# Computing the Effective Hamiltonian using a Variational Approach

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 $Abstract{\---}{A}$  numerical method for homogenization of Hamilton-Jacobi equations is presented and implemented as an  $L^\infty$  calculus of variations problem. Solutions are found by solving a nonlinear convex optimization problem. The numerical method is shown to be convergent and error estimates are provided. Several examples are worked in detail, including the cases of non-strictly convex Hamiltonians and Hamiltonians for which the cell problem has no solution.

### I. INTRODUCTION

Given the Hamiltonian H(p,x) which is smooth, convex in p, and periodic in the second variable x, we consider, for a given  $P \in \mathbb{R}^n$ , periodic solutions of the Hamilton-Jacobi equation

$$H(P + D_x u, x) = \bar{H}(P). \tag{HB}$$

For each fixed P the problem (HB) can be regarded as a nonlinear eigenvalue problem for the function function u(x) and the number  $\bar{H}(P)$ , the *effective Hamiltonian*.

In this paper, we reduce the problem of finding the (approximate) effective Hamiltonian to a finite dimensional convex optimization problem, which may solved numerically using standard methods.

Numerical computations of effective Hamiltonians have been done by [EMS95], [KBM01], with applications to front propagation and combustion, and in [Qia01], both of them using partial differential equations methods.

In this work we circumvent the difficulties of solving (HB) by computing  $\bar{H}(P)$  without finding the solution u. Our methods are based on the representation formula

$$\bar{H}(P) = \inf_{\phi \in C_{per}^1} \sup_x H(P + D_x \phi, x) \tag{1}$$

due, for strictly convex Hamiltonians, to [CIPP98].

In this paper we always assume that H to be convex but not necessarily strictly convex. This assumption has implications for the existence and smoothness of solutions of (HB). If strict convexity fails, solutions may (see  $\S IV$ -B) or may not (see  $\S IV$ -C) exist, and the degree of smoothness will depend on the Hamiltonian in question.

Computing the effective Hamiltonian is relevant in several problems, as we describe briefly next.

In homogenization problems [LPV88], [Con95], if  $w^{\epsilon}$  solves

$$-w_t^{\epsilon} + H(D_x w^{\epsilon}, \frac{x}{\epsilon}) = 0,$$

then as  $\epsilon$  goes to 0, the solution  $w^{\epsilon}$  converges to  $w^{0}$  which is a solution of the limiting problem

$$-w_t^0 + \bar{H}(D_x w^0) = 0.$$

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In the study of long time limits of viscosity solutions of Hamilton-Jacobi equations

$$-w_t + H(P + D_x w, x) = 0,$$

the difference  $w(x,t) - \bar{H}(P)t$  converges as  $t \to -\infty$  to a stationary solution of (HB) [Fat98b], [BS00]. See also [AI01], [CDI01].

In classical mechanics smooth solutions u of (HB) yield a canonical change of coordinates X(p,x) and P(p,x):  $(p=P+D_xu,\ X=x+D_Pu)$ , which simplifies the Hamiltonian dynamics

$$\dot{x} = -D_p H(p, x) \qquad \dot{p} = D_x H(p, x) \tag{2}$$

into the trivial dynamics

$$\dot{P} = 0 \qquad \dot{X} = -D_P \bar{H}(P).$$

In Aubry-Mather theory [Mat89], [Mat91], one looks for probability measures  $\mu$  on  $\mathbb{T}^n \times \mathbb{R}^n$  that minimize

$$\int L(x,v) + P \cdot v d\mu,\tag{3}$$

where L(x, v) is the Legendre transform of H(p, x), and satisfy a holonomy condition:

$$\int v D_x \phi \, d\mu = 0, \text{ for all } \phi(x) \in C^1(\mathbb{T}^n).$$

The supports of these measures are called the Aubry-Mather sets, [E99], [Fat97a], [Fat97b], [Fat98a], [Fat98b], [CIPP98], [EG01a], [EG01b], [Gom01b]. Viscosity solutions of (HB) encode important properties of the Aubry-Mather sets. In particular,

$$\int L(x,v) + P \cdot v d\mu = -\bar{H}(P),$$

the support of the Mather measure is a subset of the graph

$$(x, -D_pH(P+D_xu, x)),$$

for any viscosity solution of (HB), and if (x,p) belongs to any Mather, and (x(t),p(t)) is its orbit under (2) then

$$\frac{x(T)}{T} \to -D_P \bar{H}(P),$$

for some P, if  $\bar{H}$  is differentiable.

Equation (HB) and related stationary first and second order Hamilton-Jacobi equations are also important to the *ergodic control problem* [Ari98], [Ari97]. Effective Hamiltonians also arise in the study of *propagation of flame fronts in combustion*: in this case, solving a homogenization problem gives the effective or averaged front speed [EMS95], [KBM01].

#### II. CONVERGENCE RESULTS

We start this section by reviewing two results concerning the function  $\bar{H}(P)$ :

Proposition 1 (Lions, Papanicolao, Varadhan): There is at most one value  $\bar{H}$  for which (HB) has a periodic viscosity solution.

Proposition 2 (Contreras, Iturriaga, Paternain, Paternain): Suppose H is periodic in x and convex in p. Assume that there exists a viscosity solution u of (HB). Then

$$\bar{H} = \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x \psi, x), \tag{4}$$

in which the infimum is taken over the space  $C^1(\mathbb{T}^n)$  of periodic functions.

We should note that the original proof required strict convexity, but a simple viscosity solution argument overcomes this problem.

The next issue is the approximation of the problem (1). To this effect, consider a triangulation of  $\mathbb{T}^n$  with cells of diameter smaller than h. Let  $C(T_h)$  be the collection of piecewise linear finite elements which interpolate given nodal values

Proposition 3: Suppose H(p,x) is convex in p. Then

$$\inf_{\psi \in C^1(\mathbb{T}^n)} \sup_x H(D_x \psi, x) = \lim_{h \to 0} \inf_{\phi \in C(T_h)} \mathrm{esssup}_x H(D_x \phi, x).$$
 Proof: Fix  $\epsilon > 0$ . Let  $\psi$  be a  $C^1$  function for which

$$\sup_{x \in \mathbb{T}^n} H(D_x \psi, x) \le \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x \psi, x) + \epsilon.$$

Because  $\psi$  is  $C^1$ ,  $D_x\psi$  is uniformly continuous. Thus, for h sufficiently small, there is  $\phi \in C(T_h)$  such that  $\underset{x \in \mathbb{T}^n}{\operatorname{esssup}} |D_x\phi - D_x\psi| \leq \epsilon$ . This implies

$$\underset{x \in \mathbb{T}^n}{\text{esssup}} H(D_x \phi, x) \le \sup_{x \in \mathbb{T}^n} H(D_x \psi, x) + O(\epsilon),$$

by Lipschitz continuity of H in p. Thus, taking first  $\lim_{h\to 0}\inf_{\phi\in C(T_h)}$ , then  $\inf_{\psi\in C^1(\mathbb{T}^n)}$ , and finally  $\epsilon\to 0$ , we obtain the first inequality.

To prove the converse inequality observe that if  $\phi \in C(T_h)$ ,  $\eta_{\epsilon}$  is a smooth mollifier, and  $\psi = \eta_{\epsilon} * \phi$ , then convexity yields

$$H(D_x\psi(x), x) \le \int H(D_x\phi(y), y)\eta_{\epsilon}(x - y)dy + O(\epsilon),$$

every x, and so the result follows from

$$H(D_x\psi(x), x) \le \underset{x \in \mathbb{T}^n}{\operatorname{esssup}} H(D_x\phi(x), x) + O(\epsilon),$$

taking first  $\inf_{\psi \in C^1}$ , then  $\lim_{h \to 0} \inf_{\phi \in C(T_h)}$ , and finally  $\epsilon \to 0$ .

First observe that

$$\mathcal{H}(\phi) = \sup_{x \in \mathbb{T}^n} H(D_x \phi, x),$$

is a convex, but not strictly convex, functional. Therefore local minima are global minima.

Proposition 4: The approximate Hamiltonian

$$\bar{H}_h(P) = \inf_{\phi \in C(T_h)} \underset{x \in \mathbb{T}^n}{\text{esssup}} H(P + D_x \phi, x)$$

is convex in P.

*Proof:* Let  $P_1, P_2 \in \mathbb{R}^n$  and let  $\phi_1, \phi_2 \in C(T_h)$  be the corresponding minimizers. Let  $0 \le \lambda \le 1$ , and set  $P = \lambda P_1 + (1-\lambda)P_2$ , and  $\phi = \lambda \phi_1 + (1-\lambda)\phi_2$ . Then, for any x we have

$$H(P + D_x \phi, x)$$
  
  $\leq \lambda H(P_1 + D_x \phi_1, x) + (1 - \lambda) H(P_2 + D_x \phi_2, x),$ 

and so

$$\bar{H}_h(P) = \inf_{\phi \in C(T_h)} \underset{x \in \mathbb{T}^n}{\text{esssup}} H(P + D_x \phi, x)$$
$$\leq \lambda \bar{H}_h(P_1) + (1 - \lambda) \bar{H}_h(P_2).$$

Theorem 1: For any convex Hamiltonian H(p,x) for which (HB) has a viscosity solution

$$\bar{H} \leq \inf_{\phi \in C(T_h)} \operatorname{esssup}_{x} H(D_x \phi, x).$$

If there exists a globally  $C^2$  solution of (HB) then

$$\inf_{\phi \in C(T_h)} \operatorname{esssup}_{x} H(D_x \phi, x) = \bar{H} + O(h).$$

If (HB) has a Lipschitz solution (for instance if H(p,x) is strictly convex in p) we have

$$\inf_{\phi \in C(T_h)} \operatorname{esssup}_{x} H(D_x \phi, x) = \bar{H} + O(h^{1/2}).$$

If H is convex but not strictly convex and (HB) has a viscosity solution then

$$\inf_{\substack{\phi \in C(T_h) \\ Proof:}} \text{esssup} H(D_x \phi, x) = \bar{H} + o(1).$$

Proof: Observe that

$$\bar{H} = \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_x H(D_x \psi, x) \le \inf_{\phi \in C(T_h)} \text{esssup} H(D_x \phi, x),$$

because by convexity we can associate to each  $\phi \in C(T_h)$  a function  $\psi = \phi * \eta_{\epsilon} \in C^1(\mathbb{T}^n)$  such that  $\sup_x H(D_x \psi, x) \leq \operatorname{esssup} H(D_x \phi, x) + O(\epsilon)$ , for arbitrary  $\epsilon > 0$ .

To prove the second assertion suppose u is a  $C^2$  viscosity solution of (HB). Fix h and construct a function  $\phi_u \in C(T_h)$  by interpolating linearly the values of u at the nodal points. In each triangle  $T^i$ , the oscillation of the derivative of u is O(h), since u is  $C^2$ . Thus, we obtain

$$D_x \phi_u(x) = D_x u(x) + O(h),$$

for any x. Since  $H(D_x u, x) = \bar{H}$ , at every point  $x \in T^i$  we have  $H(D_x \phi_u, x) \leq \bar{H} + O(h)$ , which implies

$$\inf_{\phi \in C(T_h)} \operatorname{esssup}_{x \in \mathbb{T}^n} H(D_x \phi, x) \le \bar{H} + O(h).$$

If u is a Lipschitz viscosity solution, let  $\tilde{u} = \eta_{h^{1/2}} * u$ . Observe that  $|D_{xx}^2 \tilde{u}| \leq \frac{C}{h^{1/2}}$ , and

$$H(D_x\tilde{u},x) \le \bar{H} + O(h^{1/2}).$$

Construct a function  $\phi_u \in C(T_h)$  by interpolating linearly the values of  $\tilde{u}$  at the nodal points. In each triangle  $T^i$ , the oscillation of the derivative of  $\tilde{u}$  is  $O(h^{1/2})$ .



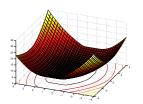


Fig. 1:  $\bar{H}(P)$  for the one-dimensional pendulum.

Thus  $D_x\phi_u(x)=D_x\tilde{u}(x)+O(h^{1/2}),$  for any x. Since  $H(D_x\tilde{u},x)\leq \bar{H}+O(h^{1/2}),$  for every point  $x\in T^i$  we have  $H(D_x\phi_u,x) \leq \bar{H} + O(h^{1/2})$ . This implies

$$\inf_{\phi \in C(T_h)} \operatorname{esssup}_{x \in \mathbb{T}^n} H(D_x \phi, x) \le \bar{H} + O(h^{1/2}).$$

The last case, for not strictly convex Hamiltonians, the sup convolution yields a function  $u_{h^{1/3}}$  that satisfies

$$H(D_x u_{h^{1/3}}, x) \le \bar{H} + o(1),$$

almost everywhere and has Lipschitz constant bounded by  $\frac{C}{h^{1/3}}$ . Define  $\tilde{u}=\eta_{h^{1/3}}*u_{h^{1/3}}$  which satisfies  $H(D_x\tilde{u},x)\leq \tilde{H}+o(1)$  and has  $|D_{xx}^2\tilde{u}|\leq \frac{C}{h^{2/3}}$ . Since in each triangle the oscillation of the derivative is  $O(h^{1/3})$  we have the result, since

$$H(D_x\phi_u, x) \le \bar{H} + o(1).$$

A corollary to the previous theorem is the following:

Corollary 1: Suppose  $\xi_h \in \mathbb{R}^n$  is a supporting plane for  $\bar{H}_h(P)$  that converges as  $h \to 0$  to  $\xi$ . Then  $\xi$  is a supporting hyperplane for  $\bar{H}(P)$ . As a consequence if  $\bar{H}(P)$  is differentiable at P then  $\xi_h$  converges to the unique supporting hyperplane of H(P) at P.

### III. NUMERICAL IMPLEMENTATION

We can make a further approximation, discretizing the spatial variable by computing the supremum only at the nodes  $x_i$ , which gives the minimax problem

$$\min_{\phi \in C(T_h)} \max_{x_i} H(D_x \phi, x_i), \tag{5}$$

for  $x_i$  at the nodal points of the finite element space.

The minimax problem (5) is a finite dimensional nonlinear optimization problem which can by solved using standard optimization routines. We carried out the implementation in MATLAB, using the Optimization Toolbox.

Fig. 2:  $\bar{H}(P)$  for the double pendulum

## IV. COMPUTATIONAL RESULTS

## A. Strictly convex Hamiltonians

We present two examples, the one-dimensional pendulum and the double pendulum.

Example 1 (one-dimensional pendulum): In this case the Hamiltonian is  $H(p,x) = \frac{p^2}{2} - \cos 2\pi x$ . the result is presented in Figure 1, and agrees with the explicit formula for H, which is known in this case.

Example 2 (Double pendulum): The double pendulum is a well known non-integrable system for which the effective Hamiltonian is not known. The Hamiltonian for the double pendulum is

$$\frac{p_x^2 - 2p_x p_y \cos(2\pi(x-y)) + 2p_y^2}{2 - \cos^2(2\pi(x-y))} + 2\cos 2\pi x + \cos 2\pi y.$$

The result is presented in Figure 2.

### B. Non strictly convex problems

In this section we study several examples in which H is convex, but not strictly convex, for which there is a viscosity solution of (HB).

Example 3 (Linear non-resonant): Consider the linear (nonresonant) Hamiltonian

$$H(p,x) = \omega \cdot p + V(x,y). \tag{6}$$

Suppose u is a smooth solution of (HB). Integrating the equation over  $\mathbb{T}^n$  yields

$$\bar{H}(0) = \int_{\mathbb{T}^n} V,\tag{7}$$

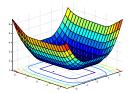
and so  $\bar{H}(P) = \bar{H}(0) + \omega \cdot P$ .

For the example  $u_x + \sqrt{2}u_y + \cos(2\pi x)$  we obtained  $D_P \bar{H} = (1, \sqrt{2})$  and  $\bar{H}(0, 0) = 0$ . In this (linear) case the optimization routine converged very quickly.

Example 4 (Vakonomic): Finally, we study an example of a non-strictly convex Hamiltonian which satisfies commutation relations related to vakonomic mechanics [AKN97],

$$H(p,x) = \frac{|f_1 \cdot Du|^2}{2} + \frac{|f_2 \cdot Du|^2}{2} + V(x,y)$$

in which the vector fields  $f_1, f_2$  do not span  $\mathbb{R}^2$  in every point but when we consider the commutator  $[f_1, f_2]$  we have that



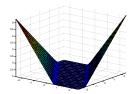


Fig. 3:  $\bar{H}(P)$  for the Vakonomic Hamiltonian.

Fig. 4:  $\bar{H}(P)$  for the quasi-periodic Hamiltonian.

 $f_1, f_2, [f_1, f_2]$  span  $\mathbb{R}^2$  in every point. In this situation (HB) has Hölder continuous viscosity solutions [EJ89], [Gom01a].

We chose  $f_1=(0,1)$ , and  $f_2=(\cos 2\pi y,\sin 2\pi y)$ , so that  $f_1,f_2,[f_1,f_2]$  always span  $\mathbb{R}^2$ . Therefore there is a Hölder continuous viscosity solution. The potential is  $V(x,y)=\cos 2\pi x+\sin 2\pi (x-y)$  The result is presented in Figure 3.

## C. Non-existence of viscosity solutions

There are situations where there do not exist viscosity solutions to (HB), but  $\bar{H}$  can still be defined by solving a more general problem, see [BS00], [BS01] and [LS03]. In some of these situations, the solution of the minimax problem (1) may exist and give a consistent result.

We work out two interesting examples and try to explain the results obtained numerically.

The problem

$$\alpha u^{\alpha} + H(P + D_x u^{\alpha}, x) = 0, \tag{8}$$

which (when  $\alpha \neq 0$ ) has a unique solution is considered in [LS03]. Sending  $\alpha \to 0$  gives the effective Hamiltonian

$$\bar{H}(P) \equiv \lim_{\alpha \to 0} \alpha u^{\alpha}. \tag{9}$$

Proposition 5: Let  $u^{\alpha}$  be a solution of (8), and suppose  $\alpha u^{\alpha}$  converges uniformly to a constant number  $\bar{H}(P)$ . Then

$$\bar{H}(P) = \lim_{\alpha \to 0} \alpha u^{\alpha} = \inf_{\phi} \sup_{x \in \mathbb{T}^n} H(P + D_x \phi, x).$$

*Proof:* 1. Define  $\bar{H}_{\alpha} \equiv -\alpha \min_{x} u^{\alpha}$  and

$$v^{\alpha} \equiv u^{\alpha} + \frac{\bar{H}_{\alpha}}{\alpha},$$

so that  $\min_x v^{\alpha} = 0$ . We will demonstrate  $\bar{H}_{\alpha} \to \bar{H}$ . We have

$$\bar{H} = \lim_{\alpha \to 0} H(P + D_x u^{\alpha}, x) = \lim_{\alpha \to 0} -\alpha u^{\alpha}$$
$$= \lim_{\alpha \to 0} \alpha (u^{\alpha} - \min_{x} u^{\alpha}) + \alpha \min_{x} u^{\alpha} = \bar{H}_{\alpha}$$

2. Let  $v_{\alpha}^{\epsilon}$  denote the sup convolution of  $v_{\alpha}$  and let  $\phi = \eta_{\epsilon} * v_{\alpha}^{\epsilon}$ . Then  $H(D_{x}\phi, x) \leq \bar{H}_{\alpha} + O(\epsilon)$ . Therefore  $\inf_{\phi} \sup_{x \in \mathbb{T}^{n}} H(D_{x}\phi, x) \leq \bar{H}_{\alpha} \to \bar{H}$ .

3. Now let  $e_{\alpha} = \sup_{x} \alpha v_{\alpha}$ , which converges to 0.

Let  $\phi$  be any function. Then  $v_{\alpha} - \phi$  has a local minimum at a point  $x_0$ . At this point

$$\alpha v_{\alpha}(x_0) + H(D_x \phi(x_0), x_0) \ge \bar{H}_{\alpha},$$

and so  $\sup_{x\in\mathbb{T}^n}H(D_x\phi,x)\geq \bar{H}_\alpha-e_\alpha\to \bar{H}$ . Therefore  $\inf_\phi\sup_{x\in\mathbb{T}^n}H(D_x\phi,x)\geq \bar{H}$ .

Example 5 (Quasiperiodic Hamiltonians): We give an example from [LS03] where there is no viscosity solution to (HB), but where  $\bar{H}(P)$  can be determined from (9). Let

$$H(p_x, p_y, x, y) = |p_x + \alpha p_y| + \sin(x) + \sin(y)$$

with  $\alpha$  irrational.

We computed  $\bar{H}(P)$  numerically from (1). The results are presented in Figure 4.

Example 6 (Linear resonant): Resonant linear Hamiltonians (6) may fail to have a viscosity solution. An example is

$$(0,1) \cdot Du + \sin(2\pi x) = \bar{H}.$$

The formula (7) yields  $\bar{H}(0) = 0$  if there were a solution of (HB). However, we have

$$\inf_{\phi} \sup_{x} H(D_x \phi, x) = 1.$$

In fact, let  $\phi$  be an arbitrary periodic function. Set  $x_0 = 1/4$ , so that  $\sin 2\pi x_0 = 1$ . Then  $\phi(x_0, y)$  is a periodic function of y and so  $D_y\phi(x_0, y) = 0$  at some  $y = y_0$ . Thus

$$\sup_{x} H(D_x \phi, x) \ge H(D_x \phi(x_0, y_0), x_0, y_0) = 1.$$

Numerically we obtained  $D_P \bar{H} = (0,1)$  and  $\bar{H}(0,0) = 1$ .

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