for $0 < \beta \leq \alpha \leq \bar{\alpha}$,

$$\begin{aligned} m_{x,\epsilon,h}(\Omega^{U,\alpha}) &= m_{x,\epsilon,h}(\Omega^{U,\alpha} - \Omega^{U,\beta}) + m_{x,\epsilon,h}(\Omega^{U,\beta}) \\ &= \theta_1 m_{x,\epsilon,h}(\Omega^{C,\beta}) + m_{x,\epsilon,h}(\Omega^{U,\beta}) \end{aligned}$$

where $-1 \leq \theta_1 \leq 1$ since $\Omega^{U,\alpha} - \Omega^{U,\beta} \subset \Omega^{C,\beta}$. So

$$|m_{x,\epsilon,h}(\Omega^{U,\alpha}) - (1 - \gamma)| \leq \frac{1}{s_U - s_L} \left[\frac{2\delta_h}{\epsilon} + \beta + \frac{E_h^{1/2} c_8}{\beta \lambda_1^{1/2} \epsilon} \right] + \frac{(\gamma + 1)E_h}{\beta^2 \lambda_1 \epsilon}.$$

Then for $\beta = h^{1/2}$ and $\bar{\alpha} \geq \alpha \geq h^{1/2}$ we obtain

$$(3.7) \quad |m_{x,\epsilon,h}(\Omega^{U,\alpha}) - (1 - \gamma)| \leq \frac{1}{s_U - s_L} \left[\frac{2c_9 h^{1/2}}{\epsilon} + h^{1/2} + \frac{c_6^{1/2} c_8 h^{1/2}}{\lambda_1^{1/2} \epsilon} \right] + \frac{(2 - \gamma)c_6 h}{\lambda_1 \epsilon}.$$

A similar result holds for $m_{x,\epsilon,h}(\Omega^{L,\alpha})$. Theorem 1 now follows from (3.6) and (3.7). $\square$

The proof of Theorem 2 will follow from the following lemma.

LEMMA 5. Assume that conditions (2.4)-(2.7) hold. Then there exists $c_{10} > 0$ such that

$$(3.8) \quad \begin{aligned} \left| \int_0^1 \left[\frac{1}{|B_\epsilon(y)|} \int_{B_\epsilon(y)} F(y, u'_h(z)) dz \right] dy - \int_0^1 [\gamma F(y, s_L) + (1 - \gamma)F(y, s_U)] dy \right| \\ \leq c_{10} \left(\frac{h^2}{\alpha^2 \epsilon} + \frac{h^{1/2}}{\epsilon} \right) + 2\rho\alpha. \end{aligned}$$

Proof. Now

$$\frac{1}{|B_\epsilon(y)|} \int_{B_\epsilon(y)} F(y, u'_h(z)) dz = \int_{-\infty}^{\infty} F(y, s) dm_{y,\epsilon,h}(s).$$

So,

$$(3.9) \quad \int_0^1 \left[\frac{1}{|B_\epsilon(y)|} \int_{B_\epsilon(y)} F(y, u'_h(z)) dz \right] dy = \int_0^1 \int_{-\infty}^{\infty} F(y, s) dm_{y,\epsilon,h}(s) dy.$$

Further, for $0 < \alpha \leq \bar{\alpha}$,

$$\begin{aligned} & \int_0^1 \int_{-\infty}^{\infty} F(y, s) dm_{y,\epsilon,h}(s) dy \\ &= \int_0^1 \left[\int_{-\infty}^{s_L - \bar{\alpha}} + \int_{s_L - \bar{\alpha}}^{s_L - \alpha} + \int_{s_L - \alpha}^{s_L + \alpha} + \int_{s_L + \alpha}^{s_U - \alpha} + \int_{s_U - \alpha}^{s_U + \alpha} \right. \\ & \quad \left. + \int_{s_U + \alpha}^{s_U + \bar{\alpha}} + \int_{s_U + \bar{\alpha}}^{\infty} \right] F(y, s) dm_{y,\epsilon,h}(s) dy \\ &= I_1 + \cdots + I_7 \end{aligned}$$

Define the function

$$(3.10) \quad \xi_\epsilon(z) = \int_{B_\epsilon(z)} \frac{1}{|B_\epsilon(y)|} dy.$$

Then a simple calculation shows that

$$\xi_\epsilon(z) = \begin{cases} \ln 2 + \frac{z}{2\epsilon} & 0 \leq z \leq \epsilon, \\ \ln \frac{2\epsilon}{z} + \frac{z}{2\epsilon} & \epsilon \leq z \leq 2\epsilon, \\ 1 & 2\epsilon \leq z \leq 1 - 2\epsilon, \\ \ln \frac{2\epsilon}{1-z} + \frac{1-z}{2\epsilon} & 1 - 2\epsilon \leq z \leq 1 - \epsilon, \\ \ln 2 + \frac{1-z}{2\epsilon} & 1 - \epsilon \leq z \leq 1. \end{cases}$$

Hence,

$$(3.11) \quad \ln 2 \leq \xi_\epsilon(z) \leq \ln 2 + 1/2, \quad z \in (0, 1).$$

Thus, by Fubini's Theorem and (3.11),

$$\begin{aligned}
(3.12) \quad I_1 &= \int_0^1 \int_{-\infty}^{s_L - \bar{\alpha}} F(y, s) dm_{y, \epsilon, h}(s) dy \leq c_3 \int_0^1 \int_{-\infty}^{s_L - \bar{\alpha}} \phi(s) dm_{y, \epsilon, h}(s) dy \\
&\leq c_3 \int_0^1 \int_{-\infty}^{\infty} \phi(s) dm_{y, \epsilon, h}(s) dy \\
&= c_3 \int_0^1 \frac{1}{|B_\epsilon(y)|} \int_{B_\epsilon(y)} \phi(u'_h(z)) dz dy \\
&= c_3 \int_0^1 \int_{B_\epsilon(z)} \frac{1}{|B_\epsilon(y)|} \phi(u'_h(z)) dy dz \\
&\leq 2c_3 \int_0^1 \phi(u'_h(z)) dz \\
&= 2c_3 E_h \leq 2c_3 c_6 h^2.
\end{aligned}$$

Similarly,

$$(3.13) \quad I_7 \leq 2c_3 c_6 h^2.$$

Next,

$$\begin{aligned}
(3.14) \quad I_2 &= \int_0^1 \int_{s_L - \bar{\alpha}}^{s_L - \alpha} F(y, s) dm_{y, \epsilon, h}(s) dy \\
&\leq c_2 \sup_{y \in (0, 1)} m_{y, \epsilon, h}((s_L - \bar{\alpha}, s_L - \alpha)) \\
&\leq c_2 \frac{E_h}{\alpha^2 \lambda_1 \epsilon} \leq \frac{c_2 c_6 h^2}{\alpha^2 \lambda_1 \epsilon}.
\end{aligned}$$

Similarly,

$$(3.15) \quad I_4 \leq \frac{c_2 c_6 h^2}{\alpha^2 \lambda_1 \epsilon}, \quad I_6 \leq \frac{c_2 c_6 h^2}{\alpha^2 \lambda_1 \epsilon}.$$

Finally, by Theorem 1 for some $-1 \leq \theta_2 \leq 1$, $-1 \leq \theta_3 \leq 1$,

$$\begin{aligned}
(3.16) \quad I_3 &= \int_0^1 \int_{s_L - \alpha}^{s_L + \alpha} F(y, s) dm_{y, \epsilon, h}(s) dy \\
&= \int_0^1 \int_{s_L - \alpha}^{s_L + \alpha} F(y, s_L) dm_{y, \epsilon, h}(s) dy + \theta_2 \rho \alpha \\
&= \int_0^1 F(y, s_L) m_{y, \epsilon, h}(\Omega^{L, \alpha}) dy + \theta_1 \rho \alpha \\
&= \int_0^1 \gamma F(y, s_L) dy + \frac{\theta_3 c_2 c_1 h^{1/2}}{\epsilon} + \theta_2 \rho \alpha.
\end{aligned}$$

Similarly, for some $-1 \leq \theta_4 \leq 1$, $-1 \leq \theta_5 \leq 1$,

$$(3.17) \quad I_5 = \int_0^1 (1 - \gamma) F(y, s_U) dy + \frac{\theta_4 c_2 c_1 h^{1/2}}{\epsilon} + \theta_5 \rho \alpha.$$

The result (3.8) now follows from (3.12) - (3.17). $\square$

We finally now turn to the proof of Theorem 2.

Proof of Theorem 2. By Fubini's Theorem, (2.8), Lemma 4, and (3.11) for $-1 \leq \theta_6 \leq 1$,

$$(3.18) \quad \begin{aligned} & \int_0^1 \left[\frac{1}{|B_\epsilon(y)|} \int_{B_\epsilon(y)} F(y, u'_h(z)) dz \right] dy \\ &= \int_0^1 \int_{B_\epsilon(z)} \frac{1}{|B_\epsilon(y)|} F(y, u'_h(z)) dy dz \\ &= \int_0^1 \int_{B_\epsilon(z)} \frac{1}{|B_\epsilon(y)|} F(z, u'_h(z)) dy dz + 2\theta_6 c_4 \epsilon \\ &= \int_0^1 \xi_\epsilon(z) F(z, u'_h(z)) dz + 2\theta_6 c_4 \epsilon. \end{aligned}$$

Further,

$$(3.19) \quad \int_0^1 \xi_\epsilon(z) F(z, u'_h(z)) dz = \int_0^1 F(z, u'_h(z)) dz + \int_0^1 (\xi_\epsilon(z) - 1) F(z, u'_h(z)) dz$$

and

$$(3.20) \quad \begin{aligned} & \left| \int_0^1 (\xi_\epsilon(z) - 1) F(z, u'_h(z)) dz \right| \\ & \leq \int_0^{2\epsilon} |F(z, u'_h(z))| dz + \int_{1-2\epsilon}^1 |F(z, u'_h(z))| dz \\ & \leq 4\epsilon(c_2 + c_3 E_h) \\ & \leq 4\epsilon c_2 + 4c_3 c_6 h^2 \epsilon. \end{aligned}$$

Thus, it follows from (3.8) and (3.18)-(3.20) that

$$(3.21) \quad \begin{aligned} & \left| \int_0^1 F(x, u'_h(x)) dx - \int_0^1 [\gamma F(x, s_L) + (1 - \gamma) F(x, s_U)] dx \right| \\ & \leq c_{10} \left(\frac{h^2}{\alpha^2 \epsilon} + \frac{h^{1/2}}{\epsilon} \right) + 2\rho\alpha + 2c_4 \epsilon + 4c_2 \epsilon + 4c_3 c_6 h^2 \epsilon. \end{aligned}$$

Finally, the proof of Theorem 2 follows from the inequality (3.21) by letting $\alpha = h^{\frac{7}{12}}$ and $\epsilon = h^{1/4}$. $\square$

Proof of Theorem 4. The proof of Theorem 4 follows the proofs of Theorems 1–3 by using $\hat{\phi}(s) \equiv \phi(s) + l(s)$ in place of $\phi(s)$, the result (2.12), and Lemma 2 in place of Lemma 1. $\square$

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