

On the quantum Guerra-Morato Action Functional

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Abstract

Given a smooth potential $W : \mathbb{T}^n \rightarrow \mathbb{R}$ on the torus, the Quantum Guerra-Morato action functional is given by

$$I(\psi) = \int \left(\frac{Dv Dv^*}{2}(x) - W(x) \right) a(x)^2 dx,$$

where ψ is described by $\psi = a e^{i \frac{u}{\hbar}}$, $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$, v, v^* are real functions, $\int a^2(x) dx = 1$, and D is derivative on $x \in \mathbb{T}^n$. It is natural to consider the constraint $\operatorname{div}(a^2 Du) = 0$. The a and u obtained from a critical solution (under variations τ) for such action functional, fulfilling such constraints, satisfy the Hamilton-Jacobi equation with a quantum potential. Denote $' = \frac{d}{d\tau}$. We show that the expression for the second variation of a critical solution is given by

$$\int a^2 D[v'] D[(v^*)'] dx.$$

Introducing the constraint $\int a^2 Du dx = V$, we also consider later an associated dual eigenvalue problem. From this follows a transport and a kind of eikonal equation.

1 Introduction

In [10] L. C. Evans considered an Action Functional which is related to Aubry-Mather theory and also present another Action Functional which he called the Guerra-Morato Action Functional. The first Functional is of Lagrangian nature and the second Functional of Hamiltonian nature. This last one is more adequate for the description of the Physics of Quantum Mechanics, and to analyze its properties is the primary goal of the present work. In [10] a few properties of this last mentioned functional were presented and we intend to provide here a more complete description of the topic. One of our goals is to characterize critical action solutions for this quantum action functional; they

are not necessarily local minimal solutions. Our main result concerns the expression for the second variation of a critical solution (see Theorem 1). We will present full proofs adapting the reasoning followed in [10] (with the necessary changes at each moment).

The Evans Functional Action (see (1.5) in [10]) plays an important role in the quantum analog of weak KAM theory.

The reason for the terminology Guerra-Morato Action Functional introduced in [10] was motivated by the paper [13] by F. Guerra and L. Morato. Related work appear in [25], [20], [?] and [22]. In fact, the expression coined by Evans, which is of a stationary nature, does not appear in this form in [13] which is of nonstationary type. Moreover, in [13] there is no assumption to constraints which is an essential issue in [10].

The papers [1], [2], [3], [18], [11], [23], [24] and [6] analyze different types of problems related to Evans Functional Action and Mather measures.

Let's consider a potential of class C^∞ given by $W : \mathbb{T}^n = (S^1)^n \rightarrow \mathbb{R}$, where S^1 is the unit circle. Under some suitable assumptions similar results hold for $W : \mathbb{R}^n \rightarrow \mathbb{R}$ but we will not address this issue here.

The classical Lagrangian is given by

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

and the associated classical (mechanical) Hamiltonian is

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

where m denotes the mass.

Taking $p = mv$, it is well known that the solutions of the Euler-Lagrange equation for L and the ones for the Hamilton equation correspond to each other via a change of coordinates. It is well known that in Classical Mechanics there exist critical action principles for the Lagrangian formulation and for Hamiltonian one (see [4]). From the point of view of Physics, solutions minimizing the action are preferred in the theory.

We denote $\hbar = \frac{1}{m}$. A wave function has the form $\psi = a e^{i \frac{u}{\hbar}}$, where a is positive and u is real.

In Quantum Mechanics the expected value of the Hamiltonian is

$$\int \left(\frac{\hbar}{2} |D\psi|^2 + W|\psi|^2 \right) dx \tag{1}$$

Given the functions $a > 0$ and u , where $a : T^n \rightarrow \mathbb{R}$ and $u : T^n \rightarrow \mathbb{R}$, consider $s = \hbar \log a$ and take $v^* = (u + s)$ and $v = (u - s)$, then

$$\frac{v + v^*}{2} = u$$

and

$$\frac{v^* - v}{2} = s = \hbar \log a.$$

Thus, we can write every function of the form $a e^{i \frac{u}{\hbar}}$, in terms of v and v^* by solving the above equation.

If u and a are periodic (in $(S^1)^n$) the same goes for $v, v^* : T^n \rightarrow \mathbb{R}$.

Likewise given v and v^* , the functions $a > 0$ and u can be determined using the above expressions.

The Guerra-Morato action functional (see (7.10) in [10]) is given by

$$I(\psi) = \int \left(\frac{Dv Dv^*}{2} - W \right) a(x)^2 dx \quad (2)$$

where ψ is described by $\psi = a e^{i \frac{u}{\hbar}}$, $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$, v, v^* are real functions and $\int a^2(x) dx = 1$. When considering critical action for such functional, we are analyzing a problem that is different from the critical action problem for the Evans Action Functional, as defined by (1.5) in [10] (see also our Remark 4).

The function ψ will be assumed to satisfy the constraints (7), (8), (9) to be defined next (see also (17), (18) and (19)). Expressions (7), (8), (9) are in some sense the *field version* of the corresponding classical constraints in Aubry-Mather theory (see [14]). The expression (8) corresponds to the assumption that a probability is holonomic and condition (9) plays the role of a homological class (see Section 2.6 in [9]).

Our main result is

Theorem 1. *If $\psi = a e^{i u/\hbar}$ is critical for the action and $a > 0$, where $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$, then the second derivative of the variation has the expression*

$$\int a^2 D[v'] D[(v^*)'] dx. \quad (3)$$

The sign of (3) will determine if the critical solution is a local minimum or a local maximum (or indeterminate).

The above functional I is Hamiltonian in nature (the Evans functional is Lagrangian in nature according to discussion on page 312 in [10]). Here we will analyze a principle of **critical action** for such an action I .

We say that a certain ψ is critical for I if any close-by variation will have zero derivative. Another issue will be whether at a given critical ψ , the functional I attains a minimum, a maximum, or neither. Our objective will be to analyze the first and second variational problems.

We point out that in Sections 2 and 3 here (in the same way as in Section 2 in [10]) the functions $v, v^* : T^n \rightarrow \mathbb{R}$, do not satisfy any other constraint different from $\int e^{\frac{v^*(x)-v(x)}{\hbar}} dx = 1$. When comparing our setting with the hypothesis (16), (17), and (18) in [25], it is clear that in [25] there are assumptions on b, b^* , which does not correspond to the freedom of our v, v^* . In the same direction, expressions (4) (5) (6), and (7) in [8] show that we are considering a different class of problems.

In Section 4 and 5 the functions v, v^* will satisfy certain relations which will be described by (32) and (33). When considering (3) (see also (32) and (33)) we get from Remarks 9 and 11 that a critical point is not necessarily a local minimum (or maximum).

In our understanding, the above expression of the functional (2), taken from Section 7.2 in [10], corresponds to a different type of problem that one considered in [13]. We also point out that [13] considered variational problems depending on time which is a different framework when compared with [10].

Remark 2. *To add the term Px to u , getting $\tilde{u} = u + Px$, is equivalent to consider the new functions $\tilde{v} = v + Px$ and $\tilde{v}^* = v^* + Px$.*

Below D will denote derivative with respect to x .

We will need a later expression (4).

As $\frac{a'}{a} = \frac{(v^*)' - v'}{2\hbar}$, then

$$-\hbar^2 \left| D\left(\frac{a'}{a}\right) \right|^2 + |Du'|^2 = D[v'] D[(v^*)'] \quad (4)$$

In the case we want to consider $\tilde{u} = u + Px$ instead of u , we get

$$-\hbar^2 \left| D\left(\frac{a'}{a}\right) \right|^2 + |D\tilde{u}'|^2 = D[\tilde{v}'] D[(\tilde{v}^*)'] = D[v'] D[(v^*)']. \quad (5)$$

Here $\tilde{\psi}$ will be considered in the form $\tilde{\psi} = a e^{i\frac{u}{\hbar}}$, where $a = e^{\frac{v^*-v}{2\hbar}}$ and $u = \frac{v^*+v}{2}$, where v and v^* are periodic functions taking real and differentiable values.

Let's assume that ψ has the "Bloch waveform"

$$\psi = e^{i\frac{1}{\hbar}Px} \tilde{\psi}$$

for some $P \in \mathbb{R}^n$ and where $\tilde{\psi} : \mathbb{T}^n \rightarrow \mathbb{C}$ was given in the above form. The introduction of the parameter P is quite important in our reasoning.

Consider a fixed vector $V \in \mathbb{R}^n$.

Let us now consider the Quantum Guerra-Morato action of the state ψ

$$A[\psi] := \int_{\mathbb{T}^n} \left(\frac{D v^*(x) D v(x)}{2} - W(x) \right) a^2(x) dx, \quad (6)$$

where we assume that

$$\int_{\mathbb{T}^n} |\psi(x)|^2 dx = \int_{\mathbb{T}^n} a(x)^2 dx = 1, \quad (7)$$

$$\int_{\mathbb{T}^n} (\overline{\psi(x)} D \psi(x) - \psi(x) D \overline{\psi(x)}) \cdot D \phi(x) dx = 0 \text{ for all } \phi \in C^1(\mathbb{T}^n), \quad (8)$$

and

$$\frac{\hbar}{2i} \int_{\mathbb{T}^n} (\overline{\psi} D \psi - \psi D \overline{\psi}) dx = V. \quad (9)$$

If ψ is differentiable then (8) implies

$$\operatorname{div}(\overline{\psi} D \psi - \psi D \overline{\psi}) = 0 \quad (10)$$

The vector field $j := \overline{\psi} D \psi - \psi D \overline{\psi}$ represents what is called the flux in quantum mechanics.

Note that

$$\frac{\hbar}{2i} (\overline{\psi} D \psi - \psi D \overline{\psi}) = \frac{\hbar}{2i} \left(a a' + a^2 \frac{i u'}{\hbar} - a a' + a^2 \frac{i u'}{\hbar} \right) = a^2 u'. \quad (11)$$

So the condition (10) can be replaced by the transport equation

$$\operatorname{div}(a^2 D u) = 0$$

and condition (9) by

$$\int a^2 D u dx = V. \quad (12)$$

Fixing v, v^* we will denote

$$V_0 := \int a^2(x) D u(x) dx = \int \left(e^{\frac{v^*(x) - v(x)}{2\hbar}} \right)^2 D \left(\frac{v^*(x) + v(x)}{2} \right) dx.$$

If we consider $\tilde{u} = \frac{v^*(x) + v(x)}{2} + P x$ instead of $u = \frac{v^*(x) + v(x)}{2}$, as in Remark 2, we get

$$\int a^2 D \tilde{u} dx = \int a^2 (D u + P) dx = V_0 + P = V = V_P. \quad (13)$$

Remark 3. *This shows that the value V , which we fix as a constraint, is coupled with the term P . Note that in the reasoning of Sections 2 and 3 the constraint (12) is not used.*

2 First variation

Consider the state ψ in polar form where

$$\psi = a e^{i \frac{u}{\hbar}}, \quad (14)$$

and where the phase u satisfies the expression

$$u(x) = P \cdot x + z(x) \quad (15)$$

for some periodic function z .

It is known from (7.11) Section 7.2 in [10] that the Guerra-Morato action is given in this case by

$$A[\psi] = \int_{\mathbb{T}^n} -\frac{\hbar^2}{2} |Da|^2 + \frac{a^2}{2} |Du|^2 - W a^2 dx, \quad (16)$$

Remark 4. *This action is different from (2.3) considered in [10] due to a change of sign in the first term under the integral (see section 7.2 in [10]). Indeed, compare (16) with (2.3) in [10].*

We are initially interested in the critical points of this action.

Note that (7), (8) and (9) become by (11) in the expressions

$$\int_{\mathbb{T}^n} a^2 dx = 1, \quad (17)$$

$$\operatorname{div}(a^2 Du) = 0, \quad (18)$$

$$\int_{\mathbb{T}^n} a^2 Du dx = V. \quad (19)$$

Let $\{(u(\tau), a(\tau))\}_{-1 \leq \tau \leq 1}$ be a differentiable family of functions indexed by τ such that it satisfies the constraints above, i.e., (17)-(19) holds for $a = a(\tau)$, and moreover $(u(0), a(0)) = (u, a)$. Let's assume that for every $\tau \in (-1, 1)$, we can write

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

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

$$j(\tau) := \int_{\mathbb{T}^n} -\frac{\hbar^2}{2m} |Da(\tau)|^2 + \frac{a^2(\tau)}{2} |Du(\tau)|^2 - W a^2(\tau) dx,$$

In the next theorems, we denote $' = \frac{d}{d\tau}$, and in turn, the derivative with respect to x will be denoted as D .

We can thus consider variations and, under the hypothesis that the choice of a, u is critical for the action, we will be able to obtain constraints for a and u .

Consider a and u fixed and we will look for conditions obtained when they are critical for the action.

Note that as the functions $a' = a'(0)$ and $u' = u'(0)$ denote the derivative with respect to the variation $\{(u(\tau), a(\tau))\}_{-1 \leq \tau \leq 1}$, with the variable τ , they can be quite general. But, for example, a' must satisfy the identity

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

which is obtained by differentiating with respect to τ , at $\tau = 0$, the expression

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

Theorem 5. *Suppose that ψ is described by $\psi = a e^{i \frac{u}{\hbar}}$. Then $j'(0) = 0$ for all variations, if and only if,*

$$\frac{\hbar^2}{2} \Delta a = a \left(\frac{|Du|^2}{2} + W - E \right) \quad (20)$$

for some real number E .

In this case, a and u satisfy the so-called Hamilton-Jacobi equation with a quantum potential.

Proof. First, let's estimate $j'(\tau)$. An easy account shows that

$$j'(\tau) = \int_{\mathbb{T}^n} \left(-\frac{\hbar^2}{m} Da \cdot Da' + aa' |Du|^2 + a^2 Du \cdot Du' - 2Waa' \right) dx.$$

Above, $a = a(\tau)$, $u = u(\tau)$. Taking derivatives at $\tau = 0$ under the assumption of constraints we obtain:

$$\operatorname{div}(2aa'Du + a^2 Du') = 0, \quad (21)$$

$$\int_{\mathbb{T}^n} (2aa'Du + a^2 Du') \, dx = 0, \quad (22)$$

Remember that $Du = P + Dz$. We multiply (21) by u and integrate in space. Then, by integrating by parts we arrive at

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

So,

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

Remember that each variation a' must satisfy the identity

$$\int_{\mathbb{T}^n} \frac{d a(\tau)}{d \tau} a dx = \int_{\mathbb{T}^n} a' a dx = 0.$$

Assume that a and u satisfy

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

for some constant E .

Thus, $j'(0) = 0$ for any variation of a and u .

The above expression means

$$\left(\frac{|Du|^2}{2} + W \right) - E = \frac{\hbar^2}{2m} \frac{\Delta a}{a}, \quad (23)$$

for some constant E .

Let's show that when $j'(0) = 0$ we get that the reciprocal holds. We assume that $a^2 > 0$.

Now,

$$\begin{aligned} j'(0) &= 2 \int_{\mathbb{T}^n} a' \left(\frac{\hbar^2}{2m} \Delta a - a \left(\frac{|Du|^2}{2} + W \right) \right) dx \\ &= 2 \int_{\mathbb{T}^n} a' g dx. \end{aligned}$$

As a' is general, the only restriction being that $\int a a' dx = 0$, we can conclude from $j'(0) = 0$, that there is a constant E such that $g = -a E$ and the result follows (similar reasoning as Theorem 2.1 in [10]).

Note that given the constraint (19) on V , the vector P has to be set, and this shows a coupling of the value E with V (and also P)

□

The next result was proved in Theorem 7.2 in [10]

Theorem 6. *If $\psi = a e^{i \frac{u}{\hbar}}$ is differentiable and critical for the Guerra-Morato action, then ψ is an eigenfunction of the Hamiltonian operator*

$$-\frac{\hbar^2}{2} \Delta \psi + W \psi = E \psi, \quad (24)$$

for some $E \in \mathbb{R}$.

Note that expression (20) is different from expression (2.8) in [10] due to a change of sign in the Laplacian term.

3 Second variation

Let us now analyze the second variation. Thus, we will take the second derivative of j with respect to τ .

Theorem 7. *Suppose that ψ is described by $\psi = a e^{i \frac{u}{\hbar}}$, where $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$ and v, v^* are real functions. If $\psi = a e^{i u/\hbar}$ is a critical point for action I then*

$$j''(0) = \int_{\mathbb{T}^n} -\frac{\hbar^2}{m} |Da'|^2 + a^2 |Du'|^2 - 2(a')^2 \left(\frac{|Du|^2}{2} + W - E \right) dx. \quad (25)$$

Proof. Note that

$$\begin{aligned} j''(\tau) = \int_{\mathbb{T}^n} & \left[-\frac{\hbar^2}{m} |Da'|^2 - \frac{\hbar^2}{m} Da \cdot Da'' \right] \\ & + [aa'' |Du|^2 + 4aa' Du \cdot Du' + a^2 Du \cdot Du''] \\ & + [(a')^2 |Du|^2 + a^2 |Du'|^2 - 2W(a')^2 - 2Waa''] dx. \end{aligned} \quad (26)$$

Taking derivative in (21) and (22) we get

$$\operatorname{div}(2(a')^2 Du + 2aa'' Du + 4aa' Du' + a^2 Du'') = 0 \quad (27)$$

and

$$\int_{\mathbb{T}^n} (2(a')^2 Du + 2aa'' Du + 4aa' Du' + a^2 Du'') dx = 0. \quad (28)$$

Now take $\tau = 0$, multiply (27) by u , integrate, and do integration by parts to get

$$\int_{\mathbb{T}^n} [2(a')^2 |Du|^2 + 2aa'' |Du|^2 + 4aa' Du' \cdot Du + a^2 Du'' \cdot Du] dx = 0. \quad (29)$$

Let's now use the expression (26). As $j'(0) = 0$, we integrate by parts $(-h^2/2m) Da \cdot Da''$ and obtain

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

Above we use the identity

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

obtained by differentiating with respect to τ twice and using $\int a^2 dx = 1$.

The reasoning above proves the claim we were looking for. \square

Note that (25) is an expression which is different from (2.12) in [10].

4 Other expression for $j''(0)$

We want to get a more appropriate expression for $j''(0)$.

Let's assume that

$$a(x) > 0, \text{ for all } x \in \mathbb{T}^n.$$

Theorem 8. If $\psi = a e^{iu/\hbar}$ is critical for the action and $a > 0$, where $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$, then

$$j''(0) = \int_{\mathbb{T}^n} \left(|Du'|^2 - \frac{\hbar^2}{m} \left| D\left(\frac{a'}{a}\right) \right|^2 \right) a^2 dx = \int a^2 D[v'] D[(v^*)'] dx. \quad (30)$$

Proof: Since ψ is critical, from (23) we have

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

So, from (4) we have

$$\begin{aligned} j''(0) &= \int a^2 |Du'|^2 - \frac{\hbar^2}{m} |Da'|^2 - 2(a')^2 \left(\frac{\hbar^2}{2m} \frac{\Delta a}{a} \right) dx \\ &= \int a^2 |Du'|^2 - \frac{\hbar^2}{m} |Da'|^2 - \frac{\hbar^2}{m} (a')^2 \frac{|Da|^2}{a^2} + \frac{2\hbar^2}{m} a' \frac{Da' \cdot Da}{a} dx \\ &= \int_{\mathbb{T}^n} a^2 |Du'|^2 - \frac{\hbar^2}{m} a^2 \left| D\left(\frac{a'}{a}\right) \right|^2 dx = \int a^2 D[v'] D[(v^*)'] dx, \end{aligned}$$

showing the claim of the theorem.

□

Note that $j''(0)$ in expression (30) may be positive or negative.

Remark 9. Remember that ψ is described by $\psi = a e^{i\frac{u}{\hbar}}$, where $u = \frac{v+v^*}{2}$, $a = e^{\frac{v^*-v}{2\hbar}}$ e v, v^* are real functions. Note that if $v = -v^*$ then the $j''(0)$ is negative. Also, if $v + v^*$ is constant, then the above expression is negative.

Remark 10. Note that in the case we consider $u = \frac{v+v^*}{2} + Px$, we also get

$$j''(0) = \int a^2 D[v'] D[(v^*)'] dx. \quad (31)$$

We point out that from Remark 3 the vector P has to be set from the constraint (19) on V .

Remark 11. Similar results hold when $x \in \mathbb{R}^n$ and not on the torus. Let's consider $x \in \mathbb{R}$ next. Note that in the case of the harmonic oscillator $H(x, p) = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$ we have the ground state ψ_0 , which is the minimum energy state $E_0 = \frac{1}{2} \hbar \omega$, is described by

$$\psi_0(x) = \left(\frac{m\omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}.$$

Thus, $|\psi_0|^2$ will determine a Gaussian density with variance $a = \sqrt{\frac{h}{2mw}}$.

Note that $v^*(x) - v(x) = -mx^2$ and $v + v^* = 0$.

Thus, $v' = -v^*'$ and

$$\frac{1}{m} \int a^2 D[v'] D[(v^*)'] dx < 0$$

That is, we just show the ground state ψ_0 is not minimum for the Guerra-Morato action I when $x \in \mathbb{R}$ (and not in the circle).

5 Dual eigenfunctions

In this section, we will assume conditions on v, v^* .

It is natural to consider the dual eigenvalue problems:

$$\begin{cases} -\frac{h^2}{2}\Delta w + hP \cdot Dw + Ww = E_h^0 w & \text{in } \mathbb{T}^n \\ w \text{ is } \mathbb{T}^n \text{ periodic} \end{cases} \quad (32)$$

and

$$\begin{cases} -\frac{h^2}{2}\Delta w^* - hP \cdot Dw^* + Ww^* = E_h^0 w^* & \text{in } \mathbb{T}^n \\ w^* \text{ is } \mathbb{T}^n \text{ periodic,} \end{cases} \quad (33)$$

where $E_h^0(P) \in \mathbb{R}$ is the main eigenvalue. We may assume the real eigenfunctions w, w^* to be positive in \mathbb{T}^n and normalized in such way that

$$\int_{\mathbb{T}^n} ww^* dx = 1. \quad (34)$$

Moreover, we can take w, w^* and E_h^0 to be twice differentiable in x and P .

Note the change of sign in the W term when compared with (3.1) and (3.2) in [10] (and also [1] and [3]).

In the same way as in [10] we employ a form of the Cole-Hopf transformation, to define

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

Then,

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

and then follows that

$$\begin{cases} -\frac{h}{2}\Delta v + \frac{1}{2}|P + Dv|^2 - W = \overline{H}_h(P) & \text{in } \mathbb{T}^n \\ v \text{ is a } \mathbb{T}^n\text{-periodic function} \end{cases} \quad (35)$$

and

$$\begin{cases} \frac{h}{2}\Delta v^* + \frac{1}{2}|P + Dv^*|^2 - W = \overline{H}_h(P) & \text{in } \mathbb{T}^n \\ v^* \text{ is a } \mathbb{T}^n\text{-periodic function} \end{cases} \quad (36)$$

for

$$\overline{H}_h(P) := \frac{|P|^2}{2} - E_h^0(P). \quad (37)$$

It follows from classical PDE estimates the bounds

$$|Dv|, |Dv^*| \leq C,$$

for a constant C depending only on P and W .

Remark 12. *The equation (35) in the one-dimensional case admits a solution*

$$v = -h \log(w) + Cx$$

where $w > 0$ solves the equation

$$w'' - 2\left(\frac{P+C}{h}\right)w' + \left(\left(\frac{P+C}{h}\right)^2 - \frac{2}{h^2}(\overline{H}_h + W)\right)w = 0.$$

Now we define

$$\sigma := ww^* = e^{\frac{v^*-v}{h}} \quad (38)$$

and

$$u := P \cdot x + \frac{v + v^*}{2}. \quad (39)$$

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 (38) of the eigenfunctions is also noted in [3] (see also [18]) but it is used for a different purpose related to Aubry-Mather Theory (see [14]).

Note that

$$a e^{\frac{i u}{h}} = e^{\frac{\frac{1}{2}(v^*-v) + i \frac{v+v^*}{2} + i P \cdot x}{h}}.$$

According to (34),

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

Theorem 13. For

$$u = P \cdot x + \frac{v + v^*}{2}, \text{ we get}$$

$$(i) \quad \operatorname{div}(\sigma Dw) = 0 \text{ in } \mathbb{T}^n. \quad (40)$$

(ii) Furthermore,

$$\frac{1}{2}|Du|^2 - W - \overline{H}_h(P) = \frac{h}{4}\Delta(v - v^*) - \frac{1}{8}|Dv - Dv^*|^2 \text{ in } \mathbb{T}^n. \quad (41)$$

We call (40) the *continuity* (or *transport*) *equation*, and regard (41) as an *eikonal equation* with an error term on the right-hand side. Note that the form of (41) is not exactly the classical Hamilton-Jacobi equation due to the minus sign multiplying the potential W (in the left-hand side of (41)). This expression is different from (3.12) in [10].

Proof. a) Note that

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

But

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

and therefore

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

This shows (i).

b) Taking into account the expression (see [10])

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

and taking $a = (P + Dv)$, $b = (P + Dv^*)$, we get

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

Therefore, we finally get

$$\begin{aligned}
\frac{1}{2}|Du|^2 - W - \overline{H}_h(P) &= \frac{1}{2} \left(\frac{1}{2}|P + Dv|^2 - W - \overline{H}_h(P) \right) \\
&\quad + \frac{1}{2} \left(\frac{1}{2}|P + Dv^*|^2 - W - \overline{H}_h(P) \right) - \frac{1}{8}|D(v - v^*)|^2 \\
&= \frac{1}{2} \left(\frac{h}{2}\Delta v \right) - \frac{1}{2} \left(\frac{h}{2}\Delta v^* \right) - \frac{1}{8}|D(v - v^*)|^2 \\
&= \frac{\hbar}{4}\Delta(v - v^*) - \frac{1}{8}|D(v - v^*)|^2.
\end{aligned}$$

□

Remark 14. *One can also show that*

$$\begin{aligned}
-\frac{h}{2}\Delta\sigma - \operatorname{div}((P + Dv)\sigma) &= 0, \\
-\frac{h}{2}\Delta\sigma + \operatorname{div}((P + Dv^*)\sigma) &= 0.
\end{aligned}$$

Indeed, note that

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

Now, add and subtract the above from (40).

Now we will show integral identities involving Du and D^2u . To simplify notation, we will denote

$$d\sigma := \sigma dx.$$

Theorem 15.

$$\int_{\mathbb{T}^n} \frac{1}{2}|Du|^2 - W d\sigma = \overline{H}_h(P) + \frac{1}{8} \int_{\mathbb{T}^n} |Dv - Dv^*|^2 d\sigma. \quad (42)$$

Proof. Note that from the above

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

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

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

□

Theorem 16. For \hbar fixed, taking derivative with respect to P

$$i) \frac{d}{dP} H_h(P) = \int Du d\sigma. \quad (43)$$

Moreover,

$$ii) \frac{d^2}{dP^2} \overline{H}_h(P) = \int_{\mathbb{T}^n} D_{xP}^2 u \otimes D_{xP}^2 u d\sigma + \frac{1}{4} \int_{\mathbb{T}^n} D_{xP}^2 (v - v^*) \otimes D_{xP}^2 (v - v^*) d\sigma. \quad (44)$$

This shows that \overline{H}_h is a convex function of P .

Proof. The proof i) is similar to the proof of item 1) in Theorem 4.1 in [10]; we just have to substitute $-W$ (of [10]) by W . Taking derivative with respect to P in (32) and (33) we get $\frac{d}{dP} E_h^0(P) = -\int Dv d\sigma$ and $\frac{d}{dP} E_h^0(P) = -\int Dv^* d\sigma$ (see page 321 in [10]).

Then, from (37) we get

$$\frac{d}{dP} H_h(P) = P - \frac{d}{dP} E_h^0(P) = P + \frac{1}{2} \int [Dv + Dv^*] d\sigma = \int Du d\sigma.$$

The proof of ii) is also similar to the one in Theorem 4.1 in [10].

The same cancellation procedure of item 2) in theorem 4.1 in [10] results in (44). \square

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