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^{∞} 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. One and two dimensional examples are worked in detail, comparing known results with the numerical ones and computing new examples. The cases of nonstrictly convex Hamiltonians and Hamiltonians for which the cell problem has no solution are treated.

Key words. Hamilton-Jacobi, homogenization, numerics, calculus of variations

AMS subject classifications. 37, 49, 65, 35

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1. Introduction. Given the Hamiltonian H(p, x), which is smooth, convex in p, and periodic in the second variable x, we are interested in finding for a given $P \in \mathbb{R}^n$ a periodic solution of the Hamilton–Jacobi equation

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

For each fixed P the problem (HB) can be regarded as a nonlinear eigenvalue problem for the function u(x) and the number $\overline{H}(P)$. We regard $\overline{H}(P)$, the *effective Hamiltonian*, as a function of the parameter P. It encodes information about H(x, p), as we shall describe below.

Problem (HB) requires that we determine for a given $P \in \mathbb{R}^n$ the pair (u, H(P)). Classical solutions do not exist for all P, so viscosity solutions [CIL92, BCD97, FS93] are used.

Solving (HB) directly involves finding the viscosity solution to a degenerate elliptic partial differential equation coupled to an unknown constant, $\bar{H}(P)$. While this may be done, it is not an easy task. We choose instead to reduce the problem of finding the (approximate) effective Hamiltonian to a finite dimensional convex optimization problem, which may be solved numerically using optimization routines.

Numerical computations of effective Hamiltonians have been done by [EMS95, KBM01], with applications to front propagation and combustion. At the time of preparation of this manuscript, the authors also discovered work by [Qia01]. The numerical approach taken by these authors was to find the effective Hamiltonian by partial differential equations methods.

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

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

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due, for strictly convex Hamiltonians, to [CIPP98], in which the infimum is taken over all periodic C^1 functions, $C^1(\mathbb{T}^n)$. This formula is a problem in the calculus of variations problem in L^{∞} . Such problems were studied by Aronsson in the 1960s [Aro66, Aro65]. Recently there has been a renewed interest in calculus of variations in L^{∞} [BJW01a, BJW01b, Bar94]. Related methods in the calculus of variations in L^{∞} were applied to the effective Hamiltonian problem in [Eva03].

In this paper we always assume that H is convex but not necessarily strictly convex. This assumption has implications for the existence and smoothness of solutions of (HB). For instance, if H is strictly convex, then there are viscosity solutions of (HB) which are Lipschitz continuous. However, if strict convexity fails, solutions may (see section 5.2) or may not (see section 5.3) exist, and the degree of smoothness will depend on the Hamiltonian in question.

1.1. Applications. Computing the effective Hamiltonian is relevant to several classes of applications: homogenization problems, the long time behavior of Hamilton–Jacobi equations, classical mechanics, Aubry–Mather theory, ergodic control, and front propagation.

In homogenization problems [LPV88, Con95], if w^{ϵ} solves

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

then, as ϵ goes to 0, the solution w^ϵ converges to $w^0,$ which is a solution of the limiting problem

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

The effective Hamiltonian also appears in the study of *long time limits of viscosity* solutions of Hamilton–Jacobi equations:

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

It turns out that $w(x,t) - \overline{H}(P)t$ converges as $t \to -\infty$ to a stationary solution of (HB) [Fat98b, BS00]; see also [AI01, CDI01].

In classical mechanics [AKN97], smooth solutions u of (HB) yield a canonical change of coordinates X(p, x) and P(p, x) defined by the equations

(2)
$$p = P + D_x u, \qquad X = x + D_P u.$$

This would simplify the Hamiltonian dynamics

(3)
$$\dot{x} = -D_p H(p, x), \qquad \dot{p} = D_x H(p, x)$$

into the trivial dynamics

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

In other words, for each P there is an invariant torus in which the dynamics is simply a rotation. However, (HB) does not admit smooth solutions in general (see section 4), and one must deal with viscosity solutions [CIL92, BCD97, FS93, Eva98].

In Aubry–Mather theory [Mat89a, Mat89b, Mat91, Mn92, Mn96], instead of looking for invariant tori, one looks for probability measures μ on $\mathbb{T}^n \times \mathbb{R}^n$ that minimize the average action

(4)
$$\int L(x,v) + P \cdot v d\mu$$

and satisfy a holonomy condition

$$\int v D_x \phi \, d\mu = 0$$

for all $\phi(x) \in C^1(\mathbb{T}^n)$.

Here L(x, v) is the Legendre transform of H(p, x), defined by

$$L(x, v) = \sup_{p} -v \cdot p - H(p, x).$$

The supports of these measures are called the Aubry–Mather sets and are the natural generalizations of invariant tori. Recent results [E99, Fat97a, Fat97b, Fat98a, Fat98b, CIPP98], some by one of the authors [EG01, EG02, Gom01b], show that viscosity solutions encode the Aubry–Mather sets. In particular, we have

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

and 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).

In the Mather set the asymptotics of the Hamiltonian dynamics are controlled by viscosity solutions. Indeed let (x, p) be any point in $\mathbb{T}^n \times \mathbb{R}^n$. Consider its flow by the Hamilton equations (3). If (x, p) belongs to any Mather set, then

$$\frac{x(T)}{T} \to Q$$

as $T \to \infty$ for some vector $Q \in \mathbb{R}^n$, with $Q = D_P \overline{H}(P)$ for some P if \overline{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]. While this article was being reviewed, the authors became aware of [FSar]. Aubry–Mather theory can also be generalized to second order equations [Gom02], and many of the techniques that we develop can be generalized appropriately.

The computation of effective Hamiltonians has applications to the propagation of flame fronts in combustion: Hamilton–Jacobi equations which are homogeneous of order one, for example $u_t = c|Du|$, can represent the evolution of a propagating front moving in the normal direction with speed c. If the front is propagating in a periodic media, an equation of the form $u_t = c(x)|Du|$ holds, where c(x) is positive and periodic in x. In this case, solving a homogenization problem gives the effective or averaged front speed. As mentioned earlier, numerical computations for this problem have been performed by [EMS95, KBM01].

2. Solvability and approximation of the homogenization problem.

2.1. Solvability of the homogenization problem. We start this section by reviewing some results concerning the function $\bar{H}(P)$. In particular, we recall the uniqueness result of \bar{H} from [LPV88], and we generalize a representation formula for \bar{H} due to [CIPP98].

PROPOSITION 2.1 (from Lions, Papanicolao, Varadhan [LPV88]). There is at most one value \bar{H} for which (HB) has a periodic viscosity solution.

Proof. Suppose, for contradiction, that (HB) admits viscosity solutions u_1 and u_2 for $\bar{H} = \bar{H}_1, \bar{H}_2$, respectively, with $\bar{H}_1 > \bar{H}_2$. We may assume $v_1 \equiv u_1 + C > u_2$ for a sufficiently large positive constant C. For ϵ sufficiently small

$$\epsilon v_1 + H(D_x v_1, x) \ge \epsilon u_2 + H(D_x u_2, x)$$

in the viscosity sense. The comparison principle [BCD97] then implies $v_1 \leq u_2$, which is a contradiction. \Box

Next we prove a representation formula for \overline{H} . Our result extends [CIPP98] to nonstrictly convex Hamiltonians H, for which the solution may fail to be Lipschitz.

PROPOSITION 2.2 (from Contreras, Iturriaga, Paternain, Paternain [CIPP98]). Suppose that H is periodic in x and convex in p (strict convexity is not required). Suppose further that there exists a viscosity solution u of (HB). Then

(5)
$$\bar{H} = \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x\psi, x),$$

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

First we recall some facts concerning the sup convolution. The proof may be found in [FS93].

LEMMA 2.3. Suppose u is a viscosity of (HB). Define

(6)
$$u_{\epsilon}(x) = \sup_{y} \left[u(y) - \frac{|x-y|^2}{\epsilon} \right].$$

Then

1. $u_{\epsilon} \rightarrow u$ uniformly as $\epsilon \rightarrow 0$,

2. u_{ϵ} is semiconvex,

3. u_{ϵ} satisfies

$$H(D_x u_{\epsilon}, x) \le \bar{H} + o(1),$$

in the viscosity sense and almost everywhere.

Proof of Proposition 2.2. Let

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

At some point x_0 , $u - \psi$ has a local minimum. By the viscosity property

$$H(D_x\psi(x_0), x_0) \ge \bar{H},$$

which implies $\bar{H}^* \geq \bar{H}$.

Let η_{ϵ} be a smoothing kernel. Set $v_{\epsilon} = u_{\epsilon} * \eta_{\epsilon}$. Then, using convexity,

$$H(D_x v_{\epsilon}(x), x) \leq \int H(D_x u_{\epsilon}(y), y) \eta_{\epsilon}(x - y) dy + o(1) \leq \bar{H} + o(1),$$

and thus $\bar{H}^* \leq \bar{H}$. \Box

Before proceeding with the discretization of this problem we will prove an elementary bound.

PROPOSITION 2.4. We have

$$\inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x \psi, x) \ge \inf_{x \in \mathbb{T}^n} H(0, x).$$

Proof. For any function $\psi \in C^1(\mathbb{T}^n)$ there is a point x_0 for which $D_x \phi(x_0) = 0$. Therefore $\sup_{x \in \mathbb{T}^n} H(D_x \psi, x) \ge H(0, x_0) \ge \inf_{x \in \mathbb{T}^n} H(0, x)$. \Box **2.2.** Approximation. The next issue we study 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 continuous piecewise linear grid functions which interpolate given nodal values. We avoid the use of the term finite elements to emphasize the pointwise nature of the approximation.

The following proposition is an approximation result: we do not assume the existence of a viscosity solution of (HB).

PROPOSITION 2.5. Suppose H(p, x) is convex in p. Then

$$\inf_{\psi \in C^1(\mathbb{T}^n)} \sup_x H(D_x\psi, x) = \lim_{h \to 0} \inf_{\phi \in C(T_h)} \operatorname{essup}_x H(D_x\phi, x).$$

Proof. Fix $\epsilon > 0$. Let ψ 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 ψ is C^1 , $D_x \psi$ is uniformly continuous. Thus, for h sufficiently small, there is $\phi \in C(T_h)$ such that

(7)
$$\operatorname{esssup}_{x \in \mathbb{T}^n} |D_x \phi - D_x \psi| \le \epsilon.$$

In fact, in each triangle along an edge e_i with length $|e_i|$ pointing in the direction ν_i we have

$$D_x \psi \cdot \nu_i = \frac{1}{|e_i|} \int_{e_i} D_x \phi \cdot dz = D_x \phi(\bar{x}) \cdot \nu_i + o(1),$$

in which \bar{x} is, for instance, the center of the triangle. Since the shape factor is bounded, there are at least n edges ν_i linearly independent such that

(8)
$$|\det[\nu]| \ge \theta$$

for some θ for all triangles. Therefore

$$D_x\psi = D_x\phi(\bar{x}) + o(1),$$

as required.

This therefore implies

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

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

$$\lim_{h \to 0} \inf_{\phi \in C(T_h)} \underset{x \in \mathbb{T}^n}{\operatorname{esssup}} H(D_x \phi, x) \le \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x \psi, x) + O(\epsilon).$$

Send $\epsilon \to 0$.

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

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

for every x, and so

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

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

$$\inf_{\psi \in C^1} \sup_x H(D_x\psi, x) \le \lim_{h \to 0} \inf_{\phi \in C(T_h)} \operatorname{essup}_{x \in \mathbb{T}^n} H(D_x\phi, x) + O(\epsilon).$$

Since ϵ is arbitrary, we have the claim. \Box

Before stating and proving an improved version of the previous proposition for the case in which (HB) has a viscosity solution, we record some important properties of the L^{∞} calculus of variations problem. 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 for any ϕ_1 and ϕ_2 we have

$$\mathcal{H}(\lambda\phi_1 + (1-\lambda)\phi_2) \le \lambda\mathcal{H}(\phi_1) + (1-\lambda)\mathcal{H}(\phi_2).$$

This in particular implies that any local minimum is a global minimum.

However, in general the minimizers are not unique, and it is not true that a minimizing sequence will converge to a viscosity solution of

$$H(D_x u, x) = \bar{H}.$$

For example, $H = p^2/2 + \cos x$ has $\overline{H} = 1$, and $u \equiv 0$ is a minimizer. However, $H(D_x u, x) \neq \overline{H}$.

A similar argument applied to the discretized problem yields that

$$\mathcal{H}_h(\phi) = \underset{x \in \mathbb{T}^n}{\mathrm{essup}} H(D_x \phi, x)$$

is convex for $\phi \in C(T_h)$, and so a local minimum is a global minimum.

PROPOSITION 2.6. The approximate Hamiltonian

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

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 $0 \leq \lambda \leq 1$, 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

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

Thus

$$\operatorname{esssup}_{x \in \mathbb{T}^n} H(P + D_x \phi, x) \le \lambda \bar{H}_h(P_1) + (1 - \lambda) \bar{H}_h(P_2),$$

and so

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

if $P = \lambda P_1 + (1 - \lambda)P_2$. \Box

THEOREM 2.7. For any convex Hamiltonian H(p, x) for which (HB) has a viscosity solution

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

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), then

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

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

$$\inf_{\phi \in C(T_h)} \operatorname{essup}_x H(D_x \phi, x) = \bar{H} + o(1).$$

Proof. Observe that

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

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

$$\sup_{x} H(D_x\psi, x) \le \operatorname{esssup}_{x} H(D_x\phi, x) + O(\epsilon),$$

for arbitrary $\epsilon > 0$, as seen in the previous proposition.

To prove the second assertion suppose that 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, proceeding as in the proof of (7), we obtain

$$D_x\phi_u(x) = D_xu(x) + O(h)$$

for any x. Since $H(D_x u, x) = \overline{H}$, at every point $x \in T^i$ we have

$$H(D_x\phi_u, x) \le \bar{H} + O(h).$$

This implies

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

If u is a Lipschitz viscosity solution, let $\tilde{u} = \eta_{h^{1/2}} * u$. Observe that

$$|D_{xx}^2 \tilde{u}| \le \frac{C}{h^{1/2}}$$

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 $O(h^{1/2})$. Thus

$$D_x\phi_u(x) = D_x\tilde{u}(x) + O(h^{1/2})$$

for any x. Since $H(D_x \tilde{u}, x) \leq \overline{H} + O(h^{1/2})$, for every point $x \in T^i$,

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

This implies

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

In the final case of nonstrictly convex Hamiltonians, the sup convolution (6) with $\epsilon = h^{1/3}$ 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 $Ch^{-1/3}$. Define $\tilde{u} = \eta_{h^{1/3}} * u_{h^{1/3}}$, which satisfies

$$H(D_x\tilde{u},x) \le \bar{H} + o(1)$$

and

$$|D_{xx}^2 \tilde{u}| \le \frac{C}{h^{2/3}}$$

Since in each triangle the oscillation of the derivative is $O(h^{1/3})$, we obtain

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

thereby proving the last statement of the theorem.

A corollary to the previous theorem is the following.

COROLLARY 2.8. Suppose $\xi_h \in \mathbb{R}^n$ is a supporting plane for $\overline{H}_h(P)$ that converges as $h \to 0$ to ξ . Then ξ is a supporting hyperplane for $\overline{H}(P)$. As a consequence, if $\overline{H}(P)$ is differentiable at P, then ξ_h converges to the unique supporting hyperplane of $\overline{H}(P)$ at P.

Proof. The previous theorem asserts that $\overline{H}(P)$ converges uniformly to $\overline{H}(P)$. In Proposition 2.6 we proved that $\overline{H}_h(P)$ is convex. Therefore the corollary follows from a standard convex analysis argument. \Box

3. Numerical implementation. In this section we discuss the numerical implementation of the fully discretized minimax problem (4). There are two parts to the discussion: (i) implementing the discrete version of the problem and (ii) solving the resulting optimization problem. If the discretization is performed properly, the resulting minimax problem is convex, and standard routines can be used to find the solution.

3.1. Discretization. In the last section we discussed the approximation of the infinite dimensional problem

$$\bar{H}(P) = \inf_{\phi \in C^1_{per}} \sup_{x} H(P + D_x \phi, x)$$

by the finite dimensional problem

$$\inf_{\phi \in C(T_h)} \operatorname{esssup}_x H(D_x \phi, x),$$

for ϕ in the space of continuous piecewise linear grid functions.

To fully discretize the problem, we make a further approximation: we discretize the spatial variable by computing the supremum only at the nodes x_i , which gives the minimax problem

(9)
$$\min_{\phi \in C(T_h)} \max_{x_i} H(D_x \phi, x_i)$$

for x_i at the nodal points of the grid function space. The spatial approximation introduces a small additional error of O(h), which is proportional to the Lipschitz constant (in the x variable) of H.

The minimax problem (9) is a finite dimensional nonlinear optimization problem which can by solved using standard optimization routines.

Discretization in one dimension. We first present the discretization scheme in one dimension. Choosing n to be the number of nodes, we get a partition of \mathbb{T} , the unit interval with periodic boundary conditions, into n intervals of length h = 1/n. For any ϕ in the grid function space $C(T_h)$, we identify ϕ with the vector of values on the nodes

 ϕ is identified with $u = (u_1, \dots, u_n) = (\phi(0), \dots, \phi(ih), \dots, \phi((n-1)h)).$

Then, choosing $x_i = (i + 1/2)h$ to be the midpoint of the interval gives the discretization

(10)
$$H(\phi_x, x) = H\left(\frac{u_{i+1} - u_i}{h}, x_i\right) \text{ on } T_i = [ih, (i+1)h]$$

As long as H(p, x) is convex in p, for each x, the right-hand side of (10) is convex in u_{i+1} and u_i . Taking the maximum over the nodes gives a convex function of nvariables to be minimized.

Discretization in two dimensions. Next, in two dimensions, take an $n \times n$ grid for \mathbb{T}^2 , the unit square with periodic boundary conditions. Create a regular tiling by triangles as follows. To each node i, j, let

$$T_{i,j}^{\pm} =$$
 the triangle with vertices $(i, j), (i \pm 1, j), (i, j \pm 1).$

For ϕ in the grid function space $C(T_h)$, we identify ϕ with the matrix of values on the nodes:

$$\phi$$
 is identified with $u = (u_{i,j}) = (\phi(ih, jh)), \quad i, j = 1, \dots, n.$

As a result we have $2n^2$ triangles on which ϕ is linear.

On each triangle, choosing $x_{i,j}^{\pm}, y_{i,j}^{\pm}$ to be a point in the middle of $T_{i,j}^{\pm}$, we get the discretization

(11)
$$H(\phi_x, \phi_y) = H^{\pm}\left(\frac{u_{i\pm 1,j} - u_{i,j}}{h}, \frac{u_{i,j\pm 1} - u_{i,j}}{h}, x_i^{\pm}, y_i^{\pm}\right) \text{ on } T_{i,j}^{\pm}.$$

As long as H(p, x) is convex in p, for each x, the right-hand side of (11) is convex in the variables $u_{i,j}$ and $u_{i\pm 1,j\pm 1}$.

Taking the maximum over the triangles gives a convex function of $2n^2$ variables to be minimized. Alternately, we can take $x_{i,j}^{\pm} = x_{i,j}, y_{i,j}^{\pm} = y^{i,j}$ and take the maximum H^{\pm} with these values to reduce the number of variables by a factor of two.

3.2. Numerical solution of the minimax problem. The implementation required only that a suitable discretization of the Hamiltonian be given. This discretization takes the form of a map from \mathbb{R}^n to \mathbb{R}^n , or a map from \mathbb{R}^{2n} to \mathbb{R}^{2n} , in the case of one and two dimensional Hamiltonians, respectively. Each component of the map is convex in each of the variables, and the map is sparse, in the sense that it depends on only a small number of other variables.

Taking the maximum of the components of the map gives a convex function which is to be minimized. In general, there are many minimizers, but the minimum is unique.

At this point, publicly available routines for convex optimization may be used to solve the problem. We carried out the implementation in MATLAB, using the Optimization Toolbox. The Optimization Toolbox contains an assortments of routines for solving multidimensional nonlinear optimization problems, some of which take advantage of sparse linear algebra. We used fminimax, which is specially designed for minimax problems but does not use sparse linear algebra. A possible alternative would have been to use the a more general solver with sparse linear algebra, which might have performed better on larger problems. For the problems we implemented, which were of modest size (128 variables in two dimensions), the minimization problem was solved in a few seconds on a laptop computer. Solving for a range of a few hundred values of P took between twenty minutes and a few hours to compute for each problem.

For background on convex optimization we refer to [Fle80]. Briefly, the minimax is solved by searching for the worst of the objective functions, then improving that function by solving a sequence of quadratic programs, which are in turn computed by solving a sequence of linear equations. The error in the solution of the optimization problem is insignificant compared to the discretization error.

3.3. Error estimates. There are three main issues which may lead to errors in the numerical computation of $\overline{H}(P)$: the error which arises from the discretization (which was discussed in the previous section), the error involved in computing the essue approximately, and the error in solving the discrete problem numerically.

To compute the essential supremum we chose to evaluate the function at a single point in each node. This gives an additional contribution to the error of O(h), depending on the Lipschitz constant of the Hamiltonian. This discretization error was nonnegligible, but it could be eliminated by computing the maximum at the endpoints of the nodes, instead of the middle of each node. Since a linear function on a segment of a triangle achieves its maximum at the nodes, this supremum would have been computed accurately up to $O(h^2)$, decreasing the discretization error at the expense of increasing the number of functions to be evaluated in the minimax.

Improved convergence estimates. Because of the improved convergence when smooth solutions exist, for most values of P we expected to get, and indeed we saw,

linear convergence. Nevertheless, there should be examples where the convergence is sublinear.

Global convergence of $\bar{H}_h(P)$ to $\bar{H}(P)$ may be better than expected. Since $\bar{H}_h(P)$ is convex, and is an upper bound for $\bar{H}(P)$, if for some values of P we get $\bar{H}_h(P)$ accurately (for instance, because there is a smooth solution of (HB)), that immediately implies improved bounds for other values of P. If, for instance, $\bar{H}_h(P) = \bar{H} + O(h)$ in a set of full measure, then immediately one gets $\bar{H}_h(P) = \bar{H}(P) + O(h)$ in the remaining points.

Secondly, in Theorem 2.7 we constructed the approximate minimizer from a viscosity solution. However, there may be other minimizers which may be smoother than the viscosity solution.

Finally, in the proof we used convolutions with a smoothing kernel, to get estimates of the form $H(D_x \tilde{u}, x) \leq \overline{H} + O(h^{\alpha})$ for some exponent α . In practice the inequality may be strict at points in which the original viscosity solution is not smooth, which could help to improve the estimates since we are taking suprema.

4. Validation. We begin by studying a one dimensional case for which explicit analytical information is available. This analytical information is used to validate the numerical method.

Theorem 2.7 gives convergence of order O(h) when there exists a smooth solution of (HB). Despite the lack of smoothness in the solution, we obtained convergence rates of O(h).

4.1. Analytical results. Consider the Hamiltonian corresponding to a one dimensional pendulum with mass and length normalized to unity,

$$H(p,x) = \frac{p^2}{2} - \cos 2\pi x$$

For this Hamiltonian one can find explicitly the solution of (HB).

PROPOSITION 4.1. The solution $(u, \bar{H}(P))$ of (HB), when H corresponds to the one dimensional pendulum, is given by

(12)
$$u(x) = \int_0^x -P + s(y)\sqrt{2(\bar{H}(P) + \cos 2\pi y)} \, dy$$

where |s(y)| = 1, with $\overline{H}(P) = 1$ for $|P| \le 4\pi^{-1}$ and

(13)
$$P = \pm \int_0^1 \sqrt{2(\bar{H}(P) + \cos 2\pi y)} \, dy$$

otherwise.

Proof. For each $P \in \mathbb{R}$ and a.e. (almost every) $x \in \mathbb{R}$, the solution u(P, x) satisfies

$$\frac{(P+D_x u)^2}{2} = \bar{H}(P) + \cos 2\pi x$$

This implies $\overline{H}(P) \ge 1$ and so

$$D_x u = -P \pm \sqrt{2(\bar{H}(P) + \cos 2\pi x)}, \quad \text{a.e. } x \in \mathbb{R}.$$

Thus (12) holds for |s(y)| = 1.

TABLE 1

Computed values for \overline{H} as a function of the number of points, comparing the sine and cosine potential, with P = 0.5 and $\overline{H}(0.5) = 1$.

Number of points $n =$	9	17	33	65
Values (using sine)	0.98480	0.99573	0.99887	0.99971
Max of sin on the grid	0.98480	0.99573	0.99887	0.99971
Values (using cosine)	1.00000	1.00000	1.00000	1.00000
Max of cosine on the grid	1.00000	1.00000	1.00000	1.00000

Because H is convex in p and u is a viscosity solution, u is semiconcave, and so the only possible discontinuities in the derivative of u are the ones that satisfy $D_x u(x^-) - D_x u(x^+) > 0$ (see [Eva98]). Therefore s can change sign from 1 to -1 at any point, but jumps from -1 to 1 can happen only when $\sqrt{2(\bar{H}(P) + \cos 2\pi x)} = 0$.

If we require 1-periodicity, then there are two cases. (i) If $\bar{H}(P) > 1$, the solution is C^1 since $\sqrt{2(\bar{H}(P) + \cos 2\pi y)}$ is never zero. These solutions correspond to invariant tori. In this case P and $\bar{H}(P)$ satisfy (13). It is easy to check that this equation has a solution $\bar{H}(P)$ whenever

$$|P| \ge \int_0^1 \sqrt{2(1+\cos 2\pi y)} dy,$$

that is, whenever $|P| > 4\pi^{-1}$. (ii) Otherwise, when $|P| \le 4\pi^{-1}$, $\overline{H}(P) = 1$ and s(x) can have a discontinuity. Indeed, s(x) jumps from -1 to 1 when $x = \frac{1}{2} + k$, with $k \in \mathbb{Z}$, and there is a point x_0 , defined by the equation

$$-\int_{0}^{1} s(y)\sqrt{2(1+\cos 2\pi y)}dy = P,$$

in which s(x) jumps from 1 to -1. In this last case the graph $(x, P + D_x u)$ is a backwards invariant set contained in the unstable manifold of the hyperbolic equilibria of the pendulum. The graph of $\bar{H}(P)$ has a flat spot near P = 0. \Box

This example also shows that (HB) does not have a unique solution. Indeed, $\cos 2\pi x$ is also 2-periodic. So if we look for 2-periodic solutions, we find out that for |P| small we can have two points where the derivative is discontinuous, and we can choose one of them freely because our only constraint is periodicity. Note, however, that the value of \overline{H} is uniquely determined and is the same whether we look for 1- or 2-periodic solutions.

4.2. Validation in one dimension. To test our numerical method we varied the number of nodes n, computing \overline{H} for n = 8, 16, 32, 64 and with P = 0.5. Here the exact value is $\overline{H} = 1$.

For each of the above values of n, the exact answer was achieved with an error bounded by 10^{-10} . However, this is an artifact of the special nature of the example, related to the fact that we resolved the maximum of $\sin(x)$ well. To illustrate this, we use a poorer choice of n values and get a larger error, as seen from Table 1. With these choices of n we see that the discrete problem is solved to within the tolerance of 10^{-6} , but the exact problem is solved only up to the resolution error of the Hamiltonian.

We repeated the same test for P = 2, which puts us in the strictly convex part of $\bar{H}(P)$. The value $\bar{H}(2) = 2.0637954$ can be obtained by solving the equation

$$2 = \int_0^1 \sqrt{2(\bar{H}(2) - \cos(2\pi x))} dx$$

TABLE 2

Computed error for \overline{H} as a function of the number of points, comparing the sine and cosine potential, with P = 2.

Number of points $n =$	8	16	32	64	96
Error (using sine) $\times 10^{-5}$	0.1912	0.0013	0.0009	0.0005	0.0183
Error (using cosine) $\times 10^{-5}$	0.1912	-0.0013	-0.0014	0.0074	0.0017



FIG. 1. $\overline{H}(P)$ for the pendulum, over the range [-2,2] (left), and an enlargement near the lower-right corner.

with respect to $\overline{H}(2)$. The error is plotted in Table 2; in this case except for the smallest (n = 8) discretization, the computed values fall within the tolerance of the scheme. The conclusion is that the dominant error comes from the discretization, not the optimization routines.

The values of $\overline{H}(P)$, computed with a resolution of 32 points, are shown in Figure 1. The largest error occurs near the corner. The location of the corner is close to the analytical value $P = 4\pi^{-1} \simeq 1.27324$.

4.3. Validation in two dimensions. In this section we study two uncoupled pendulums. This problem is a direct sum of the one dimensional case, so it is used to validate the method in two dimensions.

The Hamiltonian corresponding to two pendulums is

$$H(p_x, p_y, x, y) = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \cos 2\pi x + \cos 2\pi y$$

The effective Hamiltonian is thus

$$\bar{H}(P_x, P_y) = \bar{H}_0(P_x) + \bar{H}_0(P_y),$$

in which \bar{H}_0 is the effective Hamiltonian for a one dimensional pendulum. For instance, $\bar{H}(1.5) = 1.244638$, $\bar{H}(2.5) = 3.165327$, and thus the analytical value is $\bar{H}(1.5, 2, 5) = 4.4099660$.

As an accuracy test in the two dimensional case, we computed for P = (1.5, 2.5)and n = 8, 12, 16, 32 the value of $\overline{H}(P)$ and the corresponding error; see Table 3.

TABLE	9
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Computed values for $\overline{H}(1.5, 2.5)$ as a function of the number of points.

n	8	12	16	24	Exact
Values FE	4.6521	4.5627	4.5216	4.4836	4.4099660
Error FE	0.24	0.14	0.11	0.07	
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			. 4.		



FIG. 2. Visualization of $\overline{H}(P)$ for the potential $V(x, y) = \cos(2\pi x)$.

5. Computational results.

5.1. Strictly convex Hamiltonians. In this section we study several strictly convex Hamiltonians. Unless stated otherwise, all the numerical examples use n = 8, that is, 64 nodes and 128 triangular elements.

Example 1 (pendulum and a free particle). Potential: $V(x, y) = \cos(2\pi x)$. This potential is *y*-independent, and therefore $\bar{H}(P_1, P_2)$ for P_2 fixed should be the same as the effective Hamiltonian for the one dimensional pendulum. With P_1 fixed, \bar{H} should be a parabola in P_2 . We solved for $\bar{H}(P)$ with a resolution of .1 for $P \in [-4, 4] \times [-4, 4]$. The result is presented in Figure 2.

Example 2 (potential $V(x, y) = \cos(2\pi x)\cos(2\pi y)$). We computed $\bar{H}(P)$ with a resolution in P of .1 for $P \in [-4, 4] \times [-4, 4]$. The result is presented in Figure 3.

Example 3 (potential $V(x, y) = \cos(2\pi x) + \cos(2\pi y) + \cos(2\pi (x - y))$). We computed $\overline{H}(P)$ with a resolution of .25 in P for $P \in [-3, 3] \times [-3, 3]$. The result is presented in Figure 4.

Example 4 (double pendulum). The double pendulum is a well known nonintegrable example for which the effective Hamiltonian is not known. The Hamiltonian for the double pendulum is

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

We computed the values of $\overline{H}(P)$ with a resolution in P of .2 for P in $[-5,5] \times [-5,5]$. The result is presented in Figure 5.



FIG. 3. Visualization of $\overline{H}(P)$ for the potential $V(x,y) = \cos(2\pi x)\cos(2\pi y)$.



FIG. 4. Visualization of $\overline{H}(P)$ for the potential $V(x,y) = \cos(2\pi x) + \cos(2\pi y) + \cos(2\pi (x-y))$.

5.2. Nonstrictly 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 5 (linear nonresonant). Consider the linear (nonresonant) Hamiltonian

(14)
$$H(p,x) = \omega \cdot p + V(x,y).$$

Suppose u is a smooth viscosity solution of (HB) for this Hamiltonian. The divergence theorem yields

$$\int_{\mathbb{T}^n} \omega \cdot D_x u = 0.$$



FIG. 5. Visualization of $\overline{H}(P)$ for the double pendulum.

Therefore

(15)
$$\bar{H}(0) = \int_{\mathbb{T}^n} V$$

and $\bar{H}(P) = \bar{H}(0) + \omega \cdot P$. For the example $u_x + \sqrt{2}u_y + \cos(2\pi x)$ we obtained $D_P \bar{H} = (1, \sqrt{2})$ and $\bar{H}(0, 0) = 0$. Despite the fact that the vector (1, 1) is rationally dependent, the Hamilton–Jacobi equation $u_x + u_y + \cos(2\pi x)$ is nonresonant because of the nature of the potential. Numerically we obtained $D_P \bar{H} = (1, 1)$ and $\bar{H}(0, 0) = 0$. In this (linear) case the optimization routine converged very quickly.

Example 6 (time-periodic). Another example is a periodic time-dependent one-space-dimension Hamilton–Jacobi equation

$$-u_t + H(D_x u, x, t) = \bar{H}.$$

There exists a unique value \overline{H} for which this problem admits space-time-periodic solutions [EG02]. Moreover, this solution is Lipschitz, and thus we have a O(h) convergence.

Note also that $P = (P_t, P_x)$ but $\overline{H}(P)$ is linear in P_t , and so we may as well consider the problem

$$\inf_{\phi} \sup_{(x,t)} -\phi_t + H(P_x + D_x\phi, x, t) = \bar{H}(P_x).$$

For the forced pendulum

$$H(p,x) = \frac{p^2}{2} + \cos 2\pi x + \sin 2\pi x \sin 2\pi t.$$

We set $P_t = 0$ and plot $\overline{H}(P_x)$; see Figure 6.

Observe that the maximum of the potential $\cos 2\pi x + \sin 2\pi x \sin 2\pi t$ is $\sqrt{2}$, which coincides with the minimum of $\overline{H}(P)$.



FIG. 6. Values of $\overline{H}(P)$ for the time-periodic Hamiltonian.

Example 7 (vakonomic). Finally, we study an example of a nonstrictly convex Hamiltonian which satisfies commutation relations related to vakonomic mechanics [AKN97],

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

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

We choose V = 0, $f_1 = (0, 1)$, and $f_2 = (\cos 2\pi y, \sin 2\pi y)$. If $\sin 2\pi y = 0$, $f_2 = (0, \pm 1)$, and so f_1 and f_2 are linearly dependent. However,

$$[f_1, f_2] = 2\pi (-\sin 2\pi y, \cos 2\pi y),$$

and so the vectors $f_1, f_2, [f_1, f_2]$ always span \mathbb{R}^2 . Therefore there is a Hölder continuous viscosity solution.

In fact, this example can be reduced to a one dimensional problem. The Hamilton–Jacobi equation is

$$\frac{\cos^2 2\pi y}{2} (P_x + u_x)^2 + \frac{(1 + \sin^2 2\pi y)}{2} (P_y + u_y)^2 + \sin 2\pi y \cos 2\pi u (P_x + u_x) (P_y + u_y) = \bar{H}(P_x, P_y).$$

Since there is no explicit dependence in x, there are solutions independent of x, given by the equation

$$\frac{\cos^2 2\pi y}{2} P_x^2 + \frac{(1+\sin^2 2\pi y)}{2} (P_y + u_y)^2 + \sin 2\pi y \cos 2\pi y P_x (P_y + u_y) = \bar{H}(P_x, P_y).$$

Since this equation is strictly convex in u_y , there is a Lipschitz solution.

To remove this degeneracy we considered the potential $V(x,y) = \cos 2\pi x + \sin 2\pi (x-y)$, for which the previous reduction procedure does not work. The result is presented in Figure 7.



FIG. 7. Values of $\overline{H}(P)$ for the time-periodic Hamiltonian.

5.3. Nonexistence of viscosity solutions. There are situations where there do not exist viscosity solutions to (HB), but where \overline{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

(16)
$$\alpha u^{\alpha} + H(P + D_x u^{\alpha}, x) = 0,$$

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

(17)
$$\bar{H}(P) \equiv \lim_{\alpha \to 0} \alpha u^{\alpha}$$

These results are consistent with (HB) but determine a value $\overline{H}(P)$ even under weaker conditions, for example, as long as αu^{α} converges uniformly to a constant, which happens when

$$u^{\alpha} - \min_{x} u^{\alpha} \to \text{ bounded function of } x$$

uniformly.

For example, in the simpler case when H is strictly convex in p, we get that $u^{\alpha} - \min_{x} u^{\alpha}$ is bounded uniformly in α , since in this case the solutions u^{α} are Lipschitz independently of α .

The result (1) may also give a correct value for \overline{H} in these more general situations. PROPOSITION 5.1. Let u^{α} be a solution of (16), and suppose that αu^{α} converges uniformly to a constant number $\overline{H}(P)$. 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

$$v^{\alpha} \equiv u^{\alpha} + \frac{H_{\alpha}}{\alpha},$$

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_{α}^{ϵ} denote the sup convolution of v_{α} , and let $\phi = \eta_{\epsilon} * v_{\alpha}^{\epsilon}$. Then

$$H(D_x\phi, x) \le H_\alpha + O(\epsilon).$$

Therefore

$$\inf_{\phi} \sup_{x \in \mathbb{T}^n} H(D_x \phi, x) \le \bar{H}_{\alpha} \to \bar{H}.$$

3. Now let

$$e_{\alpha} = \sup_{x} \alpha v_{\alpha},$$

which converges to 0.

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

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

Thus

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

and so

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

Therefore $\inf_{\phi} \sup_{x \in \mathbb{T}^n} H(D_x \phi, x) \ge \overline{H}.$ \Box

Example 8 (quasiperiodic Hamiltonians). We consider an example from [LS03] for which there is no viscosity solution to (HB), yet where $\bar{H}(P)$ can be determined from (17). Let

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

with α irrational. We computed $\overline{H}(P)$ numerically from (1). The results are presented in Figure 8.

Example 9 (linear resonant). Resonant linear Hamiltonians (14) may fail to have a viscosity solution. An example is

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

The formula (15) yields $\overline{H}(0) = 0$ if there is a solution of (HB). However, we have

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

Let ϕ 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 $D_P \overline{H} = (0, 1)$ and $\overline{H}(0, 0) = 1$. This is interesting, because $\overline{H}(0, 0)$ should be 0, not 1, and this shows the nonexistence of solutions.



FIG. 8. Values of $\bar{H}(P)$ for the quasi-periodic Hamiltonian.

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