TOWARDS A QUANTUM ANALOG OF WEAK KAM THEORY

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Abstract. We discuss a quantum analogue of Mather's minimization principle for Lagrangian dynamics, and provide some formal calculations suggesting the corresponding Euler–Lagrange equation. We then rigorously construct from the dual eigenfunctions of a certain non-selfadjoint operator a candidate ψ for a minimizer, and recover aspects of "weak KAM" theory in the limit as $h \to 0$. Regarding our state ψ as a quasimode, we furthermore derive some error estimates, although it remains a open problem to improve these bounds.

1. Introduction.

This paper proposes an extension of Mather's variational principle [M1-2, M-F] and Fathi's weak KAM theory [F1-3] to quantum states. We interpret "weak KAM" theory to mean the application of nonlinear PDE methods, mostly for first–order equations, towards understanding the structure of action minimizing measures solving Mather's problem. As explained in the introduction to [E-G], a goal is interpreting these measures as providing a sort of "integrable structure", governed by an associated "effective Hamiltonian" $\bar{H}$, in the midst of otherwise possibly very chaotic dynamics. The relevant PDE are a nonlinear eikonal equation and an associated continuity (or transport) equation.

In this work we attempt to extend this viewpoint and some of the techniques to a quantum setting, in the semiclassical limit. We do so by suggesting an analogue of Mather's action minimization problem for the Lagrangian $L(v,x) = \frac{1}{2}|v|^2 - W(x)$, where the potential W is periodic, and formally computing the first and second variations. Thus motivated, we next build a candidate state ψ for a minimizer and discuss at length its properties. As in the nonquantum case, we come fairly naturally upon an eikonal PDE (with some extra terms) and an exact continuity equation. We next send $h \to 0$ and show how the usual structure of weak KAM theory appears in this limit.

More interesting is understanding if our ψ is a good quasimode, that is, a decent approximate solution of an appropriate eigenvalue problem. This turns out to be so, although our error bounds are too weak to allow for any deductions about the spectrum.

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Much of the interest in the following calculations centers upon our minimizing, subject to certain side conditions, the expected value of the Lagrangian, namely the expression

$$\int_{\mathbb{T}^n} \frac{h^2}{2}|D\psi|^2 - W|\psi|^2 dx,$$

and not the expected value of the Hamiltonian,

$$\int_{\mathbb{T}^n} \frac{h^2}{2}|D\psi|^2 + W|\psi|^2 dx.$$

It will turn out that owing to the constraints a minimizer of the former is approximately a critical point of the later. But the key question, unresolved here, is determining when the error terms are of order, say, $o(h)$ in L^2.

The calculations below represent improvements upon some ideas developed earlier in [E1]. An interesting recent paper of Anantharaman [A] presents a somewhat similar approach within a probabilistic framework, and Holcman and Kupka's forthcoming paper [H-K] is related. Likewise, Gomes [G] found some related constructions for his stochastic analogue of Aubry-Mather theory. We later discuss also some formal connections with the "stochastic mechanics" approach to quantum mechanics of Nelson [N] and also with homogenization theory for divergence–structure second–order elliptic PDE.

Action minimizing measures. Hereafter $\mathbb{T}^n$ denotes the flat torus in $\mathbb{R}^n$, the unit cube with opposite faces identified. We are given a smooth and periodic potential function $W : \mathbb{T}^n \to \mathbb{R}$ and a vector $V \in \mathbb{R}^n$. The Lagrangian is

$$L(v, x) := \frac{1}{2}|v|^2 - W(x) \qquad (v \in \mathbb{R}^n, x \in \mathbb{T}^n),$$

and the corresponding Hamiltonian is

$$H(p, x) := \frac{1}{2}|p|^2 + W(x) \qquad (p \in \mathbb{R}^n, x \in \mathbb{T}^n).$$

Mather's minimization problem is to find a Radon measure μ on the velocity–position configuration space $\mathbb{R}^n \times \mathbb{T}^n$ to minimize the generalized action

$$A[\mu] := \int_{\mathbb{R}^n} \int_{\mathbb{T}^n} \frac{1}{2}|v|^2 - W \, d\mu, \tag{1.1}$$

subject to the requirements that

$$\mu \geq 0, \ \ \mu(\mathbb{R}^n \times \mathbb{T}^n) = 1, \tag{1.2}$$

$$\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v\cdot D\phi \, d\mu = 0 \quad \text{for all } \phi \in C^1(\mathbb{T}^n), \tag{1.3}$$

and

$$\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v \; d\mu = V. \tag{1.4}$$

The identity (1.3) is a weak form of flow invariance.

Quantum action minimizing states. We propose as a quantum version of Mather's problem to find ψ minimizing the action

$$A[\psi] := \int_{\mathbb{T}^n} \frac{h^2}{2}|D\psi|^2 - W|\psi|^2 dx, \tag{1.5}$$

subject to the constraints that

$$\int_{\mathbb{T}^n} |\psi|^2 \, dx = 1, \tag{1.6}$$

$$\int_{\mathbb{T}^n} (\bar{\psi} D\psi - \psi D\bar{\psi})\cdot D\phi \, dx = 0 \quad \text{for all } \phi \in C^1(\mathbb{T}^n), \tag{1.7}$$

and

$$\frac{h}{2i}\int_{\mathbb{T}^n} \bar{\psi} D\psi - \psi D\bar{\psi} \, dx = V. \tag{1.8}$$

Here h denotes a positive constant. We always suppose that ψ has the Bloch wave form

$$\psi = e^{\frac{iP\cdot x}{h}} \hat{\psi}$$

for some $P \in \mathbb{R}^n$ and a periodic function $\hat{\psi} : \mathbb{T}^n \to \mathbb{C}$.

If ψ is smooth, condition (1.7) reads

$$\operatorname{div}(\bar{\psi} D\psi - \psi D\bar{\psi}) = 0. \tag{1.7$'$}$$

This is the analogue of the flow invariance. The vector field $\mathbf{j} := \bar{\psi} D\psi - \psi D\bar{\psi}$ represents the flux.

Remark. While it is presumably possible to introduce some sort of quantization for more general Lagrangians than $L(v,x) = \frac{1}{2}|v|^2 - W(x)$, most of the subsequent analysis would fail: we will from §3 onward rely upon some Cole-Hopf type transformations that depend upon the precise structure of this Lagrangian. □

2. First and second variations, local minimizers.

In this section we provide some formal calculations concerning the first and second variations of our problem (1.5) – (1.8). These heuristic deductions motivate the constructions and computations in §§3-8.

Let us take the complex-valued state in polar form

$$\psi = ae^{iu/h}, \tag{2.1}$$

where the phase u has the structure

$$u = P \cdot x + v \tag{2.2}$$

for some $\mathbb{T}^n$-periodic function v. Thus ψ has the requisite Bloch wave form. The action is then

$$A[\psi] = \int_{\mathbb{T}^n} \frac{h^2}{2}|Da|^2 + \frac{a^2}{2}|Du|^2 - Wa^2\,dx, \tag{2.3}$$

and the constraints (1.6)–(1.8) become

$$\int_{\mathbb{T}^n} a^2\,dx = 1, \tag{2.4}$$

$$\operatorname{div}(a^2 Du) = 0, \tag{2.5}$$

$$\int_{\mathbb{T}^n} a^2 Du\,dx = V. \tag{2.6}$$

2.1 First variation. Let $\{(u(\tau), a(\tau))\}_{-1\leq\tau\leq 1}$ be a smooth one-parameter family satisfying (2.4)–(2.6), with $(u(0), a(0)) = (u, a)$. We suppose also that for each $\tau \in (-1, 1)$, we can write

$$u(\tau) = P(\tau) \cdot x + v(\tau),$$

where $P(\tau) \in \mathbb{R}^n$ and $v(\tau)$ is $\mathbb{T}^n$–periodic. Define

$$j(\tau) := \int_{\mathbb{T}^n} \frac{h^2}{2}|Da(\tau)|^2 + \frac{a^2(\tau)}{2}|Du(\tau)|^2 - Wa^2(\tau)\,dx, \tag{2.7}$$

and hereafter write $' = \frac{d}{d\tau}$.

Theorem 2.1. *We have $j'(0) = 0$ for all variations if and only if*

$$-\frac{h^2}{2}\Delta a = a\left(\frac{|Du|^2}{2} + W - E\right) \tag{2.8}$$

for some real number E.

We interpret (2.8) as the *Euler–Lagrange equation* for our minimization problem, and call $\psi = ae^{iu/h}$ a *critical point* if this PDE is satisfied.

Proof. 1. We first compute

$$j' = \int_{\mathbb{T}^n} h^2 Da \cdot Da' + aa'|Du|^2 + a^2 Du \cdot Du' - 2Waa'\,dx.$$

Next, differentiate (2.5), (2.6):

$$\operatorname{div}(2aa'Du + a^2 Du') = 0, \tag{2.9}$$

$$\int_{\mathbb{T}^n} 2aa'Du + a^2 Du'\,dx = 0, \tag{2.10}$$

and set $\tau = 0$. Recall also that $Du = P + Dv$. Multiply (2.9) by v, integrate by parts, then take the inner product of (2.10) with P. Add the resulting expressions to find

$$\int_{\mathbb{T}^n} 2aa'|Du|^2 + a^2 Du' \cdot Du\,dx = 0.$$

Hence

$$j'(0) = \int_{\mathbb{T}^n} h^2 Da \cdot Da' - aa'|Du|^2 - 2Waa'\,dx$$

$$= 2\int_{\mathbb{T}^n} a'\left(-\frac{h^2}{2}\Delta a - \left(\frac{|Du|^2}{2} + W\right)a\right)dx.$$

Then $j'(0) = 0$ for all such a' provided

$$-\frac{h^2}{2}\Delta a - \left(\frac{|Du|^2}{2} + W\right)a = -Ea,$$

for some real constant E. This is so since the variation a' must satisfy the identity

$$\int_{\mathbb{T}^n} a'a\,dx = 0, \tag{2.11}$$

which we obtain upon differentiating (2.4). □

Remark. The foregoing deduction depends upon the implict assumption that we can construct a wide enough class of variations to permit our concluding (2.8) from the integral indentities involving a'. We will return to this point in §8. □

2.2 Second variation. We next differentiate j twice with respect to τ:

Theorem 2.2. *If $\psi = ae^{iu/h}$ is a critical point, then*

$$j''(0) = \int_{\mathbb{T}^n} h^2|Da'|^2 + a^2|Du'|^2 - 2(a')^2\left(\frac{|Du|^2}{2} + W - E\right) dx. \tag{2.12}$$

Proof. 1. We have

$$\begin{aligned} j'' = \int_{\mathbb{T}^n} & h^2|Da'|^2 + h^2 Da\cdot Da'' + (a')^2|Du|^2 \\ & + aa''|Du|^2 + 4aa'Du\cdot Du' + a^2|Du'|^2 \\ & + a^2 Du\cdot Du'' - 2W(a')^2 - 2Waa''\, dx. \end{aligned} \tag{2.13}$$

Differentiating (2.9), (2.10) again, we find

$$\operatorname{div}(2(a')^2 Du + 2aa''Du + 4aa'Du' + a^2Du'') = 0 \tag{2.14}$$

and

$$\int_{\mathbb{T}^n} 2(a')^2 Du + 2aa''Du + 4aa'Du' + a^2Du''dx = 0. \tag{2.15}$$

Set $\tau = 0$. Multiply (2.14) by v, integrate, multiply (2.15) by P, and add:

$$\int_{\mathbb{T}^n} 2(a')^2|Du|^2 + 2aa''|Du|^2 + 4aa'Du'\cdot Du + a^2Du''\cdot Du\, dx = 0. \tag{2.16}$$

2. We employ this equality in (2.13):

$$\begin{aligned} j''(0) &= \int_{\mathbb{T}^n} 2a''\left(-\frac{h^2}{2}\Delta a - a\left(\frac{|Du|^2}{2} + W\right)\right) + h^2|Da'|^2 \\ &\qquad - (a')^2|Du|^2 + a^2|Du'|^2 - 2W(a')^2\, dx \\ &= \int_{\mathbb{T}^n} 2a''(-Ea) + h^2|Da'|^2 - 2(a')^2\left(\frac{|Du|^2}{2} + W\right) \\ &\qquad\qquad + a^2|Du'|^2\, dx \\ &= \int_{\mathbb{T}^n} h^2|Da'|^2 + a^2|Du'|^2 - 2(a')^2\left(\frac{|Du|^2}{2} + W - E\right) dx. \end{aligned}$$

We have used here the identity

$$\int_{\mathbb{T}^n} a''a + (a')^2 dx = 0,$$

derived by twice differentiating (2.4). □

2.3 Local minimizers. We continue to write $\psi = ae^{iu/h}$, and now assume as well that

$$a > 0 \qquad \text{in } \mathbb{T}^n. \tag{2.17}$$

Observe that this follows from (2.8) and the strong maximum principle, provided a and u are smooth enough.

Theorem 2.3. *If $\psi = ae^{iu/h}$ is a critical point and* (2.17) *holds, then*

$$
j''(0) = \int_{\mathbb{T}^n} a^2|Du'|^2 + a^2 \left| D\left(\frac{a'}{a}\right)\right|^2 dx > 0, \tag{2.18}
$$

provided $a' \neq 0$.

In this case we call $\psi = ae^{iu/h}$ a *local minimizer.*

Proof. The Euler–Lagrange equation (2.8) asserts that

$$
-\frac{h^2}{2}\Delta a = a\left(\frac{|Du|^2}{2} + W - E\right).
$$

Hence

$$
\begin{aligned}
j''(0) &= \int_{\mathbb{T}^n} a^2|Du'|^2 + h^2|Da'|^2 - 2(a')^2\left(-\frac{h^2}{2}\frac{\Delta a}{a}\right) dx \\
&= \int_{\mathbb{T}^n} a^2|Du'|^2 + h^2|Da'|^2 + h^2(a')^2\frac{|Da|^2}{a^2} - 2h^2 a'\frac{Da'\cdot Da}{a} dx \\
&= \int_{\mathbb{T}^n} a^2|Du'|^2 + h^2a^2\left|D\left(\frac{a'}{a}\right)\right|^2 dx.
\end{aligned}
$$

The last term is strictly positive, unless $a' \equiv \lambda a$ for some constant $\lambda \neq 0$. But this is impossible, since

$$
\int_{\mathbb{T}^n} a'a\,dx = 0.
$$

□

3. Some useful identities.

Motivated by the foregoing calculations, our aim now is constructing an explicit state ψ, which will turn out to be a critical point, and indeed a local minimizer, of $A[\cdot]$, subject to (1.6) – (1.8). We start with two linear problems.

3.1 Dual eigenfunctions. Consider the dual eigenvalue problems:

$$
\begin{cases} -\frac{h^2}{2}\Delta w + hP\cdot Dw - Ww = E^0 w & \text{in } \mathbb{T}^n \\ w \text{ is } \mathbb{T}^n\text{-periodic} \end{cases} \tag{3.1}
$$

and

$$
\begin{cases} -\frac{h^2}{2}\Delta w^* - hP\cdot Dw^* - Ww^* = E^0 w^* & \text{in } \mathbb{T}^n \\ w^* \text{ is } \mathbb{T}^n\text{-periodic,} \end{cases} \tag{3.2}
$$

where $E^0 = E^0(P) \in \mathbb{R}$ is the principal eigenvalue. Note carefully the minus signs in front of the potential W. We may assume the real eigenfunctions w, w^* to be positive in $\mathbb{T}^n$ and normalized so that

$$\int_{\mathbb{T}^n} ww^* dx = 1. \tag{3.3}$$

Furthermore, we can take w, w^* and E^0 to be smooth in both the variables x and P.

We employ a form of the Cole–Hopf transformation, to define

$$\begin{cases} v := -h \log w \\ v^* := h \log w^*. \end{cases} \tag{3.4}$$

Then

$$\begin{cases} w = e^{-v/h} \\ w^* = e^{v^*/h}, \end{cases} \tag{3.5}$$

and a calculation shows that

$$\begin{cases} -\frac{h}{2}\Delta v + \frac{1}{2}|P + Dv|^2 + W = \bar{H}_h(P) & \text{in } \mathbb{T}^n \\ \quad v \text{ is } \mathbb{T}^n\text{-periodic} \end{cases} \tag{3.6}$$

and

$$\begin{cases} \frac{h}{2}\Delta v^* + \frac{1}{2}|P + Dv^*|^2 + W = \bar{H}_h(P) & \text{in } \mathbb{T}^n \\ \quad v^* \text{ is } \mathbb{T}^n\text{-periodic,} \end{cases} \tag{3.7}$$

for

$$\bar{H}_h(P) := \frac{|P|^2}{2} - E^0(P).$$

Standard PDE estimates applied to (3.6) and (3.7) provide the bounds

$$|Dv|, |Dv^*| \leq C, \tag{3.8}$$

for a constant C depending only upon P and the potential W.

3.2 Continuity and eikonal equations. Define

$$\sigma := ww^* \tag{3.9}$$

and

$$u := P \cdot x + \frac{v + v^*}{2}. \tag{3.10}$$

Note that although w, w^*, v, v^*, u and σ depend on h, we will for notational simplicity mostly not write these functions with a subscript h. The importance of the product (3.9) of the eigenfunctions is noted also in Anantharaman [A].

According to (3.3),

$$\sigma > 0 \text{ in } \mathbb{T}^n, \quad \int_{\mathbb{T}^n} \sigma \, dx = 1.$$

Theorem 3.1. (i) *We have*

$$\operatorname{div}(\sigma Du) = 0 \quad \text{in } \mathbb{T}^n. \tag{3.11}$$

(ii) *Furthermore,*

$$\frac{1}{2}|Du|^2 + W - \bar{H}_h(P) = \frac{h}{4}\Delta(v - v^*) - \frac{1}{8}|Dv - Dv^*|^2 \quad \text{in } \mathbb{T}^n. \tag{3.12}$$

We call (3.11) the *continuity* (or *transport*) *equation*, and regard (3.12) as an *eikonal equation* with an error term on the right hand side.

Proof. 1. We compute

$$\begin{aligned}
h \operatorname{div}(w^* Dw - wDw^*) &= h(w^*\Delta w - w\Delta w^*) \\
&= \frac{2}{h}\left(w^*\left(\frac{h^2}{2}\Delta w\right) - w\left(\frac{h^2}{2}\Delta w^*\right)\right) \\
&= \frac{2}{h}(w^*(-E^0 w - Ww + hP\cdot Dw) \\
&\qquad - w(-E^0 w^* - Ww^* - hP\cdot Dw^*)) \\
&= 2(w^* P\cdot Dw + wP\cdot Dw^*) = 2P\cdot D\sigma.
\end{aligned}$$

But

$$w^* Dw - wDw^* = w^*\left(-\frac{Dv}{h}w\right) - w\left(\frac{Dv^*}{h}w^*\right) = -\frac{1}{h}\sigma(Dv + Dv^*),$$

and therefore

$$P\cdot D\sigma + \frac{1}{2}\operatorname{div}\left(\sigma D(v+v^*)\right) = 0.$$

This is (3.11).

2. Recalling the formula

$$\frac{1}{2}|a-b|^2 + \frac{1}{2}|a+b|^2 = |a|^2 + |b|^2,$$

we compute

$$\begin{aligned}
\frac{1}{2}\left|P + \frac{1}{2}D(v+v^*)\right|^2 &= \frac{1}{8}|(P+Dv) + (P+Dv^*)|^2 \\
&= \frac{1}{4}|P+Dv|^2 + \frac{1}{4}|P+Dv^*|^2 - \frac{1}{8}|Dv - Dv^*|^2.
\end{aligned}$$

Hence

$$\begin{aligned}
\frac{1}{2}|Du|^2 + W - \bar{H}_h(P) &= \frac{1}{2}\left(\frac{1}{2}|P+Dv|^2 + W - \bar{H}_h(P)\right) \\
&\quad + \frac{1}{2}\left(\frac{1}{2}|P+Dv^*|^2 + W - \bar{H}_h(P)\right) - \frac{1}{8}|D(v-v^*)|^2 \\
&= \frac{1}{2}\left(\frac{h}{2}\Delta v\right) + \frac{1}{2}\left(-\frac{h}{2}\Delta v^*\right) - \frac{1}{8}|D(v-v^*)|^2,
\end{aligned}$$

owing to (3.6), (3.7). ☐

Remark. We also have the identities

$$-\frac{h}{2}\Delta\sigma - \operatorname{div}((P+Dv)\sigma) = 0 \tag{3.13}$$

$$-\frac{h}{2}\Delta\sigma + \operatorname{div}((P+Dv^*)\sigma) = 0. \tag{3.14}$$

For a quick derivation, observe first that

$$\frac{h}{2}\Delta\sigma = \operatorname{div}\left(\frac{1}{2}D(v^*-v)\sigma\right).$$

Add and substract this from (3.11). ☐

3.3 Integral identities involving Du and D²u. To simplify notation, we will hereafter write

$$d\sigma := \sigma dx. \tag{3.15}$$

Theorem 3.2. *These formulas hold:*

$$\int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 + W\,d\sigma = \bar{H}_h(P) + \frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\,d\sigma, \tag{3.16}$$

$$\int_{\mathbb{T}^n} |D^2u|^2 + \frac{1}{4}|D^2v - D^2v^*|^2\,d\sigma = -\int_{\mathbb{T}^n} \Delta W\,d\sigma. \tag{3.17}$$

Proof. 1. In view of (3.12),

$$\begin{aligned}\int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 + W - \bar{H}_h(P)\,d\sigma = \frac{h}{4}\int_{\mathbb{T}^n} \Delta(v-v^*)\sigma\,dx \\ -\frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\sigma\,dx.\end{aligned}$$

But $\sigma = ww^* = e^{\frac{v^*-v}{h}}$, and therefore

$$\begin{aligned}\int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 + W - \bar{H}_h(P)\,d\sigma &= -\frac{h}{4}\int_{\mathbb{T}^n} D(v-v^*)\cdot\frac{D(v^*-v)}{h}\sigma\,dx \\ &\quad -\frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\sigma\,dx \\ &= \frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\,d\sigma.\end{aligned}$$

2. Now differentiate the identity (3.12) twice with respect to x_k:

$$Du \cdot Du_{x_k x_k} + Du_{x_k} \cdot Du_{x_k} + W_{x_k x_k} = \frac{h}{4}\Delta(v - v^*)_{x_k x_k} - \frac{1}{4}D(v - v^*) \cdot D(v - v^*)_{x_k x_k} - \frac{1}{4}D(v - v^*)_{x_k} \cdot D(v - v^*)_{x_k}.$$

Multiply by σ and integrate:

$$\int_{\mathbb{T}^n} Du \cdot Du_{x_k x_k} + Du_{x_k} \cdot Du_{x_k} + W_{x_k x_k}\, d\sigma = \frac{h}{4}\int_{\mathbb{T}^n} \Delta(v - v^*)_{x_k x_k}\, d\sigma - \frac{1}{4}\int_{\mathbb{T}^n} D(v - v^*) \cdot D(v - v^*)_{x_k x_k}\, d\sigma - \frac{1}{4}\int_{\mathbb{T}^n} D(v - v^*)_{x_k} \cdot D(v - v^*)_{x_k}\, d\sigma.$$

According to Theorem 3.1, the first term on the left vanishes. We integrate by parts in the first term on the right, and thereby derive an expression that cancels the second term on the right. Next sum on k, to derive (3.17). □

4. First and second derivatives of $\bar{\mathbf{H}}_h$.

As explained in [E-G], the behavior of various expressions as functions of P is important:

Theorem 4.1. *We have*

$$D\bar{H}_h(P) = \int_{\mathbb{T}^n} Du\, d\sigma, \tag{4.1}$$

$$D^2\bar{H}_h(P) = \int_{\mathbb{T}^n} D^2_{xP}u \otimes D^2_{xP}u\, d\sigma + \frac{1}{4}\int_{\mathbb{T}^n} D^2_{xP}(v - v^*) \otimes D^2_{xP}(v - v^*)\, d\sigma. \tag{4.2}$$

In particular, $\bar{H}_h$ is a convex function of P.

Our notation means that the $(l, m)^{\text{th}}$ component of the first term on the right hand side of (4.2) is $\int_{\mathbb{T}^n} u_{x_i P_l} u_{x_i P_m}\, d\sigma$ and of the second term is $\frac{1}{4}\int_{\mathbb{T}^n} (v - v^*)_{x_i P_l}(v - v^*)_{x_i P_m}\, d\sigma$.

Proof. 1. We differentiate (3.1) and (3.2) with respect to P_k:

$$-\frac{h^2}{2}\Delta w_{P_k} + hP \cdot Dw_{P_k} - Ww_{P_k} - E^0 w_{P_k} = E^0_{P_k} w - hw_{x_k}, \tag{4.3}$$

$$-\frac{h^2}{2}\Delta w^*_{P_k} - hP \cdot Dw^*_{P_k} - Ww^*_{P_k} - E^0 w^*_{P_k} = E^0_{P_k} w^* + hw^*_{x_k}. \tag{4.4}$$

Multiply (4.3) by w^* and integrate over $\mathbb{T}^n$. Since w^* solves (3.2), we deduce

$$DE^0(P) = h \int_{\mathbb{T}^n} Dww^* dx = -\int_{\mathbb{T}^n} Dv\, ww^* dx = -\int_{\mathbb{T}^n} Dv\, d\sigma.$$

Similarly, we multiply (4.4) by w and integrate:

$$DE^0(P) = -h \int_{\mathbb{T}^n} Dw^* w\, dx = -\int_{\mathbb{T}^n} Dv^*\, d\sigma.$$

Then

$$D\bar{H}_h(P) = P - DE^0(P) = P + \frac{1}{2}\int_{\mathbb{T}^n} Dv + Dv^*\, d\sigma = \int_{\mathbb{T}^n} Du\, d\sigma.$$

2. Next, differentiate the identity (3.12) with respect to P_k and P_l:

$$\begin{aligned}\bar{H}_{h,P_kP_l} = Du \cdot Du_{P_kP_l} + Du_{P_k} \cdot Du_{P_l} - \frac{h}{4}\Delta(v-v^*)_{P_kP_l} \\ + \frac{1}{4}D(v-v^*)\cdot D(v-v^*)_{P_kP_l} + \frac{1}{4}D(v-v^*)_{P_k}\cdot D(v-v^*)_{P_l}.\end{aligned}$$

Multiply by σ and integrate, to discover

$$\begin{aligned}\bar{H}_{h,P_kP_l} = \int_{\mathbb{T}^n} Du \cdot Du_{P_kP_l} + Du_{P_k} \cdot Du_{P_l}\, d\sigma - \frac{h}{4}\int_{\mathbb{T}^n}\Delta(v-v^*)_{P_kP_l}\, d\sigma \\ + \frac{1}{4}\int_{\mathbb{T}^n} D(v-v^*)\cdot D(v-v^*)_{P_kP_l}\, d\sigma + \frac{1}{4}\int_{\mathbb{T}^n} D(v-v^*)_{P_k}\cdot D(v-v^*)_{P_l}\, d\sigma.\end{aligned}$$

In view of Theorem 3.1 and the periodicity of $u_{P_kP_l}$, the first term on the right vanishes. Since $\sigma = ww^* = e^{\frac{v^*-v}{h}}$, we can integrate by parts in the third term on the right, obtaining an expression that cancels the fourth term. Formula (4.2) results. □

As an application of Theorem 4.1, we modify some ideas from [E-G] and [E2] to discuss the effects of a *nonresonance condition* on the asymptotics as $h \to 0$.

We will explain in the next section that as $h \to 0$ the functions $\bar{H}_h$ converge uniformly on compact sets to the convex function $\bar{H}$, the *effective Hamiltonian* in the sense of Lions–Papanicolaou–Varadhan [L-P-V]. Let us suppose that $\bar{H}$ is differentiable at P and that $V = D\bar{H}(P)$ satisfies

$$V \cdot m \neq 0 \quad \text{for each } m \in \mathbb{Z}^n, m \neq 0. \tag{4.5}$$

Theorem 4.2. *Suppose also that $D^2\bar{H}_h(P)$ is bounded as $h \to 0$. Then*

$$\lim_{h\to 0}\int_{\mathbb{T}^n} \Phi(D_P u)\, d\sigma = \int_{\mathbb{T}^n} \Phi(X)\, dX \tag{4.6}$$

for each continuous, $\mathbb{T}^n$-periodic function Φ.

We discuss in [E-G] that this statement is consistent with the classical assertion that the Hamiltonian dynamics in the X, P variables, where $X := D_P u$, correspond to the trivial motion $\dot{X} = V, \dot{P} = 0$.

Proof. Fix any $m \in \mathbb{Z}^n$, and observe that the function

$$e^{2\pi i m\cdot D_P u} = e^{2\pi i m\cdot x} e^{\pi i m\cdot D_P(v+v^*)}$$

is $\mathbb{T}^n$-periodic. Consequently

$$\begin{aligned} 0 &= \int_{\mathbb{T}^n} Du \cdot D\left(e^{2\pi i m\cdot D_P u}\right)\, d\sigma = 2\pi i \int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_k u_{x_j} u_{x_j P_k}\, d\sigma \\ &= 2\pi i \int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_k \bar{H}_{h,P_k}\, d\sigma + 2\pi i \int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_k (u_{x_j} u_{x_j P_k} - \bar{H}_{h,P_k})\, d\sigma \\ &=: 2\pi i (A + B). \end{aligned} \tag{4.7}$$

We claim now that

$$B = O(h) \quad \text{as } h \to 0. \tag{4.8}$$

To confirm this, notice first that our differentiating (3.12) gives the identity

$$u_{x_j} u_{x_j P_k} - \bar{H}_{h,P_k} = \frac{h}{4}\Delta(v - v^*)_{P_k} - \frac{1}{4}(v - v^*)_{x_j}(v - v^*)_{x_j P_k};$$

and therefore

$$(u_{x_j} u_{x_j P_k} - \bar{H}_{h,P_k})\sigma = \frac{h}{4}\left((v - v^*)_{x_j P_k}\sigma\right)_{x_j}.$$

Hence

$$\begin{aligned} B &= \int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_k (u_{x_j} u_{x_j P_k} - \bar{H}_{h,P_k})\sigma\, dx \\ &= \int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_k \frac{h}{4}\left((v - v^*)_{x_j P_k}\sigma\right)_{x_j}\, dx \\ &= -\frac{h\pi i}{2}\int_{\mathbb{T}^n} e^{2\pi i m\cdot D_P u} m_l u_{x_j P_l} m_k (v - v^*)_{x_j P_k}\, d\sigma. \end{aligned}$$

So

$$|B| \leq Ch \int_{\mathbb{T}^n} |D^2_{xP} u|^2 + |D^2_{xP}(v - v^*)|^2\, d\sigma = O(h)$$

according to (4.2), since $D^2\bar{H}_h(P)$ is bounded. This proves (4.8).

But then (4.7) implies

$$|m \cdot D\bar{H}_h(P) \int_{\mathbb{T}^n} e^{2\pi i m \cdot D_P u}\, d\sigma| = |B| \leq O(h).$$

We will see in §5 that $\bar{H}_h \to \bar{H}$, locally uniformly. Since therefore $D\bar{H}_h(P) \to D\bar{H}(P) = V$ and since $m \cdot V \neq 0$, we deduce that

$$\lim_{h\to 0} \int_{\mathbb{T}^n} e^{2\pi i m \cdot D_P u}\, d\sigma = 0.$$

This limit holds for all $m \neq 0$, and hence

$$\lim_{h\to 0} \int_{\mathbb{T}^n} \Phi(D_P u)\, d\sigma = \int_{\mathbb{T}^n} \Phi(X)\, dX$$

for each $\mathbb{T}^n$–periodic function Φ. □

5. An identity involving exact solutions of the eikonal equation.

Assume next that $\hat{v}$ is a Lipschitz continuous almost everywhere solution of the cell problem

$$\text{(5.1)} \qquad \begin{cases} \frac{1}{2}|P + D\hat{v}|^2 + W = \bar{H}(P) & \text{in } \mathbb{T}^n \\ \hat{v} \text{ is } \mathbb{T}^n\text{-periodic.} \end{cases}$$

The term on the right hand side of (5.1) is the *effective Hamiltonian* in the sense of Lions–Papanicolaou–Varadhan [L-P-V], a central assertion of which is that for a given vector P problem (5.1) is solvable in the sense of viscosity solutions. (Our $\bar{H}$ corresponds to Mather's function α, and is equivalent also to Mañé's constant.)

Write

$$\text{(5.2)} \qquad \hat{u} := P \cdot x + \hat{v};$$

so that

$$\text{(5.3)} \qquad \frac{1}{2}|D\hat{u}|^2 + W = \bar{H}(P) \quad \text{almost everywhere in } \mathbb{T}^n.$$

Theorem 5.1. *This formula holds:*

$$\frac{1}{2}\int_{\mathbb{T}^n} |\frac{1}{2}D(v+v^*) - D\hat{v}|^2\, d\sigma + \frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\, d\sigma = \bar{H}(P) - \bar{H}_h(P). \tag{5.4}$$

Proof. We employ the identity

$$\frac{1}{2}|a-b|^2 + a\cdot(b-a) = \frac{1}{2}|b|^2 - \frac{1}{2}|a|^2$$

with

$$a = P + \frac{1}{2}D(v+v^*) = Du,\ \ b = P + D\hat{v} = D\hat{u},$$

to discover

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{T}^n} |\frac{1}{2}D(v+v^*) - D\hat{v}|^2\, d\sigma + \int_{\mathbb{T}^n} Du\cdot D(\hat{v} - \frac{1}{2}(v+v^*))\, d\sigma \\ = \int_{\mathbb{T}^n} \frac{1}{2}|D\hat{u}|^2 + W\, d\sigma - \int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 + W\, d\sigma.\end{aligned}$$

Owing to Theorem 3.1 and the periodicity of v, v^* and $\hat{v}$, the second term on the left vanishes. Consequently (5.3) and (3.16) imply

$$\frac{1}{2}\int_{\mathbb{T}^n} |\frac{1}{2}D(v+v^*) - D\hat{v}|^2\, d\sigma = \bar{H}(P) - \bar{H}_h(P) - \frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\, d\sigma.$$

□

As an application, we have the estimate:

Theorem 5.2. (i) *For each* $P \in \mathbb{R}^n$*,*

$$\bar{H}_h(P) \le \bar{H}(P) \le \bar{H}_h(P) + O(h) \quad \text{as } h \to 0. \tag{5.5}$$

(ii) *Hence*

$$\int_{\mathbb{T}^n} |\frac{1}{2}D(v+v^*) - D\hat{v}|^2\, d\sigma + \int_{\mathbb{T}^n} |Dv - Dv^*|^2\, d\sigma = O(h). \tag{5.6}$$

Proof. 1. According to (5.4), $\bar{H}_h(P) \le \bar{H}(P)$.

In addition, we have the minimax formula

$$\bar{H}(P) = \inf_{v\in C^1(\mathbb{T}^n)} \max_{x\in\mathbb{T}^n} \left\{\frac{1}{2}|P+Dv|^2 + W(x)\right\}. \tag{5.7}$$

(See for instance the appendix of [E2] for a quick proof due to A. Fathi.) Furthermore, standard PDE estimates deduce from (3.6), (3.7) the one–sided second derivative bounds

$$v_{\xi\xi} \leq C \quad \text{and } v^*_{\xi\xi} \geq -C, \tag{5.8}$$

for some constant C and any unit vector ξ. Then formula (3.12) implies

$$\frac{1}{2}|P + \frac{1}{2}D(v+v^*)|^2 + W \leq \bar{H}_h(P) + Ch.$$

Consequently, we can deduce from (5.7) that

$$\bar{H}(P) \leq \max_{x\in\mathbb{T}^n}\left\{\frac{1}{2}|P + \frac{1}{2}D(v+v^*)|^2 + W(x)\right\} \leq \bar{H}_h(P) + Ch.$$

2. Statement (ii) follows from (5.4), (5.5) □

6. Quantum Lagrangian calculations.

In this section we draw some connections between the minimization problems, both classical and quantum, discussed in §§1-2, and the explicitly constructed state ψ studied in §§3-5.

6.1 Quantum action. As before, we have $a = \sigma^{1/2} = e^{\frac{v^*-v}{2h}}$ and we continue to write $\psi = ae^{\frac{iu}{h}}$. Recall as well that the action of ψ is

$$A[\psi] := \int_{\mathbb{T}^n} \frac{h^2}{2}|D\psi|^2 - W|\psi|^2\, dx.$$

We next demonstrate that ψ satisfies the Euler–Lagrange equation (2.8).

Theorem 6.1. *We have*

$$\frac{1}{2}|Du|^2 + W - \bar{H}_h(P) = -\frac{h^2}{2}\frac{\Delta a}{a} \quad \text{in } \mathbb{T}^n. \tag{6.1}$$

In particular, ψ is a critical point of the action $A[\cdot]$, subject to (1.6) – (1.8).

According to Theorem 2.3, ψ is a local minimizer as well. *I conjecture that ψ is in fact a global minimizer*, but am unable to prove this.

Proof. Since $a = e^{\frac{v^*-v}{2h}}$, we compute

$$\begin{aligned}
-\frac{h^2}{2}\frac{\Delta a}{a} &= -\frac{h^2}{2}e^{\frac{v-v^*}{2h}}\Delta(e^{\frac{v^*-v}{2h}})\\
&= -\frac{h^2}{2}e^{\frac{v-v^*}{2h}}(\frac{1}{2h}\Delta(v^*-v) + \frac{1}{4h^2}|D(v^*-v)|^2)e^{\frac{v^*-v}{2h}}\\
&= \frac{h}{4}\Delta(v-v^*) - \frac{1}{8}|D(v-v^*)|^2\\
&= \frac{1}{2}|Du|^2 + W - \bar{H}_h(P),
\end{aligned}$$

the last equality being (3.12). □

We now compute the action of ψ. To do so, we first introduce $\bar{L}_h$, the Legendre transform of $\bar{H}_h$, and also write

$$V_h := D\bar{H}_h(P) = \int_{\mathbb{T}^n} Du\, d\sigma. \tag{6.2}$$

Theorem 6.2. *The quantum action of ψ is*

$$A[\psi] = \bar{L}_h(V_h). \tag{6.3}$$

Proof. Let us employ (3.11) and (3.13), to deduce

$$\begin{aligned}
A[\psi] &= \int_{\mathbb{T}^n} \frac{h^2}{2}|D\psi|^2 - W|\psi|^2 dx \\
&= \int_{\mathbb{T}^n} \frac{h^2}{2}|Da|^2 + \frac{a^2}{2}|Du|^2 - Wa^2 dx \\
&= \int_{\mathbb{T}^n} \frac{h^2}{2}|Da|^2\, dx + \int_{\mathbb{T}^n} |Du|^2 a^2\, dx - \int_{\mathbb{T}^n} \left(\frac{1}{2}|Du|^2 + W\right) a^2\, dx \\
&= \frac{1}{8}\int_{\mathbb{T}^n} |Dv - Dv^*|^2\, d\sigma + \int_{\mathbb{T}^n} (P + \frac{1}{2}D(v+v^*)) \cdot Du\, d\sigma \\
&\qquad - \int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 + W\, d\sigma \\
&= P \cdot V_h - \bar{H}_h(P) = \bar{L}_h(V_h).
\end{aligned}$$

□

6.2 Convergence as h→0. We now determine the behavior of σ and u, defined by (3.9), (3.10), as $h \to 0$. For the remainder of this section we for clarity add subscripts "h" to display the dependence on this parameter. Thus

$$\sigma_h = w_h w_h^*, \quad u_h = P \cdot x + \frac{v_h + v_h^*}{2}, \quad \text{etc.}$$

Define a measure μ_h on velocity-position configuration space by requiring

$$\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} \Phi(v,x)\, d\mu_h := \int_{\mathbb{T}^n} \Phi(Du_h(x), x)\, d\sigma_h \tag{6.4}$$

for each continuous $\Phi : \mathbb{R}^n \times \mathbb{T}^n \to \mathbb{R}$. In view of estimate (3.8) the measures $\{\mu_h\}_{h>0}$ have uniformly bounded support, and we can consequently obtain a sequence $h_j \to 0$ and a probabilitly measure μ such that

$$\mu_{h_j} \rightharpoonup \mu \quad \text{weakly as measures.}$$

We may also suppose that

$$V_{h_j} \to V \quad \text{in } \mathbb{R}^n. \tag{6.5}$$

Theorem 6.3. *The measure μ solves Mather's minimization problem* (1.1) – (1.4).

Proof. 1. First we check that μ satisfies the constraints (1.2) – (1.4), the first of which is clear since μ is a probability measure. If furthermore $\phi \in C^1(\mathbb{T}^n)$, then

$$\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v \cdot D\phi \, d\mu = \lim_{j\to\infty} \int_{\mathbb{T}^n} Du_{h_j} \cdot D\phi \, d\sigma_{h_j} = 0,$$

since $\operatorname{div}(\sigma_h Du_h) = 0$. This is (1.3); and (1.4) similarly holds since

$$\int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v \, d\mu = \lim_{j\to\infty} \int_{\mathbb{T}^n} Du_{h_j} \, d\sigma_{h_j} = \lim_{j\to\infty} V_{h_j} = V.$$

2. Recall from (5.5) that $\bar{H}_h \to \bar{H}$, uniformly on compact sets. Therefore Theorem 6.2 and (6.5) imply

$$\begin{aligned}
\bar{L}(V) &= \lim_{j\to\infty} \bar{L}_{h_j}(V_{h_j}) \\
&= \lim_{j\to\infty} \int_{\mathbb{T}^n} \frac{h_j^2}{2}|Da_{h_j}|^2 + \frac{a_{h_j}^2}{2}|Du_{h_j}|^2 - W a_{h_j}^2 \, dx \\
&= \lim_{j\to\infty} \frac{1}{8}\int_{\mathbb{T}^n} |Dv_{h_j} - Dv_{h_j}^*|^2 \, d\sigma_{h_j} + \lim_{j\to\infty}\int_{\mathbb{T}^n} \frac{1}{2}|Du_{h_j}|^2 - W \, d\sigma_{h_j} \qquad (6.6) \\
&= \lim_{j\to\infty} \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} \frac{1}{2}|v|^2 - W \, d\mu_{h_j} \\
&= \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} \frac{1}{2}|v|^2 - W \, d\mu = A[\mu].
\end{aligned}$$

Here we recalled (5.6) to ensure that the first term on the third line goes to 0.

3. Suppose now ν is any other measure satisfying (1.2) – (1.4). Let $u^\epsilon = \eta_\epsilon * \hat{u}$, where η_ϵ is a standard mollifier and as before $\hat{u}$ solves the eikonal equation (5.3) for any $P \in \partial\bar{L}(V)$. Then

$$\frac{1}{2}|Du^\epsilon|^2 + W \le \bar{H}(P) + C\epsilon$$

for some constant C, everywhere on $\mathbb{T}^n$. Therefore

$$\begin{aligned}
A[\nu] = \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} \frac{1}{2}|v|^2 - W \, d\nu &\ge \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} \frac{1}{2}|v|^2 + \frac{1}{2}|Du^\epsilon|^2 \, d\nu - \bar{H}(P) - C\epsilon \\
&\ge \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v \cdot Du^\epsilon \, d\nu - \bar{H}(P) - C\epsilon \\
&= \int_{\mathbb{R}^n}\int_{\mathbb{T}^n} v \cdot Dv^\epsilon \, d\nu + P \cdot V - \bar{H}(P) - C\epsilon \\
&= \bar{L}(V) - C\epsilon.
\end{aligned}$$

This holds for each $\epsilon > 0$, and so $\bar{L}(V)$ is less than or equal to the action of any measure ν satisfying $(1.2) - (1.4)$. But then (6.6) guaranties that the measure μ is a minimizer. $\square$

Anantharaman [A] provides interesting and additional information about the limit minimizing measure.

Limits of the eikonal equations. Upon passing if necessary to a further subsequence, we deduce from $(3.6), (3.7)$ that

$$v_{h_j} \to v, \quad v^*_{h_j} \to v^* \quad \text{uniformly on } \mathbb{T}^n,$$

where v, v^* are viscosity solutions of the respective PDE

$$\frac{1}{2}|P + Dv|^2 + W = \bar{H}(P) \quad \text{in } \mathbb{T}^n \tag{6.7}$$

and

$$-\frac{1}{2}|P + Dv^*|^2 - W = -\bar{H}(P) \quad \text{in } \mathbb{T}^n. \tag{6.8}$$

In particular the Lipschitz continuous functions v, v^* solve $(6.7), (6.8)$ almost everywhere. Therefore

$$u_{h_j} \to u := P \cdot x + \frac{v + v^*}{2} \text{ uniformly on } \mathbb{T}^n,$$

where

$$\frac{1}{2}|Du|^2 + W \leq \bar{H}(P) \quad \text{almost everywhere.} \tag{6.9}$$

Finally, write

$$\sigma := \text{proj}_x \, \mu.$$

for the projection μ onto $\mathbb{T}^n$. Then

$$\sigma_{h_j} \rightharpoonup \sigma \quad \text{weakly as measures.}$$

Applying the regularity theory from [E-G], we deduce that Dv, Dv^*, and therefore Du, exist for each point in $\text{spt}\,\sigma$, and

$$\frac{1}{2}|Du|^2 + W = \bar{H}(P) \quad \text{on } \text{spt}\,\sigma. \tag{6.10}$$

7. Quantum Hamiltonian calculations.

7.1 Quasimodes.

The observations in the last section show that our construction in §3 is a sort of semi-classical "quantization" of weak KAM theory.

We next show that ψ built above is an approximate solution of the stationary Schrödinger equation

$$-\frac{h^2}{2}\Delta\psi + W\psi = E\psi \quad \text{ in } \mathbb{T}^n.$$

Notice the plus sign in front of the potential W. As usual, $a = \sigma^{1/2} = e^{\frac{v^*-v}{2h}}$ and $\psi = ae^{\frac{iu}{h}}$. Then

$$\begin{aligned}-\frac{h^2}{2}\Delta\psi + W\psi - E\psi &= \left(\frac{1}{2}|Du|^2 + W - E\right)\psi - \frac{ih}{2}\frac{\operatorname{div}(a^2Du)}{a^2}\psi - \frac{h^2}{2}\frac{\Delta a}{a}\psi \\ &=: A + B + C.\end{aligned} \tag{7.1}$$

In view of Theorem 3.1, $B \equiv 0$. Now take

$$E = \bar{H}_h(P).$$

According to Theorem 6.1,

$$A \equiv C;$$

that is, *the formal* $O(1)$*–term identically equals the formal* $O(h^2)$*–term in the expansion* (7.1). Therefore

$$-\frac{h^2}{2}\Delta\psi + W\psi - E\psi = 2(\frac{1}{2}|Du|^2 + W - \bar{H}_h(P))\psi \tag{7.2}$$

for $E = \bar{H}_h(P)$. It is sometimes useful to rewrite this as

$$-\frac{h^2}{2}\Delta\psi = (|Du|^2 + W - \bar{H}_h(P))\psi. \tag{7.3}$$

Theorem 7.1. *If* $E = \bar{H}_h(P)$,

$$-\frac{h^2}{2}\Delta\psi + W\psi - E\psi = O(h),$$

the right hand side estimated in $L^2(\mathbb{T}^n)$.

Proof. Define the remainder term

$$R := 2(\frac{1}{2}|Du|^2 + W - \bar{H}_h(P))\psi. \tag{7.4}$$

Then

$$\frac{1}{4}\int_{\mathbb{T}^n} |R|^2\,dx = \int_{\mathbb{T}^n} \left(\frac{h}{4}\Delta(v-v^*) - \frac{1}{8}|D(v-v^*)|^2\right)^2 d\sigma$$
$$= \int_{\mathbb{T}^n} \frac{h^2}{16}(\Delta(v-v^*))^2 - \frac{h}{16}\Delta(v-v^*)|D(v-v^*)|^2 + \frac{1}{64}|D(v-v^*)|^4\,d\sigma.$$

Observe now that

$$\begin{aligned}
-\frac{h}{16}\int_{\mathbb{T}^n} \Delta(v-v^*)|D(v-v^*)|^2\,d\sigma &= -\frac{h}{16}\int_{\mathbb{T}^n} \Delta(v-v^*)|D(v-v^*)|^2 e^{\frac{v^*-v}{h}}\,dx \\
&= \frac{1}{16}\int_{\mathbb{T}^n} |D(v-v^*)|^2 D(v-v^*)\cdot D(v^*-v)\,d\sigma \\
&\quad + \frac{h}{8}\int_{\mathbb{T}^n} D(v-v^*)\cdot D^2(v-v^*)D(v-v^*)\,d\sigma \\
&= -\frac{1}{16}\int_{\mathbb{T}^n} |D(v-v^*)|^4\,d\sigma \\
&\quad + \frac{h}{8}\int_{\mathbb{T}^n} D(v-v^*)\cdot D^2(v-v^*)D(v-v^*)\,d\sigma.
\end{aligned}$$

Since $\frac{1}{16} > \frac{1}{64}$, we derive for some constant C the estimate:

$$\int_{\mathbb{T}^n} |R|^2\,dx + \int_{\mathbb{T}^n} |D(v-v^*)|^4\,d\sigma \le Ch^2\int_{\mathbb{T}^n} |D^2(v-v^*)|^2\,d\sigma. \tag{7.5}$$

We deduce finally from (7.5) and (3.17) that R is of order at most $O(h)$ in $L^2(\mathbb{T}^n)$. □

Remark. The $O(h)$–error term is not especially good, and indeed M. Zworski has outlined for me some other constructions building quasimodes with similar error estimates in quite general circumstances. Estimate (7.5) does show that if $E = \bar{H}_h(P)$ and *if*

$$\int_{\mathbb{T}^n} |D^2(v-v^*)|^2\,d\sigma = o(1), \tag{7.6}$$

we would then have the better error bound

$$-\frac{h^2}{2}\Delta\psi + W\psi - E\psi = o(h) \quad \text{as } h \to 0$$

in $L^2(\mathbb{T}^n)$. We may hope that assertion (7.6) is true in some generality, although it can fail, as the following shows:

Example. Assume that $P = 0$ and that the potential W attains its maximum at a unique point $x_0 \in \mathbb{T}^n$, where $\Delta W(x_0) < 0$. In this situation we can readily check that $\bar{H}(0) = W(x_0)$.

Since $P = 0$, we can take $w \equiv w^*$; whence $v \equiv -v^*$ and so $u \equiv 0$. Then according to (3.16) and (5.15),

$$\lim_{h\to 0} \int_{\mathbb{T}^n} W\, d\sigma = W(x_0) = \max_{\mathbb{T}^n} W.$$

So the weak limit of the measures σ as $h \to 0$ is the unit mass at x_0. Consequently, the identity (3.17) implies

$$\lim_{h\to 0} \int_{\mathbb{T}^n} |D^2(v - v^*)|^2\, d\sigma = -4\Delta W(x_0) > 0.$$

This example is from the forthcoming paper of Y. Yu [Y], who provides a very complete analysis of our problem in one dimension. In particular, if $n = 1$ and $\bar{H}(P) > \min \bar{H}$, the error term is indeed $o(h)$ in L^2 as $h \to 0$. □

7.2 **Comparison with stochastic mechanics** There are formal connections with the Guerra–Morato and Nelson variational principle in stochastic quantum mechanics, as set forth in Nelson [N], Guerra–Morato [G-M], Yasue [Ya], Carlen [C], etc. (I thank A. Majda for some of these references.)

I attempt here to explain the link by recasting their form of the action into our setting and notation, disregarding the probabilistic interpretations. In effect, then, the action of Guerra–Morato becomes

$$\tilde{A}[\psi] := \int_{\mathbb{T}^n} \left(\frac{1}{2} Dv^* \cdot Dv - W \right) a^2\, dx \tag{7.10}$$

for $\psi = ae^{iu/h}$, $a = e^{\frac{v^*-v}{2h}}$, $u = \frac{1}{2}(v+v^*)$, $P = 0$. (The Lagrangian density $\left(\frac{1}{2}Dv^* \cdot Dv - W\right) a^2$ here should be compared with formula (93) in Guerra–Morato [G-M]. See also (14.31) in Nelson [N].) We rewrite this, observing that

$$-\frac{h^2}{2}|Da|^2 + \frac{a^2}{2}|Du|^2 = \frac{a^2}{2} Dv^* \cdot Dv.$$

Consequently

$$\tilde{A}[\psi] = \int_{\mathbb{T}^n} -\frac{h^2}{2}|Da|^2 + \frac{a^2}{2}|Du|^2 - Wa^2\, dx. \tag{7.11}$$

This action differs from ours due to the sign change in the first term.

Theorem 7.2. *Let $\psi = ae^{iu/h}$ be a smooth critical point of the action $\tilde{A}[\cdot]$, subject to the constants* (1.6)–(1.8). *Then for some real constant E:*

$$-\frac{h^2}{2}\Delta\psi + W\psi = E\psi \qquad \text{in } \mathbb{T}^n, \tag{7.12}$$

and so ψ is an exact solution of this stationary Schrödinger equation.

Proof. We deduce, as in the proof of Theorem 2.1, that

$$-\frac{h^2}{2}\Delta a + a\left(\frac{|Du|^2}{2} + W - E\right) = 0,$$

with a sign change as compared with (2.8). Thus if we write out (7.1), we have

$$-\frac{h^2}{2}\Delta\psi + W\psi - E\psi = A + B + C,$$

and $B \equiv 0$, $A + C \equiv 0$. □

8. Connections with linear elliptic homogenization

This section works out some relationships between $\bar{H}_h$ and homogenization theory for divergence—structure, second order elliptic PDE: see for instance Bensoussan–Lions–Papanicolaou [B-L-P]. Our conclusions are very similar to those of Capdeboscq [Cp], and the calculations in Pedersen [P] are related as well.

Let $A = ((a_{ij}))$ be symmetric, positive definite, and $\mathbb{T}^n$-periodic. Suppose U is a bounded, open subset of $\mathbb{R}^n$, with a smooth boundary. We consider this boundary value problem for an elliptic PDE with rapidly varying coefficients:

$$\begin{cases} -\left(a_{ij}\left(\frac{x}{\varepsilon}\right)u^{\varepsilon}_{x_i}\right)_{x_j} = f & \text{in } U \\ u^{\varepsilon} = 0 & \text{on } \partial U. \end{cases}$$

Then $u^{\varepsilon} \rightharpoonup u$ weakly in $H^1_0(U)$, u solving the limit problem

$$\begin{cases} -\bar{a}_{ij}u_{x_i x_j} = f & \text{in } U \\ u = 0 & \text{on } \partial U. \end{cases}$$

The *effective diffusion coefficient matrix* $\bar{A} = ((\bar{a}_{ij}))$ is determined as follows [B-L-P]. For $j = 1, \dots, n$, let χ^j solve the *corrector problem*

$$\begin{cases} -(a_{kl}\chi^j_{x_k})_{x_l} = (a_{jl})_{x_l} & \text{in } \mathbb{T}^n \\ \chi^j \text{ is } \mathbb{T}^n\text{-periodic.} \end{cases} \tag{8.1}$$

Let us then for $i, j = 1, \dots, n$ define

$$\bar{a}_{ij} := \int_{\mathbb{T}^n} a_{ij} - a_{kl}\chi^i_{x_k}\chi^j_{x_l}\,dx. \tag{8.2}$$

Theorem 8.1. *Define $V_h = D\bar{H}_h(P)$. Then*

$$\bar{A}P = V_h, \tag{8.3}$$

where $\bar{A} = ((\bar{a}_{ij}))$ is the effective diffusion coefficient matrix corresponding to

$$A := a^2 I = ((a^2\delta_{ij})). \tag{8.4}$$

Notice in (8.4) that $a^2 = \sigma = ww^*$ depends on both h and P.

Proof. For the special case of the diagonal matrix A given by (8.4), the corrector PDE (8.1) reads

$$\begin{cases} -(a^2\chi^j_{x_k})_{x_k} = (a^2)_{x_j} & \text{in } \mathbb{T}^n \\ \chi^j \text{ is } \mathbb{T}^n\text{-periodic.} \end{cases} \tag{8.5}$$

Now $u = x \cdot P + \frac{1}{2}(v + v^*)$ solves

$$\operatorname{div}(\sigma Du) = 0,$$

and therefore

$$-\operatorname{div}\left(a^2\frac{1}{2}D(v+v^*)\right) = \operatorname{div}(a^2P) = D(a^2)\cdot P.$$

Hence

$$\frac{v+v^*}{2} = P_i\chi^i. \tag{8.6}$$

Consequently, for $j = 1, \dots, n$

$$\begin{aligned} V_{h,j} &= \int_{\mathbb{T}^n} u_{x_j}\,d\sigma = \int_{\mathbb{T}^n} (\chi^i + x_i)_{x_j} P_i\,d\sigma \\ &= P_j - \int_{\mathbb{T}^n} \chi^i P_i \sigma_{x_j}\,dx = P_j + \int_{\mathbb{T}^n} \chi^i P_i (a^2\chi^j_{x_k})_{x_k}\,dx \\ &= P_j - \int_{\mathbb{T}^n} P_i a^2 \chi^i_{x_k}\chi^j_{x_k}\,dx = (\bar{A}P)_j. \end{aligned}$$

□

Remark: constructing a family of variations. We return finally to a point left open in §2. Recall that we introduced a one parameter family of variations $\{(u(\tau), a(\tau))\}_{-1\le\tau\le1}$ satisfying the constraints (2.4)–(2.6), with $(u(0), a(0)) = (u, a)$. We assumed also that

$$u(\tau) = P(\tau)\cdot x + v(\tau), \tag{8.7}$$

for $P(\tau) \in \mathbb{R}^n$ and $v(\tau)$ is $\mathbb{T}^n$–periodic.

To finish up the proof of Theorem 2.1 we needed to know that $a' := \frac{da}{d\tau}$ was arbitrary, subject only to the integral identity (2.11). We show next we can indeed do so, provided

$$a > 0 \quad \text{in } \mathbb{T}^n. \tag{8.8}$$

To confirm this, take a smooth function $a(\cdot)$ of τ satisfying (2.4) and $a(0) = a$. For a given $P \in \mathbb{R}^n$, we invoke the Fredholm alternative to solve

$$-\operatorname{div}(a^2(\tau)Dv) = \operatorname{div}(a^2(\tau)P)$$

for a periodic function $v = v(\tau)$. Then $u(\tau) = P \cdot x + v(\tau)$ solves $\operatorname{div}(a(\tau)^2 Du(\tau)) = 0$, and the issue is whether for small τ we can select $P = P(\tau)$ so that

$$\int_{\mathbb{T}^n} a^2(\tau)Du(\tau)\,dx = V. \tag{8.9}$$

We next introduce the function $\mathbf{\Psi} = \{\Psi^1, \dots, \Psi^n\}$ defined by

$$\mathbf{\Psi}(P) := \int_{\mathbb{T}^n} a^2 Du\,dx = P + \int_{\mathbb{T}^n} a^2 Dv\,dx.$$

Now since $-\operatorname{div}(a^2 Dv) = \operatorname{div}(a^2 P)$, we have

$$-(a^2 v_{x_k P_l})_{x_k} = (a^2)_{x_l};$$

and so

$$v_{P_l} = \chi^l$$

in the notation above. Therefore, as in the proof of Theorem 8.1, we can calculate

$$\begin{aligned}
\Psi^k_{P_l} &= \delta_{kl} + \int_{\mathbb{T}^n} a^2 v_{x_k P_l}\,dx = \delta_{kl} - \int_{\mathbb{T}^n} (a^2)_{x_k} v_{P_l}\,dx \\
&= \delta_{kl} + \int_{\mathbb{T}^n} (a^2 v_{x_i P_k})_{x_i} v_{P_l}\,dx = \delta_{kl} - \int_{\mathbb{T}^n} a^2 v_{x_i P_k} v_{x_i P_l}\,dx \\
&= \bar{a}_{kl}.
\end{aligned}$$

In other words, $D\mathbf{\Psi}(P) = \bar{A}$ and the latter matrix is nonsingular. Hence the Implicit Function Theorem ensures for small τ that we can find $P = P(\tau)$ satisfying (8.9). $\square$

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