EFFECTIVE HAMILTONIANS AND QUANTUM STATES

Lawrence C. Evans
Department of Mathematics
University of California, Berkeley

Abstract. We recount here some preliminary attempts to devise quantum analogues of certain aspects of Mather's theory of minimizing measures [M1-2, M-F], augmented by the PDE theory from Fathi [F1,2] and from [E-G1]. This earlier work provides us with a Lipschitz continuous function u solving the eikonal equation a.e. and a probability measure σ solving a related transport equation.

We present some elementary formal identities relating certain quantum states ψ and u, σ. We show also how to build out of u, σ an approximate solution of the stationary Schrödinger eigenvalue problem, although the error estimates for this construction are not very good.

1. Introduction.

This paper records a few observations and comments concerning the possible implications for quantum mechanics of Fathi's "weak KAM" theory from [F1-2] and the recent paper [E-G1], which discusses connections between the "effective Hamiltonian" introduced by Lions–Papanicolaou–Varadhan [L-P-V], Mather's theory of action minimizing measures [M1-2, M-F], and Hamiltonian dynamics. See also Weinan E [EW] for more on these approaches.

We will discuss the Hamiltonian

$$H(p,x) := \frac{1}{2}|p|^2 + V(x), \tag{1.1}$$

defined for momentum variables $p \in \mathbb{R}^n$ and position variables $x \in \mathbb{T}^n$, where $\mathbb{T}^n$ denotes the flat torus in $\mathbb{R}^n$. The smooth potential V is $\mathbb{T}^n$-periodic. The corresponding stationary Schrödinger equation is

$$\hat{H}\psi = -\frac{\hbar^2}{2}\Delta\psi + V\psi = E\psi \quad \text{in } \mathbb{R}^n, \tag{1.2}$$

E denoting the energy level and $\hbar$ Planck's constant.

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The basic structure available from the references cited above for the case of the Hamiltonian (1.1) is this. Fix a vector $P \in \mathbb{R}^n$. Then there exists a $\mathbb{T}^n$-periodic, Lipschitz continuous function $v : \mathbb{R}^n \to \mathbb{R}$ solving the cell problem

$$\frac{|P + Dv|^2}{2} + V(x) = \bar{H}(P) \quad \text{in } \mathbb{R}^n$$

in the viscosity sense. The term $\bar{H}(P)$ on the right-hand side defines a convex function, the *effective Hamiltonian* $\bar{H} : \mathbb{R}^n \to \mathbb{R}$, as introduced by Lions–Papanicolaou–Varadhan [L-P-V]. We define

$$u := P \cdot x + v, \tag{1.3}$$

to transform this PDE into the form

$$\frac{|Du|^2}{2} + V(x) = \bar{H}(P) \quad \text{in } \mathbb{R}^n. \tag{1.4}$$

This is the *eikonal equation*. Furthermore we have a nonnegative Radon probability measure σ defined on $\mathbb{T}^n$, called the *Mather measure*, satisfying

$$\operatorname{div}(\sigma Du) = 0 \quad \text{in } \mathbb{R}^n \tag{1.5}$$

in the weak sense. This is a stationary form of a *transport equation*.

The primary question introduced in this paper asks to what extent we can utilize u and σ, satisfying (1.3) – (1.5), to glean information about Bloch wave solutions of Schrödinger's equation (1.2). The formal connection is that if we write

$$\psi = a\, e^{i\, s/\hbar},$$

then

$$\frac{|Ds|^2}{2} + V = E + \frac{\hbar^2}{2}\,\frac{\Delta a}{a} \tag{1.6}$$

and

$$\operatorname{div}(a^2 Ds) = 0. \tag{1.7}$$

The interesting problem, for which this paper provides some very minor progress, is of course to find rigorous statements consistent with the formal similarities between between (1.5) and (1.7) and between (1.4) and (1.6) for small $\hbar$. The following sections discuss two different approaches to this issue.

In §2, I derive two elementary identities connecting the quantities u, σ, s and a as above. These formulas record by how much the quantum state ψ fails to minimize the classical action.

In §3 following, we take the function u and the measure σ and manufacture from them a quasimode, that is, an approximate solution of (1.2) for the energy level $E = \bar{H}(P)$. However, we can only estimate the error term to be $O(\hbar)$ in L^2, which as M. Zworski tactfully pointed out to me is not very good: It is not difficult by other means to build approximations with the same error bound. I provide these computations mostly in hopes of interesting the real experts in this problem.

The papers [E-G2] and Gomes [G1-3] present some further developments of the PDE theory from [E-G1], and a good introduction to Mather's theory is Contreras–Iturriaga [C-I]. We also note here that our functions $\bar{H}, \bar{L}$ are equivalent to Mather's α, β: see the appendix to [E-G2].

2. Quantum analogues of action minimizers.

This section records two formal identities relating our solutions u, σ of the eikonal and transport PDE, with a solution of the stationary Schrödinger equation.

2.1 Notation. Define the usual Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2}\Delta + V$$

and assume that ψ is an eigenstate, normalized so that $\int_{\mathbb{T}^n} |\psi|^2 dx = 1$:

$$-\frac{\hbar^2}{2}\Delta\psi + V\psi = E\psi \quad \text{in } \mathbb{T}^n. \tag{2.1}$$

We suppose we can write ψ in the WKB form

$$\psi = a\, e^{i\, s/\hbar}, \tag{2.2}$$

with real, smooth amplitude a and phase s. Then

$$\frac{|Ds|^2}{2} + V = E + \frac{\hbar^2}{2}\,\frac{\Delta a}{a}, \tag{2.3}$$

$$\operatorname{div}(a^2 Ds) = 0. \tag{2.4}$$

We will assume as well that

$$a^2 Ds = \frac{\hbar}{i} D\psi\,\bar{\psi} \quad \text{is periodic.}$$

Next define

$$Q := \int_{\mathbb{T}^n} Ds\, a^2 dx \;=\; \int_{\mathbb{T}^n} \mathbf{j}\, dx, \tag{2.5}$$

the average of the quantum flux $\mathbf{j} := \frac{\hbar}{2i}(D\psi\,\bar{\psi} - D\bar{\psi}\,\psi)$. We introduce also the *Lagrangian operator*

$$\hat{L} = -\frac{\hbar^2}{2}\Delta - V$$

and define the *quantum action*

$$\langle\psi|\hat{L}|\psi\rangle := \int_{\mathbb{T}^n} \frac{\hbar^2}{2}|D\psi|^2 - V|\psi|^2\,dx = \int_{\mathbb{T}^n} \frac{\hbar^2}{2}|Da|^2 + \frac{|Ds|^2}{2}a^2 - Va^2 dx. \tag{2.6}$$

Fix now any $P \in \mathbb{R}^n$ and recall from above the *eikonal equation*

$$\frac{|Du|^2}{2} + V = \bar{H}(P), \tag{2.7}$$

where $u = P\cdot x + v$ and v is periodic. As noted before, the convex function $\bar{H}$ is the effective Hamiltonian, the convex dual of which is the *effective Lagrangian* $\bar{L}$.

We want to derive some identities relating these various quantum and classical objects.

2.2 Minimization of the quantum action.

Lemma 2.1. *For each $P \in \mathbb{R}^n$ we have the equality*

$$\langle\psi|\hat{L}|\psi\rangle - \bar{L}(Q) + \bar{H}(P) + \bar{L}(Q) - P\cdot Q = \frac{\hbar^2}{2}\int_{\mathbb{T}^n}|Da|^2 dx + \tfrac{1}{2}\int_{\mathbb{T}^n}|Du - Ds|^2\,a^2 dx. \tag{2.8}$$

In particular, if we take $P \in \partial\bar{L}(Q)$, then

$$\langle\psi|\hat{L}|\psi\rangle - \bar{L}(Q) = \frac{\hbar^2}{2}\int_{\mathbb{T}^n}|Da|^2\,dx + \tfrac{1}{2}\int_{\mathbb{T}^n}|Du - Ds|^2\,a^2 dx. \tag{2.9}$$

Proof. The left-hand side of (2.8) equals

$$\begin{aligned}\langle\psi|\hat{L}|\psi\rangle + \bar{H}(P) - P\cdot Q = &\int_{\mathbb{T}^n}\frac{\hbar^2}{2}|Da|^2 + \frac{|Ds|^2}{2}a^2 - Va^2 dx\\ &+ \int_{\mathbb{T}^n}\left(\frac{|Du|^2}{2} + V\right)a^2 dx - \int_{\mathbb{T}^n}P\cdot Ds\,a^2 dx,\end{aligned}$$

where we used (2.5),(2.7). This expression equals

$$\frac{\hbar^2}{2}\int_{\mathbb{T}^n}|Da|^2 dx + \tfrac{1}{2}\int_{\mathbb{T}^n}(|Du|^2 + |Ds|^2)a^2 dx - \int_{\mathbb{T}^n}(P + Dv)\cdot Ds\,a^2 dx,$$

since v, $a^2 Ds$ are periodic and $\operatorname{div}(a^2 Ds) = 0$. The foregoing then reads

$$\frac{\hbar^2}{2}\int_{\mathbb{T}^n}|Da|^2 dx + \tfrac{1}{2}\int_{\mathbb{T}^n}|Du - Ds|^2 a^2\,dx,$$

since $Du = P + Dv$. $\square$

Interpretation. The naive WKB approximation is certainly false in general, and we can understand the right-hand sides of formulas (2.8), (2.9) as recording quantitatively the failure of the PDE (1.4), (1.5) to approximate (1.6), (1.7).

The left-hand sides of (2.8), (2.9) record by how much the quantum action of ψ differs from the minimum of the classical action. Indeed according to Mather's theory, $\bar{L}(Q)$ is the minimum of the action

$$A[\mu] := \int_{\mathbb{R}^n} \int_{\mathbb{T}^n} \frac{1}{2}|p|^2 - V(x)\, d\mu.$$

taken among all flow–invariant probability measures μ on the classical phase space $R^n \times \mathbb{T}^n$, with given rotation vector

$$Q := \int_{\mathbb{R}^n} \int_{\mathbb{T}^n} p\, d\mu.$$

To understand the quantum analogue of this, we first recall that since $\bar{H}(P) + \bar{L}(Q) \geq P \cdot Q$, with equality if and only if $P \in \partial \bar{L}(Q)$, this should be our optimal choice for P. Then (2.9) asserts firstly that

$$\bar{L}(Q) \leq \langle \psi | \hat{L} | \psi \rangle$$

for all quantum states ψ satisfying (2.1), now for the given average flux

$$Q = \int_{\mathbb{T}^n} \mathbf{j}\, dx.$$

So the classical minimum of the action is a lower bound for the quantum action. Secondly, equality holds in the limit $\hbar \to 0$ if and only if the naive WKB approximation is valid, in the sense that the right-hand side of (2.9) goes to zero. The really interesting issue would be to understand under what, if any, circumstances both sides of (2.9) vanish as $\hbar \to 0$. $\square$

2.3 An identity for a periodic phase. Now assume in addition to (2.1)–(2.4) that we can write the phase s in the form

$$s = P \cdot x + r$$

where r is *periodic*. Under this strong hypothesis on the structure of the phase, we can derive a second formal identity:

Lemma 2.2. *We have*

$$\frac{1}{2} \int_{\mathbb{T}^n} |Du - Ds|^2\, a^2\, dx + E = \frac{\hbar^2}{2} \int_{\mathbb{T}^n} |Da|^2\, dx + \bar{H}(P). \tag{2.10}$$

Proof. Let us first subtract (2.3) from (2.7), to find

$$\frac{|Du|^2}{2} - \frac{|Ds|^2}{2} = \bar{H}(P) - E - \frac{\hbar^2}{2}\, \frac{\Delta a}{a}\ .$$

We rewrite:

$$\tfrac{1}{2}|Du - Ds|^2 + Ds \cdot (Du - Ds) = \bar{H}(P) - E - \frac{\hbar^2}{2}\,\frac{\Delta a}{a},$$

and then multiply by a^2 and integrate:

$$\tfrac{1}{2}\int_{\mathbb{T}^n} |Du - Ds|^2 a^2\, dx + \int_{\mathbb{T}^n} D(u-s)\cdot Ds\, a^2\, dx \;=\; \bar{H}(P) - E + \frac{\hbar^2}{2}\int_{\mathbb{T}^n} |Da|^2\, dx.$$

But $D(u-s) = D(v-r)$ and v, r are periodic. Hence $\int_{\mathbb{T}^n} D(u-s)\cdot Dsa^2\, dx = 0$. $\square$

3. Building approximate solutions.

We recall that the Lipschitz function u solves the eikonal equation (1.4) and the probability measure σ satisfies (1.5). Then formally the function

$$\psi := \sigma^{\frac{1}{2}} e^{\frac{iu}{\hbar}} \tag{3.1}$$

solves (1.2) up to an error term of order $O(\hbar^2)$, for $E = \bar{H}(P)$. This however makes no sense at all, since u is only Lipschitz continuous and σ is merely a measure: The square root in (3.1) is undefined and ψ is not smooth enough to insert into the left-hand side of the PDE (1.2). We will, naively, try to repair these defects by mollifying.

3.1. Mollifiers. Take $\zeta : \mathbb{R}^n \to \mathbb{R}$ is a smooth function, satisfying

$$\zeta \geq 0, \qquad \operatorname{spt}\zeta = B(0,1), \qquad \zeta(z) = \zeta(|z|). \tag{3.2}$$

Write

$$\eta(z) := c\zeta^4(z),$$

the constant $c > 0$ adjusted so that $\int_{B(0,1)} \eta\, dz = 1$. Fix $\epsilon > 0$ and define $\eta_\epsilon(z) := \frac{1}{\epsilon^n}\,\eta\big(\frac{z}{\epsilon}\big)$.

Lemma 3.1. *We have the estimates*

$$|D\eta| \leq C\eta^{\frac{3}{4}}, \quad |D^2\eta| \leq C\eta^{\frac{1}{2}}. \tag{3.3}$$

Proof. Compute $|D\eta| = c4\zeta^3|D\zeta| \leq C\zeta^3 \leq C\eta^{\frac{3}{4}}$; and similarly

$$|D^2\eta| \leq C\zeta^2|D\zeta|^2 + C\zeta^3|D^2\zeta| \leq C\zeta^2 \leq C\eta^{\frac{1}{2}}.$$

$\square$

The paper [EG1] contains the proof of

Lemma 3.2. *The gradient $Du(x)$ exists for each point $x \in \operatorname{spt}(\sigma)$, and*

$$|Du(y) - Du(x)| \leq C|x - y| \tag{3.4}$$

for a.e. point $y \in \mathbb{T}^n$ and each $x \in \operatorname{spt}(\sigma)$.

Next we define $u^\epsilon = \eta_\epsilon * u$ and $\sigma^\epsilon = \eta_\epsilon * \sigma$; that is,

$$u^\epsilon(x) \;=\; \int_{\mathbb{R}^n} \eta_\epsilon(x-y)u(y)dy \;=\; \frac{1}{\epsilon^n}\int_{B(x,\epsilon)} \eta\Big(\frac{x-y}{\epsilon}\Big)u(y)dy \tag{3.5}$$

and

$$\sigma^\epsilon(x) \;=\; \int_{\mathbb{R}^n} \eta_\epsilon(x-y)d\sigma(y) \;=\; \frac{1}{\epsilon^n}\int_{B(x,\epsilon)} \eta\Big(\frac{x-y}{\epsilon}\Big)d\sigma(y). \tag{3.6}$$

We need next to control how well the smoothed functions u^ϵ solve the eikonal equation, at least near $\operatorname{spt}(\sigma)$.

Lemma 3.3. *For each point $x \in \mathbb{T}^n$,*

$$\Big|\frac{|Du^\epsilon(x)|^2}{2} + V(x) - \bar{H}(P)\Big| \leq C(\epsilon^2 + \operatorname{dist}(x, \operatorname{spt}(\sigma))^2). \tag{3.7}$$

Proof. We have

$$Du^\epsilon(x) = \int_{\mathbb{R}^n} \eta_\epsilon(x-y)Du(y)dy. \tag{3.8}$$

Also

$$\frac{|Du(y)|^2}{2} + V(y) = \bar{H}(P)$$

for a.e. point $y \in B(x,\epsilon)$. Therefore

$$\begin{aligned}\frac{|Du^\epsilon(x)|^2}{2} + V(x) - \bar{H}(P) &= \frac{|Du^\epsilon(x)|^2}{2} + V(x) - \frac{|Du(y)|^2}{2} - V(y)\\ &= Du^\epsilon(x)\cdot(Du^\epsilon(x) - Du(y)) - \tfrac{1}{2}|Du^\epsilon(x) - Du(y)|^2 + V(x) - V(y).\end{aligned}$$

Multiply by $\eta_\epsilon(x-y)$ and integrate with respect to y:

$$\begin{aligned}&\frac{|Du^\epsilon(x)|^2}{2} + V(x) - \bar{H}(P)\\ &\quad= -\tfrac{1}{2}\int_{\mathbb{R}^n} \eta_\epsilon(x-y)|Du^\epsilon(x) - Du(y)|^2 dy\\ &\qquad+ \int_{\mathbb{R}^n} \eta_\epsilon(x-y)[V(x) + DV(x)\cdot(y-x) - V(y)]dy,\end{aligned}$$

where we used (3.8) and the radiality of η. Consequently

$$
\begin{aligned}
&|\frac{|Du^\epsilon(x)|^2}{2} + V(x) - \bar{H}(P)| \\
&\le C\epsilon^2 + \tfrac{1}{2}\int_{\mathbb{R}^n} \eta_\epsilon(x-y)|\int_{\mathbb{R}^n} \eta_\epsilon(x-z)(Du(z)-Du(y))dz|^2 dy \qquad (3.9)\\
&\le C\epsilon^2 + \frac{C}{\epsilon^{2n}} \int_{B(x,\epsilon)}\int_{B(x,\epsilon)} |Du(z)-Du(y)|^2 dz dy
\end{aligned}
$$

Take $x \in \operatorname{spt}(\sigma)$, $|x-x^*| = \operatorname{dist}(x, \operatorname{spt}(\sigma))$. Then according to Lemma 3.2,

$$
\begin{aligned}
\frac{1}{\epsilon^{2n}} \int_{B(x,\epsilon)}\int_{B(x,\epsilon)} |Du(z)-Du(y)|^2 dz dy &\le \frac{C}{\epsilon^n}\int_{B(x,\epsilon)} |Du(y)-Du(x^*)|^2 dy \\
&\le \frac{C}{\epsilon^n}\int_{B(x,\epsilon)} |y-x^*|^2 dy \le C(\epsilon^2 + \operatorname{dist}(x,\operatorname{spt}(\sigma))^2).
\end{aligned}
$$

We use this estimate in (3.9) to finish the proof of (3.7). □

We must also control the size of the Laplacian applied to u^ϵ:

Lemma 3.4. *For each point $x \in \mathbb{T}^n$, we have the bound*

$$
|\Delta u^\epsilon(x)| \le C + C\frac{\mathit{dist}(x, \mathit{spt}(\sigma))}{\epsilon}.
$$

Proof. Observe that

$$
\begin{aligned}
\Delta u^\epsilon(x) &= \frac{1}{\epsilon^{n+1}} \int_{B(x,\epsilon)} D\eta(\frac{x-y}{\epsilon}) \cdot Du(y) dy \\
&= \frac{1}{\epsilon^{n+1}} \int_{B(x,\epsilon)} D\eta(\frac{x-y}{\epsilon}) \cdot (Du(y) - Du(x^*)) dy,
\end{aligned}
$$

where $x^* \in \operatorname{spt}(\sigma)$, $|x-x^*| = \operatorname{dist}(x,\operatorname{spt}(\sigma))$. Thus

$$
|\Delta u^\epsilon(x)| \;\le\; \frac{C}{\epsilon^{n+1}}\int_{B(x,\epsilon)} |y-x^*| dy \;\le\; C + C\frac{\operatorname{dist}(x,\operatorname{spt}(\sigma))}{\epsilon}.
$$

□

3.2. Approximate solutions. We hereafter set

$$
\epsilon = \hbar^{\frac{1}{2}} \qquad (3.10)
$$

and define

$$
\psi_\epsilon(x) := (\sigma^\epsilon(x))^{\frac{1}{2}}\; e^{\frac{iu^\epsilon(x)}{\hbar}} \qquad (x \in \mathbb{T}^n).
$$

Theorem 3.1. *We have*

$$\psi_\epsilon \in H^2(\mathbb{T}^n), \qquad \int_{\mathbb{T}^n} |\psi_\epsilon|^2\,dx = 1, \tag{3.11}$$

and

$$-\frac{\hbar^2}{2}\Delta\psi_\epsilon + V\psi_\epsilon = \bar{H}(P)\psi_\epsilon + e_\epsilon, \tag{3.12}$$

where the error term e_ϵ satisfies the estimate

$$\|e_\epsilon\|_{L^2(\mathbb{T}^n)} \le C\hbar. \tag{3.13}$$

Proof. 1. Let $0 < \lambda \le \epsilon^4 = \hbar^2$ and define

$$\psi_{\varepsilon,\lambda} := (\sigma^\epsilon + \lambda)^{\frac{1}{2}}\ e^{iu^\epsilon/\hbar}. \tag{3.14}$$

Set $\psi = \psi_{\varepsilon,\lambda}$. We then compute

$$-\frac{\hbar^2}{2}\Delta\psi + V\psi - \bar{H}(P)\psi = A + B + C,$$

for

$$A := \left(\frac{|Du^\epsilon|^2}{2} + V - \bar{H}(P)\right)\psi, \tag{3.15}$$

$$B := -\frac{i\hbar}{2}\left(\frac{\operatorname{div}((\sigma^\epsilon + \lambda)Du^\epsilon)}{\sigma^\epsilon + \lambda}\right)\psi, \tag{3.16}$$

$$C := -\frac{\hbar^2}{2}\left(\frac{\Delta\sigma^\epsilon}{\sigma^\epsilon + \lambda} - \frac{1}{4}\frac{|D\sigma^\epsilon|^2}{(\sigma^\epsilon + \lambda)^2}\right)\psi. \tag{3.17}$$

We must estimate the L^2-norm of each term.

Estimate of A. We have

$$\begin{aligned}
\int_{\mathbb{T}^n} |A|^2 dx &= \int_{\mathbb{T}^n} \left|\frac{|Du^\epsilon|^2}{2} + V - \bar{H}(P)\right|^2 (\sigma_\epsilon + \lambda)dx \\
&\le C\lambda + \int_{\mathbb{T}^n}\int_{\mathbb{R}^n} \left|\frac{|Du^\epsilon(x)|^2}{2} + V(x) - \bar{H}(P)\right|^2 \eta_\epsilon(x-y)\,d\sigma(y)dx \\
&\le C\hbar^2 + C\int_{2\mathbb{T}^n}\int_{\mathbb{T}^n} (\epsilon^4 + \operatorname{dist}(x, \operatorname{spt}(\sigma))^4)\eta_\epsilon(x-y)\,dxd\sigma(y),
\end{aligned}$$

according to Lemma 3.3. Since $\eta_\epsilon(x-y)=0$ if $|x-y|\geq\epsilon$, we deduce

$$\int_{\mathbb{T}^n}|A|^2dx \leq C\hbar^2. \tag{3.18}$$

Estimate of B. Recalling (3.14), we compute

$$\begin{aligned}\int_{\mathbb{T}^n}|B|^2dx &\leq C\hbar^2\int_{\mathbb{T}^n}\frac{|\mathrm{div}((\sigma^\epsilon+\lambda)Du^\epsilon)|^2}{\sigma^\epsilon+\lambda}\,dx\\ &\leq C\hbar^2\int_{\mathbb{T}^n}\frac{\lambda^2|\Delta u^\epsilon|^2}{\sigma^\epsilon+\lambda}\,dx + C\hbar^2\int_{\mathbb{T}^n}\frac{|\mathrm{div}(\sigma^\epsilon Du^\epsilon)|^2}{\sigma^\epsilon+\lambda}\,dx\\ &=: B_1+B_2.\end{aligned} \tag{3.19}$$

We next recall Lemma 3.4, to estimate that

$$B_1 \leq C\hbar^2\lambda\int_{\mathbb{T}^n}|\Delta u^\epsilon|^2dx \leq C\hbar^2\frac{\lambda}{\epsilon^2}\leq C\hbar^2. \tag{3.20}$$

We also have $\mathrm{div}(\sigma Du)=0$, and so

$$\mathrm{div}(\int_{B(x,\epsilon)}\eta_\epsilon(x-y)Du(y)\,d\sigma(y))=0.$$

Hence

$$\begin{aligned}\mathrm{div}(\sigma^\epsilon Du^\epsilon) &= \mathrm{div}(\int_{B(x,\epsilon)}\eta_\epsilon(x-y)(Du^\epsilon(x)-Du(y))\,d\sigma(y))\\ &= \frac{1}{\epsilon^n}\int_{B(x,\epsilon)}\eta(\frac{x-y}{\epsilon})\Delta u^\epsilon(x)\,d\sigma(y)\\ &\quad+\frac{1}{\epsilon^{n+1}}\int_{B(x,\epsilon)}D\eta(\frac{x-y}{\epsilon})\cdot(Du^\epsilon(x)-Du(y))\,d\sigma(y)\\ &=: B_3+B_4.\end{aligned} \tag{3.21}$$

Now

$$|B_3|\leq\frac{C}{\epsilon^n}\int_{B(x,\epsilon)}\eta(\frac{x-y}{\epsilon})d\sigma(y), \tag{3.22}$$

according to Lemma 3.4. Furthermore, Lemma 3.2 implies

$$\begin{aligned}|B_4| &\leq \frac{C}{\epsilon^{n+1}}\int_{B(x,\epsilon)}|D\eta|(\frac{x-y}{\epsilon})|Du^\varepsilon(x)-D(y)|\,d\sigma(y)\\ &\leq \frac{C}{\epsilon^n}\int_{B(x,\epsilon)}|D\eta|(\frac{x-y}{\epsilon})d\sigma(y).\end{aligned} \tag{3.23}$$

Combine (3.21)–(3.23):

$$|\mathrm{div}(\sigma^\epsilon Du^\epsilon)| \le \frac{C}{\epsilon^n}\int_{B(x,\epsilon)} \eta + |D\eta|\, d\sigma.$$

Thus

$$\begin{aligned}
\frac{|\mathrm{div}(\sigma^\epsilon Du^\epsilon)|^2}{\sigma^\epsilon+\lambda} &\le \frac{C}{\epsilon^{2n}} \frac{\left(\int_{B(x,\epsilon)} \eta + |D\eta| d\sigma\right)^2}{\frac{1}{\epsilon^n}\int_{B(x,\epsilon)} \eta\, d\sigma + \lambda} \\
&\le \frac{C}{\epsilon^n} \frac{\left(\int_{B(x,\epsilon)} \eta^{\frac12}\, d\sigma\right)^2}{\int_{B(x,\epsilon)} \eta\, d\sigma + \lambda\epsilon^n} \qquad \text{by Lemma 3.1} \\
&\le \frac{C}{\epsilon^n} \frac{\left(\int_{B(x,\epsilon)} \eta\, d\sigma\right)\sigma(B(x,\epsilon))}{\int_{B(x,\epsilon)} \eta\, d\sigma + \lambda\epsilon^n} \le C\ \frac{\sigma(B(x,\epsilon))}{\epsilon^n},
\end{aligned}$$

and therefore

$$\begin{aligned}
B_2 &\le C\hbar^2 \int_{\mathbb{T}^n} \frac{\sigma(B(x,\epsilon))}{\epsilon^n}\ dx \\
&= \frac{C\hbar^2}{\epsilon^n}\int_{\mathbb{T}^n}\int_{2\mathbb{T}^n} \chi_{B(0,\epsilon)}(x-y) d\sigma(y) dx \le C\hbar^2.
\end{aligned}$$

This inequality and (3.19), (3.20) imply

$$\int_{\mathbb{T}^n} |B|^2 dx \le C\hbar^2. \tag{3.24}$$

Estimate of C. The definition (3.17) gives

$$\int_{\mathbb{T}^n} |C|^2 dx \le C\hbar^4 \int_{\mathbb{T}^n} \frac{|\Delta\sigma^\epsilon|^2}{\sigma^\epsilon+\lambda}\ dx + C\hbar^4\int_{\mathbb{T}^n} \frac{|D\sigma^\epsilon|^4}{(\sigma^\epsilon+\lambda)^3}\ dx =: C_1 + C_2. \tag{3.25}$$

We note also that

$$\Delta\sigma^\epsilon(x) = \frac{1}{\epsilon^{n+2}}\int_{B(x,\epsilon)} \Delta\eta\left(\frac{x-y}{\varepsilon}\right) d\sigma(y),$$

and so

$$\begin{aligned}
\frac{|\Delta\sigma^\epsilon|^2}{\sigma^\epsilon+\lambda} &\le \frac{C}{\epsilon^{2n+4}} \frac{\left(\int_{B(x,\epsilon)} |\Delta^2\eta| d\sigma\right)^2}{\frac{1}{\epsilon^n}\int \eta\, d\sigma + \lambda} \\
&\le \frac{C}{\epsilon^{n+4}} \frac{\left(\int_{B(x,\epsilon)} \eta^{\frac12}\, d\sigma\right)^2}{\int_{B(x,\epsilon)} d\sigma + \lambda\epsilon^n} \qquad \text{by Lemma 3.1} \\
&\le \frac{C}{\epsilon^{n+4}} \frac{\left(\int_{B(x,\epsilon)} \eta d\sigma\right)\sigma(B(x,\epsilon))}{\int_{B(x,\epsilon)} \eta d\sigma + \lambda\epsilon^n} \le \frac{C}{\epsilon^4}\ \frac{\sigma(B(x,\epsilon))}{\epsilon^n}.
\end{aligned}$$

Consequently

$$C_1 \le \frac{C\hbar^4}{\epsilon^4}\int_{\mathbb{T}^n} \frac{\sigma(B(x,\epsilon))}{\epsilon^n}\, dx \le C\hbar^2. \tag{3.26}$$

Furthermore

$$D\sigma^\epsilon(x) = \frac{1}{\epsilon^{n+1}}\int_{B(x,\epsilon)} D\eta\big(\frac{x-y}{\epsilon}\big)d\sigma(y),$$

and hence

$$\begin{aligned}\frac{|D\sigma^\epsilon|^4}{(\sigma^\epsilon+\lambda)^3} &\le \frac{C}{\epsilon^{4n+4}}\,\frac{\big(\int_{B(x,\epsilon)}|D\eta| d\sigma\big)^4}{(\frac{1}{\epsilon^n}\int \eta d\sigma+\lambda)^3} \le \frac{C}{\epsilon^{n+4}}\,\frac{\big(\int_{B(x,\epsilon)}\eta^{\frac{3}{4}} d\sigma\big)^4}{(\int \eta d\sigma+\lambda\epsilon^n)^3}\\ &\le \frac{C}{\epsilon^{n+4}}\,\frac{\big(\int \eta d\sigma\big)^3\sigma(B(x,\epsilon))}{(\int_{B(x,\epsilon)} \eta d\sigma+\lambda\epsilon^n)^3} \le \frac{C}{\epsilon^4}\,\frac{\sigma(B(x,\epsilon))}{\epsilon^n}.\end{aligned}$$

As before, we deduce that

$$C_2 \le \frac{C\hbar^4}{\epsilon^4} \;=\; C\hbar^2.$$

This and (3.26) imply

$$\int_{\mathbb{T}^n}|C|^2dx \le C\hbar^2. \tag{3.27}$$

We combine inequalities (3.18), (3.24) and (3.27), to discover

$$-\frac{\hbar^2}{2}\Delta\psi_{\epsilon,\lambda}+V\psi_{\epsilon,\lambda} = \bar{H}(P)\psi_{\epsilon,\lambda}+e_{\epsilon,\lambda}$$

where

$$\|e_{\epsilon,\lambda}\|_{L^2(\mathbb{T}^n)} \;\le\; C\hbar.$$

Now let $\lambda \to 0$:

$$-\frac{\hbar^2}{2}\Delta\psi_{\epsilon}+V\psi_{\epsilon} \;=\; \bar{H}(P)\psi_{\epsilon}+e_{\epsilon},$$

with

$$\|e_{\epsilon}\|_{L^2(\mathbb{T}^n)} \;\le\; C\hbar.$$

□

In closing, we repeat that the $O(\hbar)$ estimate here is not satisfactory. It remains an interesting problem somehow to build from u, σ an approximate solution with an L^2-error of order $o(\hbar)$.

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