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Motion in periodic potentials

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Abstract. We consider motion in a periodic potential in a classical, quantum, and semiclassical context. Various results on the distribution of asymptotic velocities are proven.

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1. Introduction

For a function $V : \mathbb{R}^d \to \mathbb{R}$ which is periodic on a regular lattice $\mathcal{L} \subset \mathbb{R}^d$ we study the evolutions

$$\mathrm{i}h\partial_t W(t) = H^h W(t) \qquad W(0) = Id \qquad \text{on } L^2(\mathbb{R}^d) \tag{1}$$

$$\partial_t \Phi^t = X_H \circ \Phi^t \qquad \Phi^0 = Id \qquad \text{on } \mathbb{R}^{2d} \tag{2}$$

where $H^h = -\frac{h^2}{2}\Delta + V(q)$, $H(p,q) = \frac{p^2}{2} + V(q)$ and $X_H(p,q) = (-\nabla V(q), p)$. This is done in the limits $t \to \infty$ and $h \to 0$.

Why should one get interested in well known things? In view of currently very active research on transport (anomalous or not) in condensed-matter physics it is first desirable to put on a firm mathematical ground the folklore that 'motion in crystals is ballistic'; second one should try to obtain at least semiclassical information on quantities such as the *distribution of asymptotic velocities*.

We investigate the asymptotic velocity $\lim_{t\to\infty} q(t)/t$ and the asymptotic behaviour of $q^2(t)/t^\alpha$ where $\alpha = 2$ characterizes by definition ballistic, $\alpha = 1$ diffusive motion.

Our results and the skeleton of the article are as follows.

In section 2 we show for a large class of V that the quantum motion is ballistic (theorem 2.3). This class of potentials is not optimal in view of singularities; it includes, however, the Coulomb case. The modulus of the asymptotic velocity is bounded from above in a natural way (corollary 2.4).

In section 3 we treat the classical motion in smooth potentials. In $d = 2$ dimensions the motion is ballistic for high enough energies E; for $d \geqslant 3$ this is true for initial conditions outside a set of measure $\sim 1/\sqrt{E}$. There always exist fast orbits (of speed $\sim \sqrt{E}$), with a dense set of directions. This is even true for the ergodic case, where the asymptotic speed is zero with probability one, whereas almost all orbits are unbounded (theorem 3.1).

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The motion is never Anosov (theorem 3.3).

In particular this means that a gas of particles in a 'periodic' container is not Anosov if the interactions are smooth. So there may be small regions of regular motions and it seems unlikely that such a gas is ergodic.

In contrast, the planar motion in periodic potentials with coulombic ($-1/r$ type) singularities is known to be of Anosov type and diffusive, [12]. In section 4 we show that the distribution of asymptotic velocities—which are zero on a set of full measure—is dense in a disk of approximate radius $\sqrt{E}$ (theorem 4.3).

Concerning semiclassics we show in section 5 that the quantum asymptotic velocities are always contained in a thickened convex hull of the classical ones for h small; they concentrate in measure inside the convex hull of the support of the classical probability distribution (theorem 5.3).

In particular in the classically ergodic case the positive speed of the quantal motion is only a quantum fluctuation vanishing in the semiclassical limit. The same is also known to be true for coulombic potentials, see [13].

The above results are basically consequences of the Birkhoff ergodic theorem. This is interesting in so far as our technique is likely to be applicable in different semiclassical situations. On the other hand more specific information is needed to prove sharper results concerning the distribution of asymptotic velocities.

This is done in section 6, where we consider separable potentials. There we have fast semiclassical convergence to the classical velocity distribution (theorem 6.1).

2. Quantum ballistic motion

Now we shall prove that the evolution of a quantum system in a rather general periodic medium is ballistic and that the asymptotic velocity exists. The latter is related to the band functions.

It is known that for a certain class of singular potentials the spectrum of the Hamiltonian is absolutely continuous, see Thomas [21], Reed and Simon [19], Knauf [13]. It has been conjectured that absolute continuity implies ballistic motion. Our proof in d dimensions is based on Bloch theory.

We consider potentials $V : \mathbb{R}^d \to \mathbb{R}$ which are periodic w.r.t. a regular lattice $\mathcal{L} \subset \mathbb{R}^d$

$$V(q + \ell) = V(q) \qquad (q \in \mathbb{R}^d, \ell \in \mathcal{L})$$

so that we may consider it as a function $V : \mathbb{T} \to \mathbb{R}$ on the unit cell $\mathbb{T} := \mathbb{R}^d/\mathcal{L}$, and calculate its Fourier transform $\mathcal{F}V : \mathcal{L}^* \to \mathbb{C}$. Our assumptions on the regularity of the potential are:

(A_q): $d = 2$**:** $V \in L^p(\mathbb{T})$ with $p > 1$
$d = 3$**:** $V \in L^2(\mathbb{T})$ and
$d > 3$**:** $\mathcal{F}(V) \in l^p(\mathcal{L}^*)$ with $p < (d-1)/(d-2)$.

(A_q) implies that V is form small with respect to $-\Delta$ and even operator small for $d \neq 2$, see [3].

$$\text{Denote } D := -\mathrm{i}h\nabla \qquad \text{then } H^h := \frac{D^2}{2} \dot{+} V$$

is defined by its quadratic form with form domain $Q(H^h) = Q(-\Delta) = H^1(\mathbb{R}^d)$; for $d \neq 2$ the operator domain is $D(H^h) = H^2(\mathbb{R}^d)$.

We denote by

$$O(t) := W^*(t) O W(t)$$

(with the solution $W(t) := \exp(-\mathrm{i}H^h t/h)$ of (1)) the Heisenberg time evolution of an operator O.

The symmetries of H^h allow for a decomposition with respect to the group of lattice translations: let $\mathcal{L}^*$ be the dual lattice with unit cell $\mathbb{T}^*$ and denote by

$$U : L^2(\mathbb{R}^d) \to L^2\left(\mathbb{T}^*, \frac{\mathrm{d}k}{|\mathbb{T}^*|}; L^2(\mathbb{T}, \mathrm{d}q)\right) \equiv \int_{\mathbb{T}^*}^{\oplus} L^2(\mathbb{T}, \mathrm{d}q) \frac{\mathrm{d}k}{|\mathbb{T}^*|}$$

the unitary operator defined by extension from Schwarz space of

$$U\psi(k, q) \equiv (U\psi)_k(q) := \sum_{\ell \in \mathcal{L}} \mathrm{e}^{-\mathrm{i}k(q+\ell)} \psi(q + \ell) \qquad (\psi \in \mathcal{S}(\mathbb{R}^d)).$$

The following facts are known in the literature and will be used below.

Theorem 2.1. *Let V satisfy (A_q). Then*

(1) $UH^hU^{-1} = \int_{\mathbb{T}^*}^{\oplus} H^h(k) \frac{\mathrm{d}k}{|\mathbb{T}^*|}$ with $H^h(k) = \frac{1}{2}(D+hk)^2 \dot{+} V$ on $L^2(\mathbb{T})$, with form domain $Q(H^h(k)) = H^1(\mathbb{T})$;

(2) $k \mapsto H^h(k)$ is a type (B) analytic family;

(3) the spectrum of H^h is absolutely continuous;

(4) $H^h(k)$ has compact resolvent, $H^h(k) = \sum_{n=1}^{\infty} E_n^h(k) P_n^h(k)$ where $E_n^h(k)$ are the eigenvalues in ascending order, $P_n^h(k)$ the eigenprojections;

(5) for every n the following are Lebesgue nullsets:

$$\{k \in \mathbb{T}^* | E_n^h \text{ is not differentiable at } k\}$$
$$\{k \in \mathbb{T}^* | P_n^h \text{ is not differentiable at } k\}$$
$$\{k \in \mathbb{T}^* | \nabla_k E_n^h(k) = 0\}.$$

Proof. (1)–(4) are proven in [19], respectively in [13] for $d = 2$. (5) is proven in [23, 21], see also [5]. □

Remark 2.2. We emphasize that while the assumptions (A_q) are sufficient for absolute continuity, for $d > 2$ they are far from necessary for self-adjointness. It would be interesting to understand what happens in the gap!

The result on ballistic transport in the quantum case is given below (see also the recent article [5] by Gerard and Nier).

Theorem 2.3. *Let V satisfy (A_q). It holds for ψ with*
$(D\psi, D\psi) + (q\psi, q\psi) < \infty$:

$$\bar{D}\psi := \lim_{t\to\infty} \frac{q(t)\psi}{t} = U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus} \sum_{n=1}^{\infty} P_n(k)(D + hk) P_n(k) \frac{\mathrm{d}k}{|\mathbb{T}^*|}\right) U\psi$$
$$= U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus} \sum_{n=1}^{\infty} h^{-1} \nabla_k E_n P_n(k) \frac{\mathrm{d}k}{|\mathbb{T}^*|}\right) U\psi$$

and

$$\lim_{t\to\infty} \frac{(\psi, q^2(t)\psi)}{t^2} = \int_{\mathbb{T}^*}^{\oplus} \sum_{n=1}^{\infty} |h^{-1} \nabla_k E_n|^2 \| P_n U\psi(k) \|^2_{L^2(\mathbb{T})} \frac{\mathrm{d}k}{|\mathbb{T}^*|} > 0.$$

Proof. The map

$$\psi \mapsto \frac{1}{T}\int_0^T D(t)\psi\,\mathrm{d}t - U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus}\sum_{n=1}^{\infty} P_n(k)(D+hk)P_n(k)\frac{\mathrm{d}k}{|\mathbb{T}^*|}\right)U\psi$$

is uniformly bounded from $H^1 \to L^2$, consequently it is sufficient to prove the assertion for ψ in a dense set; indeed first by the form smallness of V we have the estimate

$$\|\langle D\rangle\psi\|^2 = \langle\psi,(1+D^2)\psi\rangle \leqslant c_1|\langle\psi,H\psi\rangle| + c_2\|\psi\|^2 \leqslant c_3\langle\psi,(1+D^2)\psi\rangle$$

so

$$\left\|\frac{1}{T}\int_0^T D(t)\psi\,\mathrm{d}t\right\| \leqslant \|\langle D\rangle(H+\mathrm{i})^{-1/2}\|\|(H+\mathrm{i})^{1/2}\psi\| \leqslant c\|\psi\|_{H^1}$$

second

$$\begin{aligned}
&\left\|U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus}\sum_{n=1}^{\infty}P_n(k)(D+hk)P_n(k)\frac{\mathrm{d}k}{|\mathbb{T}^*|}\right)U\psi\right\|^2\\
&\qquad= \int_{\mathbb{T}^*}\sum_{n=1}^{\infty}\|P_n(k)(D+hk)(H(k)+\mathrm{i})^{-1/2}P_n(k)U(H+\mathrm{i})^{1/2}\psi(k)\|^2_{L^2(\mathbb{T})}\frac{\mathrm{d}k}{|\mathbb{T}^*|}\\
&\qquad\leqslant \int_{\mathbb{T}^*}\|(D+hk)(H(k)+\mathrm{i})^{-1/2}\|^2\|U(H+\mathrm{i})^{1/2}\psi(k)\|^2\frac{\mathrm{d}k}{|\mathbb{T}^*|} \leqslant \text{constant}\|\psi\|^2_{H^1}.
\end{aligned}$$

Let ψ be such that

$$U\psi = \left(\int_{\mathbb{T}^*}^{\oplus}\sum_{n=1}^{N}P_n(k)\frac{\mathrm{d}k}{|\mathbb{T}^*|}\right)U\psi.$$

The set of these is dense in $H^1(\mathbb{R}^d)$. Then

$$\begin{aligned}
&\left\|U\left(\frac{1}{T}\int_0^T D(t)\psi\,\mathrm{d}t\right) - \left(\int_{\mathbb{T}^*}^{\oplus}\sum_{n=1}^{N}P_n(k)(D+hk)P_n(k)\frac{\mathrm{d}k}{|\mathbb{T}^*|}\right)U\psi\right\|^2\\
&\qquad\leqslant \int_{\mathbb{T}^*}\left\|\sum_{m,n}^{\infty,N}\frac{1}{T}\int_0^T \exp(\mathrm{i}(E_m(k)-E_n(k))t/h)\,\mathrm{d}t\;P_m(k)(D+hk)P_n(k)U\psi(k)\right.\\
&\qquad\qquad\left.-\sum_{n=1}^{N}P_n(k)(D+hk)P_n(k)U\psi(k)\right\|^2_{L^2(\mathbb{T})}\frac{\mathrm{d}k}{|\mathbb{T}^*|}\\
&\qquad= \int_{\mathbb{T}^*}\sum_{\substack{m=1\\ m\neq n}}^{\infty}\left\|P_m(k)\sum_{n=1}^{N}\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}(E_m(k)-E_n(k))t/h}\,\mathrm{d}t\,(D+hk)P_n(k)U\psi(k)\right\|^2\frac{\mathrm{d}k}{|\mathbb{T}^*|}\\
&\qquad\to 0 \qquad (T\to\infty)
\end{aligned}$$

by dominated convergence, which is applicable because $\|P_m(k)\sum_n\ldots\| = \mathrm{O}(1/T)$ for $m\neq n$, almost all k, and is uniformly majorized by

$$\text{constant}\times\sup_{n=1,\ldots,N}\|P_m(k)(D+hk)P_n(k)U\psi(k)\|^2_{L^2(\mathbb{T})}$$

which is summable w.r.t. m and k.

In [18] it was shown that for $\psi\in H^1(\mathbb{R}^d)\cap D(|q|)$:

$$q(T)\psi = q\psi + \int_0^T D(t)\psi\,\mathrm{d}t.$$

It follows

$$\lim_{T\to\infty} \frac{q(T)\psi}{T} = \lim_{T\to\infty} \frac{1}{T} \int_0^T D(t)\psi \, \mathrm{d}t = U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus} \sum_{n=1}^{\infty} P_n(k)(D+hk)P_n(k) \frac{\mathrm{d}k}{|\mathbb{T}^*|} \right) U\psi.$$

It remains to establish the identity

$$P_n(k)(D+hk)P_n(k) = h^{-1}\nabla_k E_n(k) P_n(k)$$

for almost every $k \in \mathbb{T}^*$. This follows from:

$$\nabla_k PHP = E(\nabla_k P)P + EP(\nabla_k P) + P(\nabla_k H)P = E\nabla_k P + P(\nabla_k H)P$$
$$\nabla_k PHP = E\nabla_k P + P\nabla_k E \qquad \nabla_k H = h(D+hk)$$

all valid in the quadratic-form sense for almost every k by properties 2.1.

This was the first assertion; the second one is a consequence thereof. The positivity is inferred from theorem 2.1. □

As a corollary we get an estimate for the group velocity in one band.

Corollary 2.4. *For every n there is a set of a full measure of k's such that*

$$\left| \frac{\nabla_k E_n^h(k)}{h} \right|^2 \leqslant 2(E_n^h(k) - \inf_{\{\|\psi\|=1, P_n(k)\psi=\psi\}} \langle \psi, V\psi \rangle_{L^2(\mathbb{T})}).$$

Proof. Let $\psi \in L^2(\mathbb{T})$, k such that E_n, P_n are differentiable at k.

$$|h^{-2}\nabla_k E_n(k)|^2 \|P_n(k)\psi\|^2 = \|P_n(k)(D+hk)P_n(k)\psi\|^2 \leqslant \|(D+hk)P_n(k)\psi\|^2$$
$$= 2(E_n(k)\|P_n(k)\psi\|^2 - \langle P_n(k)\psi, VP_n(k)\psi\rangle)$$

implies the inequality. □

3. Classical motion: smooth potentials

The classical motion in a $\mathcal{L}$-periodic potential V on $\mathbb{R}^d$ is described by Hamilton's equations (2) on phase space $P := T^*\mathbb{R}^d$ for $H : P \to \mathbb{R}$, $H(p,q) = \frac{1}{2}p^2 + V(q)$. If $V \in C^2(\mathbb{R}^d, \mathbb{R})$ (as we assume in this section), the flow $\Phi^t : P \to P$ exists uniquely for all times $t \in \mathbb{R}$.

We will analyse its restrictions $\Phi_E^t := \Phi^t \restriction_{\Sigma_E}$ to the energy shells

$$\Sigma_E := H^{-1}(E).$$

Alternatively we study motion on the phase space $\hat{P} := T^*\mathbb{T}$ over the configuration torus (and mark corresponding objects with a hat). Using the phase-space projection $\Pi : P \to \hat{P}$ arising from the projection $\pi : \mathbb{R}^d \to \mathbb{T} = \mathbb{R}^d/\mathcal{L}$ of configuration spaces, we thus consider the flow $\hat{\Phi}^t : \hat{P} \to \hat{P}$ generated by the Hamiltonian function $\hat{H} : \hat{P} \to \mathbb{R}$, $\hat{H} \circ \Pi = H$, and its compact energy shells $\hat{\Sigma}_E := \hat{H}^{-1}(E)$ with the restricted flows $\hat{\Phi}_E^t := \hat{\Phi}^t \restriction_{\hat{\Sigma}_E}$.

The Liouville measures $\hat{\lambda}$ of the phase-space regions $\hat{H}^{-1}([V_{\min}, E])$ $E \in \mathbb{R}$, are now finite, a fact which enables us to use notions of ergodic theory.

The energy scales $V_{\min} := \inf_{q\in\mathbb{R}^d} V(q)$,

$$V_{\text{mean}} := \int_{\mathbb{T}} V(q)\, \mathrm{d}q/|\mathbb{T}|$$

and $V_{\max} := \sup_{q\in\mathbb{R}^d} V(q)$ of the dynamics will be used repeatedly.

As a consequence of Birkhoff's ergodic theorem for $\hat{\lambda}$—almost all $\hat{x}_0 \in \hat{P}$

$$\bar{v}^{\pm}(\hat{x}_0) := \lim_{T\to\pm\infty} \frac{1}{T} \int_0^T \hat{p}(t, \hat{x}_0)\, \mathrm{d}t$$

exist and are equal. In this case we set $\bar{v} := \bar{v}^{\pm}$, and otherwise $\bar{v} := 0$, thus defining the *asymptotic velocity*

$$\bar{v} : \hat{P} \to \mathbb{R}^d$$

which is a measurable phase-space function.

We denote its lift $\bar{v} \circ \Pi : P \to \mathbb{R}^d$ to the original phase space P by the same symbol and thus have

$$\lim_{t\to\pm\infty} \frac{q(t, x_0)}{t} = \bar{v}(x_0)$$

λ—almost everywhere.

$\hat{\Phi}^t$ is called *ballistic at* $\hat{x} \in \hat{P}$ if $\bar{v}(\hat{x}) \neq 0$ (observe that by the above definition this implies existence and equality of $\bar{v}^{\pm}$).

We are particularly interested in the energy dependence of the asymptotic velocity and thus introduce the *energy–velocity map*

$$A := (\hat{H}, \bar{v}) : \hat{P} \to \mathbb{R}^{d+1}. \tag{3}$$

A is measurable and generates an image measure $\nu := \hat{\lambda} A^{-1}$ on $\mathbb{R}^{d+1}$.

Example. In the simplest case $V = 0$ of *free motion* ν is a smooth measure on the paraboloid

$$A(\hat{P}) = \{(\tfrac{1}{2}v^2, v) | v \in \mathbb{R}^d\}.$$

As in the above example, in the general case ν is invariant under $(h, v) \mapsto (h, -v)$, since the motion is reversible.

The equality $H = \frac{1}{2}\bar{v}^2$ is in the general case replaced by the estimate $|\bar{v}(x)| \leqslant \sqrt{2(H(x) - V_{\min})}$.

For regular values of the energy E one may consider the probability distribution of the asymptotic velocities $\bar{v}$ w.r.t. the normalized Liouville measure $\hat{\lambda}_E$ on the energy shell $\hat{\Sigma}_E$. By the above bound this is supported within a ball of radius $\sqrt{E - V_{\min}}$.

Unlike in the above example, in general it is not expected to depend weak-*-continuously on E, see remark 3.2(1) below.

Here are our results on classical ballistic motion for $V \in C^2$ potentials:

Theorem 3.1.

(1) For $d = 1$ the motion is ballistic at $x = (p, q) \in P$ iff $E := H(x) > V_{\max}$, with asymptotic velocity

$$\bar{v}(x) = \frac{\mathrm{sign}(p)}{l^{-1} \int_0^l (2(E - V(q)))^{-\frac{1}{2}}\, \mathrm{d}q}$$

($l > 0$ being the period of $\mathcal{L}$).

(2) For $d > 1$ and $E > V_{\max}$ there exists a set $B_E \subset \Sigma_E$ for which the motion is ballistic, whose directions

$$\{\bar{v}(x)/\|\bar{v}(x)\| | x \in B_E\}$$

are dense in S^{d-1}*, with moduli*

$$\frac{\sqrt{2}(E - V_{\max})}{\sqrt{E - V_{\mathrm{mean}}}} \leqslant \|\bar{v}(x)\| \leqslant \sqrt{2(E - V_{\min})} \qquad (x \in B_E). \tag{4}$$

(3) For $d = 2$ *and* $V \in C^5(\mathbb{R}^d, \mathbb{R})$ *there exists a threshold* $E_{\mathrm{th}} \geqslant V_{\max}$ *above which the flows* Φ_E^t $(E > E_{\mathrm{th}})$ *are ballistic* $\hat{\lambda}_E$*, almost everywhere.*

E_{th} *is given by the following condition. For* $E > E_{\mathrm{th}}$ *there are two geometrically different minimal tori* $\mathbb{T}_1^2, \mathbb{T}_2^2 \subset \hat{\Sigma}_E$ *(by 'geometrically different' we mean: not related by time-reversal symmetry* $\mathcal{I}(\hat{p}, \hat{q}) := (-\hat{p}, \hat{q})$*).*

(4) We assume here that V *is* $3d$ *times continuously differentiable. Then for* $d > 2$ *there exists a threshold energy* $E_{\mathrm{th}} \geqslant V_{\max}$ *and for* $E > E_{\mathrm{th}}$ *subsets* $\hat{B}_E \subset \hat{\Sigma}_E$ *of measures*

$$\hat{\lambda}_E(\hat{B}_E) \geqslant 1 - \sqrt{E_{\mathrm{th}}/E}$$

such that on $\hat{B}_E$ *the motion is ballistic.*

(5) If the flow $\hat{\Phi}_E^t$ *on the energy shell is ergodic w.r.t.* $\hat{\lambda}_E$*, then* $\bar{v} = 0$ *with* $\hat{\lambda}_E$ *probability one. However, if in addition* $E > V_{\max}$*, the trajectories are unbounded with probability one:*

$$\hat{\lambda}_E\left(\left\{\hat{x}_0 \in \hat{\Sigma}_E \,\middle|\, \limsup_T \left\| \int_0^T \hat{p}(t, \hat{x}_0)\,\mathrm{d}t \right\| = \infty \right\}\right) = 1.$$

(6) For $d \geqslant 2$ *there are smooth* $\mathcal{L}$*-periodic potentials* V *and energies* $E > V_{\max}$ *whose energy shell contains a set of bounded orbits of positive measure:*

$$\hat{\lambda}_E\left(\left\{\hat{x}_0 \in \hat{\Sigma}_E \,\middle|\, \limsup_T \left\| \int_0^T \hat{p}(t, \hat{x}_0)\,\mathrm{d}t \right\| < \infty \right\}\right) > 0.$$

Example. Consider first in $d = 1$ dimensions the potential $V(q) = \cos(q)$. With the formula of theorem 3.1 for $E \geqslant 1$ the asymptotic speed equals

$$\bar{v}(E) = \frac{\pi\sqrt{E - 1}}{\sqrt{2}\,\mathrm{Elliptic}\mathcal{K}(2/(1 - E))}$$

(Elliptic$\mathcal{K}$ being the complete elliptic integral of the first kind) and $\bar{v}(E) = 0$ for $-1 \leqslant E \leqslant 1$.

For $d = 2$ this leads to a distribution of asymptotic velocities for energy E of the potential $V(q) = \cos(q_1) + \cos(q_2)$ depicted in figure 1. Observe that there is a positive probability for motion along the axes.

Proof.

(1) $\bar{v}(x_0) = l/T$ where $T := \int_0^l \frac{\mathrm{d}q}{\dot{q}}$ is the time needed for the spatial period l.

(2) The idea is to construct periodic but non-contractible orbits on the torus. These are covered by ballistic orbits in the configuration space $\mathbb{R}_q^d$.

For $E > V_{\max}$ we consider the geodesic motion on $\mathbb{T}$ in the *Jacobi metric*

$$\hat{g}_E(\hat{q}) := (E - V(\hat{q})) \cdot \sum_{i=1}^{d} d\hat{q}_i \otimes d\hat{q}_i. \tag{5}$$

The geodesics of that metric are known to coincide with the solution curves $t \mapsto \hat{q}(t, \hat{x}_0)$, $\hat{x}_0 \in \hat{\Sigma}_E$, up to a time reparametrization $\tau \mapsto t(\tau)$.

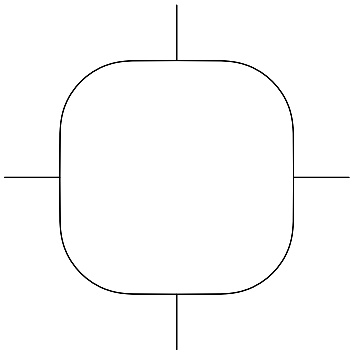

Figure 1. Distribution of asymptotic velocities $\bar{v}$ for the separable potential $V(q) = \cos(q_1) + \cos(q_2)$ and energy $E = 3$.

In every nontrivial homotopy class l of the fundamental group $\pi_1(\mathbb{T}) \cong \mathcal{L}$ we find a shortest closed geodesic $\hat{c} : S^1 \to \mathbb{T}$ (with $S^1 := \mathbb{R}/\mathbb{Z}$). The length

$$L(\hat{c}) = \int_0^1 \left\| \frac{\mathrm{d}\hat{c}(\tau)}{\mathrm{d}\tau} \right\| \cdot \sqrt{E - V(\hat{c}(\tau))}\, \mathrm{d}\tau \tag{6}$$

($\|\cdot\|$ denoting Euclidean norm) of that geodesic in the Jacobi metric is the infimum of the lengths of the curves in its homotopy class l. Let the corresponding solution curve $t \mapsto \hat{q}(t, \hat{x}_0)$ on the torus have period T.

We have $q(nT, x_0) = q(0, x_0) + n \cdot l$ for motion in configuration space $\mathbb{R}^d_q$, starting from a point $x_0 \in \Pi^{-1}(\hat{x}_0)$. Therefore the asymptotic velocity $\bar{v}(x_0)$ of this orbit exists and equals $\bar{v}(x_0) = l/T$. So our task is to estimate T from below and above.

The upper bound

$$\|\bar{v}(x)\| \leqslant \sqrt{2(E - V_{\min})}$$

follows from the general bound $\|p\| \leqslant \sqrt{2(E - V_{\min})}$ if $(p, q) \in \Sigma_E$.

In order to prove the lower bound for $\|\bar{v}\|$, we derive an upper bound for the period T and argue as follows. The length $L(\hat{c})$ of our minimal geodesic $\hat{c}$ is shorter than the lengths of all the homotopic straight lines $\tilde{c} \equiv \tilde{c}_{\hat{q}} : S^1 \to \mathbb{T}$,

$$\tilde{c}(\tau) := \hat{q} + \tau \cdot l \pmod{\mathcal{L}}$$

starting from a point $\hat{q} \in \mathbb{T}$. However, by formula (6) the length $L(\tilde{c}) = \|l\| \cdot \int_0^1 \sqrt{E - V(\tilde{c}(\tau))}\, \mathrm{d}\tau$. By concavity of $x \mapsto \sqrt{E - x}$

$$\int_0^1 \sqrt{E - V(\tilde{c}(\tau))}\, \mathrm{d}\tau \leqslant \sqrt{E - V_{\text{mean}}}$$

for some $\hat{q}$. So we obtain

$$L(\hat{c}) \leqslant L(\tilde{c}) \leqslant \|l\| \cdot \sqrt{E - V_{\text{mean}}}. \tag{7}$$

On the other hand the period

$$T = \int_0^1 \frac{\mathrm{d}t}{\mathrm{d}\tau}\, \mathrm{d}\tau = \int_0^1 \left\| \frac{\mathrm{d}\hat{c}(\tau)}{\mathrm{d}\tau} \right\| \Big/ \sqrt{2(E - V(\tilde{c}(\tau)))}\, \mathrm{d}\tau \leqslant L(\hat{c})/(\sqrt{2}(E - V_{\max})).$$

Together with (7) this gives $T \leqslant \|l\| \cdot \sqrt{E - V_{\text{mean}}}/(\sqrt{2}(E - V_{\max}))$ from which the lower estimate for the asymptotic speed $\|\bar{v}(x_0)\| = \|l\|/T$ in (4) follows.

The asymptotic *direction* $\bar{v}(x_0)/\|\bar{v}(x_0)\|$ of our ballistic orbit equals $l/\|l\|$, but the directions of lattice points $l \in \mathcal{L} \setminus \{0\}$, seen from the origin are dense in S^{d-1}.

(3) We show that under the existence assumption for the tori $\mathbb{T}_1, \mathbb{T}_2 \subset \hat{\Sigma}_E$ the motion is ballistic $\hat{\lambda}_E$ almost everywhere.

For $E > V_{\max}$ and $d = 2$ the energy shell $\hat{\Sigma}_E$ is diffeomorphic to $S^1 \times \mathbb{T}^2$, S^1 representing the circle of directions $\hat{p}/\|\hat{p}\|$.

By the minimality condition the tori

$$\mathbb{T}_1, \mathbb{T}_2 \subset \hat{\Sigma}_E \subset \hat{P} \sim \mathbb{R}^2 \times \mathbb{T}$$

(and their time inverses) $\mathcal{I}(\mathbb{T}_1), \mathcal{I}(\mathbb{T}_2)$) project diffeomorphically to the configuration torus $\mathbb{T}$. Thus we may represent them as graphs of functions $\hat{P}_1, \hat{P}_2 : \mathbb{T} \to \mathbb{R}^2$. For $i = 1, 2$ the mapping

$$\hat{P}_i/\|\hat{P}_i\| : \mathbb{T} \to S^1$$

are the local direction, and is by minimality topologically trivial. So their complement

$$\hat{\Sigma}_E - (\mathbb{T}_1 \cup \mathbb{T}_2 \cup \mathcal{I}(\mathbb{T}_1) \cup \mathcal{I}(\mathbb{T}_2))$$

in the energy shell of four components diffeomorphic to thickened two-tori. These components roughly correspond to sectors of directions in which the particle is forced to move.

The problem which has to be overcome is that these sectors of directions depend on the point q, and that their union for all q may have a total opening angle of more than π. Thus it may happen that the particle goes backward for some time.

Without loss of generality we consider *the* component $\hat{C} \subset \hat{\Sigma}_E - (\mathbb{T}_1^2 \cup \mathbb{T}_2^2)$ which consists of points $(\hat{p}, \hat{q}) \in \hat{\Sigma}_E$ which are linear combinations $\hat{p} = \alpha_1 \hat{P}_1(\hat{q}) + \alpha_2 \hat{P}_2(\hat{q})$ of the points $(\hat{P}_i(\hat{q}), \hat{q}) \in \mathbb{T}_i^2$ with *positive* coefficients α_i.

On the invariant tori $\mathbb{T}_i^2$ the motion is conditionally periodic with frequency vectors $\omega_i \in \mathbb{R}^2 \setminus \{0\}$. If we consider the Lagrangian manifolds $M_i \subset \Sigma_E$ which under Π project to the tori $\mathbb{T}_i^2$, these manifolds are not only diffeomorphic to $\mathbb{R}^2$, but by our minimality assumption they project under $\mathbf{\Pi} : P \to \mathbb{R}^2$, $(p, q) \mapsto q$ diffeomorphically to the configuration plane $\mathbb{R}^2$. Thus they induce two flows

$$\Psi_i^t : \mathbb{R}^2 \to \mathbb{R}^2 \qquad \Psi_i^t := \mathbf{\Pi} \circ \Phi^t \circ (\mathbf{\Pi} \restriction_{M_i})^{-1}.$$

These are nearly linear in the sense

$$\Psi_i^t(q_0) = q_0 + \omega_i \cdot t + \mathcal{O}(t^0) \tag{8}$$

with $\mathcal{O}(t^0)$ uniform in q_0, since they come from a conditionally periodic motion on a torus. The flow lines of Ψ_1 and Ψ_2 both foliate the configuration plane and are transversal to each other. Since both foliations project under $\pi : \mathbb{R}^2 \to \mathbb{T}^2$ to foliations of the (compact!) torus, the angles under which these foliations intersect are bounded away from 0 and π, see figure 2. However, Ψ_1 and Ψ_2 do not commute in general. Nevertheless, we may use them to find an adapted coordinate system

$$\Psi : \mathbb{R}^2 \to \mathbb{R}^2 \qquad (s_1, s_2) \mapsto \Psi_1^{\mathbb{R}} \circ \Psi_2^{s_2}(q_0) \cap \Psi_1^{s_1} \circ \Psi_2^{\mathbb{R}}(q_0)$$

since the orbit $\Psi_1^{\mathbb{R}} \circ \Psi_2^{s_2}(q_0)$ through the point $\Psi_2^{s_2}(q_0)$ has a unique intersection with the orbit $\Psi_1^{s_1} \circ \Psi_2^{\mathbb{R}}(q_0)$ through $\Psi_2^{\mathbb{R}}(q_0)$. By the above remarks we have

$$\Psi(s_1, s_2) = q_0 + \omega_1 \cdot s_1 + \omega_2 \cdot s_2 + \mathcal{O}(1)$$

and the Jacobian of Ψ is uniformly bounded.

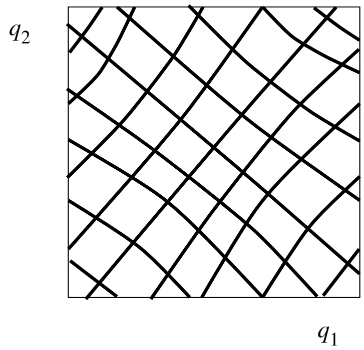

Figure 2. The two foliations of the configuration torus.

We consider the component $C = \Pi^{-1}(\hat{C})$ of Σ_E and an initial point $x_0 = (p_0, q_0) \in C$. By compactness of $\mathbb{T}$ the angle between $\hat{P}_1(\hat{q})$ and $\hat{P}_2(\hat{q})$ is bounded away from 0 and π. Thus for some $c > 0$ each point $(p, q) \in C$ has a momentum vector p which is a linear combination $p = \alpha_1 p_1 + \alpha_2 p_2$ with $(p_i, q) \in M_i$ and $\alpha_1 + \alpha_2 \geqslant c$.

Thus the Ψ-coordinates s_1, s_2 are increasing along the trajectory $t \mapsto q(t, x_0)$, and there exists a $c' > 0$ with $\frac{\mathrm{d}}{\mathrm{d}t}(s_1(t) + s_2(t)) \geqslant c'$.

The linear coordinate $\tilde{q} : \mathbb{R}^2 \to \mathbb{R}$, $\tilde{q} := (\omega_1/\|\omega_1\| + \omega_2/\|\omega_2\|) \cdot q$ on the configuration plane increases (at least) linearly along the trajectory. Namely, by (8) the trajectory meets the inequality

$$\tilde{q}(q(t, x_0)) = \left(\frac{\omega_1}{\|\omega_1\|} + \frac{\omega_2}{\|\omega_2\|}\right) \cdot \Psi(s_1(t), s_2(t)) = \left(\|\omega_1\| + \frac{\omega_1 \cdot \omega_2}{\|\omega_2\|}\right) s_1(t)$$
$$+ \left(\|\omega_2\| + \frac{\omega_1 \cdot \omega_2}{\|\omega_1\|}\right) s_2(t) + \mathcal{O}(1) \geqslant c_{II}(s_1(t) + s_2(t)) \geqslant c_I c_{II} \cdot t$$

if t is large. That is, *if* the asymptotic velocities $\bar{v}^{\pm}(x_0)$ exist and are equal, they must be non-zero.

The existence of such minimal tori for large E follows under our differentiability assumption $V \in C^5(\mathbb{R}^2, \mathbb{R})$ from the results of [17] by Pöschel.

(4) In the Jacobi metric (5) the perturbation of the integrable part equals $(1 - V(q)/E) \sum_{i=1}^{d} dq_i \otimes dq_i$. Since $\hat{V} \in C^{3d}(\mathbb{T}, \mathbb{R})$, the norm of the perturbation is finite and proportional to E^{-1}. The unperturbed part of the Hamiltonian function for geodesic motion in that metric is just the Hamiltonian of free motion. So up to a linear transformation the momenta coincide with the action variables of this integrable system, and the non-degeneracy condition of the frequencies is satisfied. These depend analytically on the action variables, and the perturbation is C^{3d} and of size $\varepsilon = \mathcal{O}(1/E)$ We can apply the result by Pöschel on the measure of KAM tori for a perturbation of order ε [17, corollary 2], which says that the measure of the complement of the KAM tori is of order $\sqrt{\varepsilon}$.

(5) If $\lambda_E(\{\bar{v} = 0\}) < 1$, there exists an index $j \in \{1, \ldots, d\}$ with probabilities

$$\lambda_E(\{\bar{v}_j > 0\}) = \lambda_E(\{\bar{v}_j < 0\}) > 0.$$

However, this contradicts ergodicity, since these two exclusive events are flow invariant.

To show that the trajectories are unbounded with probability one if $E > V_{\max}$, we consider the flow-invariant measurable events $E_n \subset \hat{\Sigma}_E$, $n \in \mathbb{N}$ defined by

$$E_n := \left\{ \hat{x}_0 \in \hat{\Sigma}_E \,\middle|\, \exists t_1, t_2 \in \mathbb{R} : \left\| \int_{t_1}^{t_2} \hat{p}(t, \hat{x}_0)\, \mathrm{d}t \right\| \geqslant n \right\}.$$

We know from part 2 of the theorem that there are ballistic trajectories. Each point $\hat{x} \in \hat{\Sigma}_E$ on such a ballistic trajectory is contained in all the sets E_n. By absolute continuity of $\| \int_{t_1}^{t_2} \hat{p}(t, \hat{x}_0)\, \mathrm{d}t \|$ w.r.t. the initial condition $\hat{x}_0$ we conclude that for all $n \in \mathbb{N}$ the Liouville measure $\lambda_E(E_n) > 0$, but the flow being ergodic, and E_n flow invariant, $\lambda_E(E_n)$ can only be zero or one. Thus, the set $\cap_{n\in\mathbb{N}} E_n$ of unbounded trajectories has measure one.

(6) To construct potentials $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$, $d \geqslant 2$, which have energies $E > V_{\max}$ with many bounded orbits on the energy shell, one writes $V(q) := \sum_{\ell\in\mathcal{L}} W(q - \ell)$ with $W \in C_0^\infty(\mathbb{R}^d, \mathbb{R})$, $W(q) := \tilde{W}(|q|)$, with $\tilde{W}(r) = 0$ for $r \geqslant \frac{1}{2} \min_{\ell\in\mathcal{L}} \|\ell\|$, so that the supports of the lattice-translated W do not overlap. As long as the particle is captured near a lattice point ℓ, the motion is one in a potential centrally symmetric around ℓ, and the angular momentum around that point is constant.

Thus one reduces the dimension by considering the effective potential $\tilde{W}_L(r) := \tilde{W}(r) + \frac{L^2}{2r^2}$ for angular momentum L. For a given choice of $L \neq 0$ one chooses $\tilde{W} \leqslant 0$ so that the effective potential has a strictly positive non-degenerate minimum r_0: $\tilde{W}_L(r_0) > 0$, $\frac{\mathrm{d}}{\mathrm{d}r}\tilde{W}_L(r_0) = 0$, $\frac{\mathrm{d}^2}{\mathrm{d}r^2}\tilde{W}_L(r_0) > 0$. Then the assertion holds for $E = \tilde{W}_L(r_0) + \varepsilon$, since $V_{\min} \leqslant 0$.

Whether one can construct for $d \geqslant 3$ potentials with a positive measure of bounded orbits on energy shells of *arbitrarily large* energy, is a much more complicated question. □

Parts 2 and 3 of the above theorem show that the minimal KAM tori play an important role in the distribution of asymptotic velocities. However, it is known [14] that for $d \geqslant 2$ an energy shell can only be foliated by such a tori if V is constant. This suggests that tori which do not diffeomorphically project to the configuration torus are important for the high-energy distribution of asymptotic velocity, see figures 3 and 4. Indeed, in the separable case $V(q) = \sum V_j(q_j)$ with V_j non-constant, the probability to move in each of the directions $\ell_1, \ldots, \ell_d$ is positive (figure 1). In the non-separable case such as the one depicted in figure 5, it can be proven by perturbation arguments that there are lattice-rational directions in which the particle moves with positive probability. If for every probability measure ν_E which is absolutely continuous w.r.t. λ_E

$$D(\nu_E) := \lim_{t\to\pm\infty} \frac{\int_{\Sigma_E} (q(t, x_0) - q_0)^2\, \mathrm{d}\nu_E(x_0)}{|t|}$$

exist and is positive, we call Φ_E^t *diffusive*.

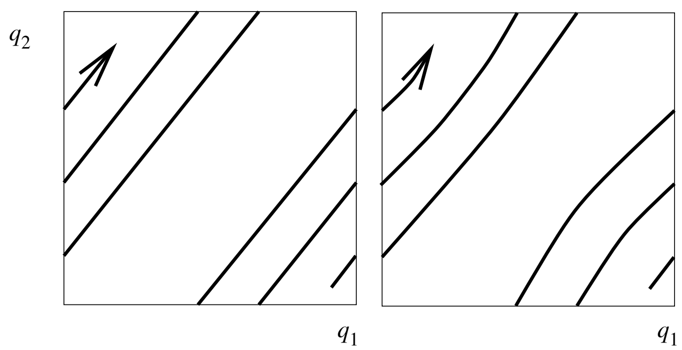

Figure 3. Motion on unperturbed (left) and perturbed (right) invariant torus.

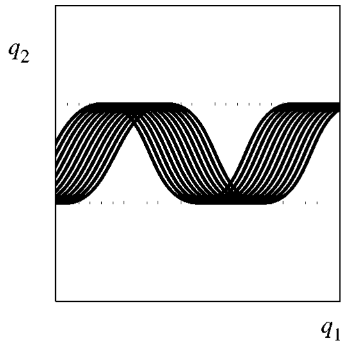

Figure 4. Motion on an invariant torus which does not project diffeomorphically onto the configuration torus.

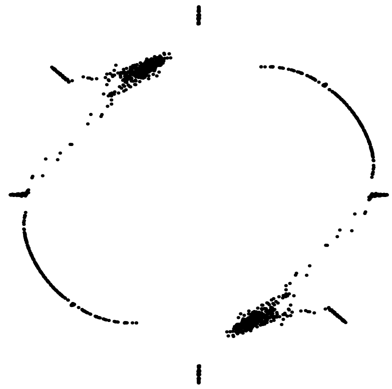

Figure 5. Distribution of asymptotic velocities $\bar{v}$ for the non-separable potential $V(q) = \cos(q_1) + \cos(q_1 + q_2)$ and energy $E = 3$ (numerical).

Moreover, we say that the flow Φ_E^t is *diffusive in the strong sense* if $q(t, x_0)/\sqrt{|t|}$ converges weakly to a Gaussian distribution with a positive covariance matrix. An example of a strongly diffusive flow is given in [12].

Remarks 3.2.

(1) Conversely to the third statement, for $d = 2$ a lowering of the energy may lead to the destruction of the second to last KAM torus, which in turn may lead to a discontinuous decrease of the group velocities.

As only for $d = 2$ the d-dimensional KAM tori have codimension one in the $(2d - 1)$-dimensional energy shell $\hat{\Sigma}_E$, for $d \geqslant 3$ Arnold diffusion may lead to initial conditions of positive measure which are not ballistic.

(2) By the statement (4) there always exists a threshold energy above which the motion is not diffusive.

(3) The mean classical velocity $\bar{v}$ for $d = 1$ equals the velocity expectation

$$\frac{\langle \psi - \mathrm{i}\nabla\psi \rangle}{\langle \psi, \psi \rangle}$$

of the WKB function

$$\psi(q) := \frac{1}{(E - V(q))^{1/4}} \exp\left(\pm\,\mathrm{i} \int_0^q \sqrt{2(E - V(q'))}\,\mathrm{d}q' \right).$$

Theorem 3.3. *If $d \geqslant 2$, then there is no energy E for which Φ_E^t is an Anosov flow.*

Proof. If $V = 0$, the motion is integrable and thus never Anosov. So we may assume V is non-constant. The Hamiltonian is *optical*, that is, strictly convex on each fibre.

Then for $E \leqslant V_{\max}$ the energy shell Σ_E touches the zero section of $T^*\mathbb{R}^d$. Thus by theorem 1 of Paternain and Paternain [16] Φ_E^t is not Anosov.

For $E > V_{\max}$ theorem 3 of [14] which generalizes a theorem of Hopf [7] says that the flow Φ_E^t has conjugate points if V is non-constant. Thus by theorem 1 of [16] the flow cannot be Anosov either. □

Remarks 3.4.

(1) Of course theorem 3.3 does not imply that motions in smooth potentials on $\mathbb{T}$ cannot be ergodic. In contrast, Donnay and Liverani gave in [4] a method to construct such ergodic $C^\infty(\mathbb{T})$ potentials for $d = 2$ freedoms. These potentials were constructed in such a way that for a given energy they contained circularly symmetric pits with a *parabolic* circular trajectory. Any decrease of the energy then makes this trajectory elliptic and the motion non-ergodic.

Our theorem shows that non-hyperbolic trajectories such as in that example must necessarily appear. In general we conjecture that for $d = 2$ these trajectories lead to anomalous diffusion effects and are incompatible with diffusivity in the strong sense.

Sinai and Kubo gave examples of repelling continuous potentials on a torus which lead to ergodic flows. However, in this case the potentials could not be chosen to be C^1 so that they too cannot serve as counterexamples to our theorem. See [4] for a discussion.

(2) Motion of k particles on a d-dimensional configuration space with periodic boundary conditions and mutual forces of potential type can be described by the motion of one particle on a (kd)-dimensional torus. Thus theorem 2 implies that it will be very hard to show ergodicity of gases if the interparticle forces are smooth.

(3) A geometric version of the above theorem is: geodesic flows on a torus $(\mathbb{T}, g)$ are never Anosov. This follows from the generalizations of Hopf's theorem by Burago and Ivanov [2], together with [16, theorem 1].

This is clearly not a mere consequence of the topology of the unit tangent bundle $S^{d-1} \times \mathbb{T}$, since for $d = 2$ this is a three-torus, and the simplest example of an Anosov flow (a suspension of Arnold's cat map) is one on $\mathbb{T}^3$.

4. Classical motion: coulombic potentials in $d = 2$

We now treat motion in a planar crystal with attracting coulombic forces. We fix the locations of the nuclei within the crystal by selecting $m \geqslant 1$ points $s_1, \ldots, s_m \in \mathcal{D}$ in the fundamental domain

$$\mathcal{D} := \{x_1\ell_1 + x_2\ell_2 | x_1, x_2 \in [0, 1)\} \subset \mathbb{R}^2_q$$

of the lattice $\mathcal{L} \subset \mathbb{R}^2_q$ with basis ℓ_1, ℓ_2. The nuclei attract the electron with the *charges* $Z_1, \ldots, Z_m > 0$. That is, we assume the potential of the form $V(q) \sim -Z_i/|q - s_i|$ for q near s_i. Now by the periodicity of the crystal the potential is singular at the points of

$$\mathcal{S} := \{s_i + \ell | i \in \{1, \ldots, m\}, \ell \in \mathcal{L}\}$$

and thus only defined in the punctured configuration plane $\tilde{M} := \mathbb{R}^2_q \setminus \mathcal{S}$. Sometimes we identify the plane with $\mathbb{C}$.

Definition 4.1. A potential $V \in C^\infty(\tilde{M}, \mathbb{R})$ which is $\mathcal{L}$-periodic

$$V(q + \ell) = V(q) \qquad (q \in \tilde{M}, \ell \in \mathcal{L})$$

is called *coulombic* if for $\varepsilon > 0$ small the functions $f_1, \ldots, f_m$,

$$f_i(Q) := \begin{cases} V(s_i + Q^2) \cdot Q\bar{Q} & 0 < |Q| < \varepsilon \\ -Z_i & Q = 0 \end{cases}$$

are C^∞.

The reason for the somewhat odd-looking definition is that we want to regularize the Coulomb singularities by using the so-called Levi-Civita transformation.

Observe that $V_{\max} := \sup_{q\in\tilde{M}} V(q)$ and V_{mean} are still well-defined finite quantities.

The classical motion is generated by the Hamiltonian function

$$\tilde{H}(p,q) := \tfrac{1}{2}p^2 + V(q) \qquad ((p,q) \in T^*\tilde{M}).$$

Due to collisions with the singularities in $\mathcal{S}$ the Hamiltonian flow on the cotangent bundle $T^*\tilde{M}$ of the punctured plane $\tilde{M}$ does not exist for all times.

However, as described in lemma 4.2 below, the flow can be smoothly regularized.

Lemma 4.2. *There exists a unique smooth extension (P, ω, H) of the Hamiltonian system $(T^*\tilde{M}, dq_1 \wedge dp_1 + dq_2 \wedge dp_2, \tilde{H})$, where the phase space P is a smooth four-dimensional manifold with*

$$P := T^*\tilde{M} \cup \bigcup_{\mathcal{S}} \mathbb{R} \times S^1 \tag{9}$$

as a set, ω is a smooth symplectic two-form on P with

$$\omega \restriction_{T^*\tilde{M}} = dq_1 \wedge dp_1 + dq_2 \wedge dp_2$$

and $H : P \to \mathbb{R}$ is a smooth Hamiltonian function with $H \restriction_{T^*\tilde{M}} = \tilde{H}$.

The smooth Hamiltonian flow

$$\Phi^t : P \to P \qquad (t \in \mathbb{R}) \tag{10}$$

generated by H is complete.

For all energies E which are regular values of V, the energy shell

$$\Sigma_E := \{x \in P \mid H(x) = E\} \tag{11}$$

is a smooth, three-dimensional manifold, and we write $\Phi_E^t := \Phi^t \restriction_{\Sigma_E}$.

Proof. The construction works locally near the singularities $s \in \mathcal{S}$. We shortly explain the method by considering the simplest case. For more details see [9, proposition 2.3], where a scattering potential is considered.

One may linearize the *Kepler flow* with Hamiltonian function

$$\tilde{H}_K(p,q) := \tfrac{1}{2}p^2 - Z/|q|$$

in a suitable neighbourhood of $\mathbb{R}^2_p \times \{0\}$ in the phase space $T^*(\mathbb{R}^2_q \setminus \{0\})$, using the canonical coordinates $\tilde{H}_K$, $\tilde{T}$, $\tilde{L}$ and $\tilde{\varphi}$, where $\tilde{L}(p,q) := p \wedge q$ is the angular momentum, $\tilde{T}(p,q)$ is the time needed to come from the phase-space point (p,q) to the pericentre of the Keplerian conic section and $\tilde{\varphi}(p,q)$ is the angle between the direction of that pericentre and, say, the 1-direction. Except $\tilde{T}$ these phase-space functions are constant along the Kepler flow, and the collision points correspond to $\tilde{T} = 0$, $\tilde{L} = 0$. The remaining coordinates $(\tilde{H}_K, \tilde{\varphi})$ take values in a cylinder $\mathbb{R} \times S^1$.

Similarly, because the singularities of V are of the Kepler form, one may thus complete the phase space $T^*\tilde{M}$ by gluing one cylinder for each singularity in $\mathcal{S}$. □

So after this regularization the Hamiltonian flow exists for all time, and we are in a similar situation as in the case of a smooth periodic potential treated in section 3. In particular we also consider the motion over the configuration torus $\mathbb{T}$.

Theorem 4.3. *If $\Delta \ln(E_{\mathrm{th}} - V) > 0$, then for all $E \geqslant E_{\mathrm{th}}$ the intersection of the set $\bar{v}(\hat{\Sigma}_E) \subset \mathbb{R}^2$ of asymptotic velocities for energy E with the disk of radius*

$$\frac{\sqrt{2}(E - V_{\mathrm{max}})}{\sqrt{E - V_{\mathrm{mean}}}}$$

is dense.

Remark 4.4. Since the motion is diffusive [12] and thus in particular the asymptotic velocity can only be non-zero on a set of measure zero, this should be considered as a 'very large deviation' result.

The ballistic orbits which we construct are of 'stop and go' type, that is, they periodically change between fast motion in a given direction and localized motion. Such orbits are somewhat special to our coulombic potential and do not exist in the general case. Compare, however, with theorem 3.1(2).

Proof. Although lemma 4.2 solves the problem of collision orbits and regularizes the motion without changing it otherwise, we will now introduce a second regularization which is more useful when one tries to construct orbits with prescribed asymptotic velocity, although it leads to a different phase space and a new time parametrization.

For coulombic potentials, the Jacobi metric (5) becomes singular near the positions $\mathcal{S}$ of the nuclei. However this is only a coordinate singularity, and Gaussian curvature does not diverge. This can be seen by considering the case of the Kepler flow and the regularizing complex coordinate $Q \in \mathbb{C}$ with $Q^2 = q$, that is, the *Levi-Civita transformation*. It turns out that in this coordinate the Jacobi metric, originally defined only for $Q \neq 0$, can be smoothly extended to a non-singular Riemannian metric on the whole complex Q plane. Note that the Q plane is a two-fold branched covering of the original q plane, with a branch point at the position $q = 0$ of the singularity.

In [12] this local construction was globalized using the toral Riemann surfaces $\mathbb{T} = M/\mathcal{L}$, its four-fold covering torus $\mathbb{T}^2 := M/(2\mathcal{L})$ (with projection $\Pi_{\mathbb{T}^2,\mathbb{T}} : \mathbb{T}^2 \to \mathbb{T}$) and the compact Riemann surface

$$\begin{aligned} M_4 &:= \left\{ (q, Q) \in \mathbb{T}^2 \times \mathbb{P} \,\middle|\, Q^2 = \frac{\prod_{i=1}^m \sigma(q - s_i + \ell_1)\sigma(q - s_i + \ell_1 + \ell_2)}{\prod_{i=1}^m \sigma(q - s_i)\sigma(q - s_i + \ell_2)} \right\} \\ \sigma(z) &:= z \prod_{w \in 2\mathcal{L}\backslash\{0\}} (1 - z/w)\exp(z/w + \tfrac{1}{2}(z/w)^2) \end{aligned} \qquad (12)$$

being the Weierstrass σ-function and $\mathbb{P} := \mathbb{C} \cup \infty$ the Riemann sphere. The map $\Pi_{M_4,\mathbb{T}^2} : M_4 \to \mathbb{T}^2$, $(q, Q) \mapsto q$ is a two-fold branched covering with branch points at the singularities, all branch numbers equalling one.

Thus by the Riemann–Hurwitz relation the genus $\mathcal{G}(M_4)$ of M_4 equals $\mathcal{G}(M_4) = 2m+1$ (m being the number of singularities in the fundamental domain). Since thus the genus is $\geqslant 3$, by Gauss–Bonnet the integrated Gaussian curvature $\int_{M_4} K_E \, \mathrm{d}M_4 = -4\pi(\mathcal{G}(M_4) - 1)$ of the lifted Jacobi metric $g_{4,E}$ on M_4 becomes negative. Due to the branched covering construction the metric $g_{4,E}$, originally not defined at the branch points, can be *smoothly* extended to these points by taking limits. So the geodesic flow $\phi^t_{4,E}$ on the unit tangent bundle $T_1 M_4$ of the surface $(M_4, g_{4,E})$ is smooth and defined for all times.

In terms of the potential V the Gaussian curvature K_E equals

$$K_E(q) = \frac{(E - V(q))\Delta V(q) + (\nabla V(q))^2}{2(E - V(q))^3} = -\frac{\Delta \ln(E_{\mathrm{th}} - V(q))}{2(E - V(q))} \qquad (13)$$

with Δ and ∇ denoting the Euclidean Laplacian and gradient, respectively.

For many coulombic potentials V the Gaussian curvature of M_4 becomes strictly negative ($K_E(x) < 0$ for all $x \in M_4$) if E is large enough. Clearly this can only happen if $\Delta V < 0$ in (13), and negativity of (13) is then preserved if one enlarges the energy E.

Similar to the proof of theorem 3.1(2) we construct ballistic orbits in $\mathbb{R}^2_q$ by finding closed geodesics of minimal length. However, due to the presence of singularities, these geodesics are not constructed on $\mathbb{T}$ but on the smooth Riemannian surface $(M_4, g_{4,E})$.

Since $(M_4, g_{4,E})$ is closed, there exists a closed geodesic in every non-trivial conjugacy class of the fundamental group $\pi_1(M_4)$. Moreover, if the Gaussian curvature K_E is strictly negative (as is the case if $\Delta \ln(E_{\text{th}} - V) > 0$ and $E \geqslant E_{\text{th}}$), then this geodesic $c : S^1 \to M_4$ is essentially unique within its conjugacy class. Namely, any other closed geodesic in that class coincides with c up to a shift of the initial point (see e.g. Klingenberg [11, theorem 3.8.14]).

As we are interested in ballistic trajectories on $\mathbb{R}^2_q$, we seek closed trajectories on $\mathbb{T}$ which are, however, non-contractible curves on the configuration torus. How many such orbits can we construct by projecting closed geodesics in M_4 to $\mathbb{T}$?

This question can be answered by considering the covering projection

$$\Pi_{M_4,\mathbb{T}} := \Pi_{\mathbb{T}^2,\mathbb{T}} \circ \Pi_{M_4,\mathbb{T}^2}. \tag{14}$$

This continuous map induces a homomorphism

$$(\Pi_{M_4,\mathbb{T}})_* : \pi_1(M_4) \to \pi_1(\mathbb{T})$$

of fundamental groups. We claim that the image subgroup $\text{Im} \subset \pi_1(\mathbb{T})$ equals

$$\text{Im} = \pi_1(\mathbb{T}^2) \cong 2\mathcal{L} \tag{15}$$

that is, consists of the equivalence classes of all loops $c : S^1 \to \mathbb{T}$ which surround the torus $\mathbb{T} \cong S^1 \times S^1$ in both basic directions an even number of times (this statement is of course independent of the base).

Equation (15) follows from the definition (14) if we show that the homomorphism

$$(\Pi_{M_4,\mathbb{T}^2})_* : \pi_1(M_4) \to \pi_1(\mathbb{T}^2)$$

is onto. To show this, we consider loops in $\mathbb{T}^2$ based at $b \in \mathbb{T}^2$, where we assume the base point b not to be a one of the $4m$ branch points of $\Pi_{M_4,\mathbb{T}^2}$, see (12), so that it has exactly two preimage points $b_0, b_1 \in M_4$.

Now we can uniquely lift any based loop $c : S^1 \to \mathbb{T}^2$ which avoids the branch points, to a path $\tilde{c} : [0, 1] \to M_4$ starting at $\tilde{c}(0) := b_0$ and ending either at $\tilde{c}(1) = b_0$ or at $\tilde{c}(1) = b_1$.

On the other hand, we can find one fixed based loop $l : S^1 \to \mathbb{T}^2$ which is contractible in $\mathbb{T}^2$ and is covered by a path $\tilde{l} : [0, 1] \to M_4$ connecting the points $\tilde{l}(0) = b_1$ and $\tilde{l}(1) = b_0$. Thus either $\tilde{c}$ or $\tilde{c} * \tilde{l}$ ($*$ denoting concatenation of paths) is a loop in M_4 based at b_0, and in both cases the image w.r.t. $\Pi_{M_4,\mathbb{T}^2}$ is freely homotopic to c. This shows that the image subgroup Im equals $(\Pi_{M_4,\mathbb{T}^2})_*(\pi_1(M_4)) = \pi_1(\mathbb{T}^2)$ and thus (15).

We need the above information in order to construct fast orbits in a given asymptotic direction, but we also need orbits with asymptotic speed zero in order to construct our 'stop and go orbits'.

With this aim we note that the kernel $\text{Ker}((\Pi_{M_4,\mathbb{T}})_*) \subset \pi_1(M_4)$ of our homomorphism is non-trivial. Indeed it contains the commutator subgroup

$$\text{Comm}(\pi_1(M_4)) = \{ghg^{-1}h^{-1} | g, h \in \pi_1(M_4)\}$$

of the fundamental group, which is the smallest normal subgroup F with $\pi_1(M_4)/F$ Abelian. The fundamental group of M_4 is non-Abelian, since the genus $\mathcal{G}(M_4) \geqslant 3$. So there exists a non-trivial

$$s \in \operatorname{Ker}((\Pi_{M_4,\mathbb{T}})_*) \qquad s \neq \mathrm{id}.$$

By shortening a loop in the conjugacy class of $s \in \pi_1(M_4)$, we obtain a closed geodesic $\tilde{s} : S^1 \to M_4$, our *stop geodesic*. After a reparametrization of time the projected geodesic $\Pi_{M_4,\mathbb{T}} \circ \tilde{s} : S^1 \to \mathbb{T}$ is a solution curve of the flow $\hat{\Phi}^t$ with initial conditions $\hat{x}_s \in \hat{\Sigma}_E$ and period T_s. This *stop orbit* has asymptotic velocity $\bar{v}(\hat{x}_s) = 0$.

Now in order to show our denseness result, we consider an arbitrary velocity $v \in \mathbb{R}^2$ with modulus

$$\|v\| \leqslant \frac{\sqrt{2}(E - V_{\max})}{\sqrt{E - V_{\mathrm{mean}}}} \tag{16}$$

and seek for any $\varepsilon > 0$ an $\hat{x}_0 \in \hat{\Sigma}_E$ with $\|\bar{v}(\hat{x}_0) - v\| < \varepsilon$.

This is easy if $v = 0$ because then we set $\hat{x}_0 := \hat{x}_s$ for our stop orbit with $v(\hat{x}_s) = 0$. So we assume that $v \neq 0$ and first approximate the *direction* $v/\|v\|$.

We can find a lattice vector $\ell' \in \mathcal{L} \cong \pi_1(\mathbb{T})$ with

$$\left\| \frac{v}{\|v\|} - \frac{\ell'}{\|\ell'\|} \right\| < \frac{\varepsilon}{2} \frac{\sqrt{E - V_{\mathrm{mean}}}}{\sqrt{2}(E - V_{\max})}. \tag{17}$$

Given ℓ', we now construct a closed geodesic $\tilde{g} : S^1 \to M_4$ whose associated periodic orbit on $\mathbb{T}$ starting at some point $\hat{x}_g \in \hat{\Sigma}_E$ has asymptotic direction

$$\frac{\bar{v}(\hat{x}_g)}{\|\bar{v}(\hat{x}_g)\|} = \frac{\ell'}{\|\ell'\|} \tag{18}$$

and speed

$$\|\bar{v}(\hat{x}_g)\| \geqslant \frac{\sqrt{2}(E - V_{\max})}{\sqrt{E - V_{\mathrm{mean}}}}. \tag{19}$$

As in the proof of theorem 3.1(2) we consider the closed straight lines

$$k : S^1 \to \mathbb{T} \qquad k(\tau) := q_0 + \tau \cdot \ell \pmod{\mathcal{L}}$$

with direction $\ell := 4\ell'$ and initial point $q_0 \in \mathbb{T}$. Since the loop k is at least four-periodic, we can lift k to M_4 obtaining a *loop* $\tilde{k} : S^1 \to M_4$ (namely, the lift of k to $\mathbb{T}^2$ is at least two-periodic and the branched covering $\Pi_{M_4,\mathbb{T}^2}$ is only two-sheeted).

Similar to (7), by an appropriate choice of the initial point q_0 we can ensure that the length $L(\tilde{k}) = \|\ell\| \cdot \int_0^1 \sqrt{E - V(k(\tau))}\,\mathrm{d}\tau$ of the corresponding loop in the Jacobi metric is bounded by

$$L(\tilde{k}) \leqslant \|\ell\|\sqrt{E - V_{\mathrm{mean}}}.$$

By shortening the loop $\tilde{k}$ we obtain a geodesic $\tilde{g} : S^1 \to M_4$ which projects to a closed orbit on the torus starting at some $\hat{x}_g \in \hat{\Sigma}_E$.

By the argument already used in the proof of theorem 3.1(2) the period T_g of that orbit is $\leqslant \|\ell\| \frac{\sqrt{E - V_{\mathrm{mean}}}}{\sqrt{2}(E - V_{\max})}$ so that the asymptotic velocity $\bar{v}(\hat{x}_g) = \ell/T_g$ meets (19). (18) is immediate from the construction since $\ell'/\|\ell'\| = \ell/\|\ell\|$.

Now this *go orbit* is too fast for our purposes. Therefore we find integers $p, q \in \mathbb{N}$ with

$$\left\| \frac{p}{q} - \frac{T_g}{T_s} \left(\frac{\|\bar{v}(\hat{x}_g)\|}{\|v\|} - 1 \right) \right\| < \delta \tag{20}$$

and consider for $n \in \mathbb{N}$ the group elements

$$o_n := s^{n\cdot p} \cdot g^{n\cdot q} \in \pi_1(M_4).$$

By curve shortening we find a geodesic $\tilde{o}_n : S^1 \to M_4$ in the conjugacy class of o_n. We denote the period of the unit speed reparametrized $\tilde{o}_n$ by $\tilde{T}_n$, and the period of the corresponding closed orbit on the torus by T_n, and claim that

$$\lim_{n\to\infty} \frac{T_n}{n(p \cdot T_s + q \cdot T_g)} = 1. \tag{21}$$

This follows from

(1) the Anosov property of the geodesic flow on the unit tangent bundle T_1M_4 of $(M_4, g_{4,E})$ proven in [12] and

(2) the formula $T_n = \int_0^{\tilde{T}_n} \frac{\mathrm{d}t}{\mathrm{d}\tau}\,\mathrm{d}\tau = \int_0^{\tilde{T}_n} \frac{\mathrm{d}\tau}{2(E-V(q(\tau)))}$ for the period. So the time reparametrization factor $1/(2(E-V(q)))$, seen as a function on T_1M_4, is Hölder continuous.

By (1) the geodesic flow line of $\tilde{o}_n$ approximates the *go geodesic* exponentially in n, then switches to the *stop geodesic* in n-uniformly bounded time, approximates that geodesic exponentially in n, and finally switches back to the *go geodesic* in n-uniformly bounded time.

Thus by (2) the ratio of times in (21) goes to one as $n \to \infty$.

Let $\hat{x}_n \in \hat{\Sigma}_E$ be a point on the torus orbit corresponding to the *stop and go geodesic* $\tilde{o}_n$. Then $\bar{v}(\hat{x}_n) = nq\,\ell/T_n$ and $\bar{v}(\hat{x}_g) = \ell/T_g$ so that by (21)

$$\lim_{n\to\infty} \|\bar{v}(\hat{x}_n)\| = \frac{\|\ell\|}{T_g + (p/q)T_s} = \|\bar{v}(\hat{x}_g)\| \Bigg/ \left(1 + \frac{pT_s}{qT_g}\right).$$

The choice (20) of p/q implies that

$$\lim_{n\to\infty} |\|\bar{v}(\hat{x}_n)\| - \|v\|| < \varepsilon/2 \tag{22}$$

for $\delta > 0$ small.

The geometric inequality

$$\|v - \bar{v}(\hat{x}_n)\| \leqslant |\|\bar{v}(\hat{x}_n)\| - \|v\|| + \left\| \frac{v}{\|v\|} - \frac{\bar{v}(\hat{x}_n)}{\|\bar{v}(\hat{x}_n)\|} \right\| \cdot \|v\|$$

together with (16)–(18) and (22) gives the result $\|v - \bar{v}(\hat{x}_n)\| < \varepsilon$ for n large. □

5. Semiclassics: smooth potentials

We now compare the quantum system in the semiclassical limit with the classical one and thus mimick the definitions of section 3.

The Schrödinger operators $H^h(k)$ on $L^2(\mathbb{T})$, $k \in \mathbb{T}^*$ have the eigenvalues $E_n^h(k)$. The *semiclassical asymptotic velocities* are defined by

$$\bar{v}_n^h(k) := \begin{cases} h^{-1}\nabla_k E_n^h(k) & \text{gradient exists} \\ 0 & \text{otherwise.} \end{cases}$$

We equip the *semiclassical phase space* $\hat{P}^h := \mathbb{N} \times \mathbb{T}^*$ with the *semiclassical measure* $\hat{\lambda}^h := (2\pi h)^d \mu_1 \times \mu_2$, where μ_1 denotes counting measure on $\mathbb{N}$ and μ_2 Haar measure on the Brillouin zone $\mathbb{T}^*$.

In order to compare classical with semiclassical quantities, we introduce the *energy-velocity map*

$$A^h : \hat{P}^h \to \mathbb{R}^{d+1} \qquad \text{with } A^h(n,k) := (E_n^h(k), \bar{v}_n^h(k))$$

and the image measure $\nu^h := \hat{\lambda}^h (A^h)^{-1}$.

Our conjecture, which we shall prove in some special cases is as follows.

Conjecture 5.1. For all $\mathcal{L}$-periodic potentials $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$

$$w^* - \lim_{h \searrow 0} \nu^h = \nu$$

(which means

$$\lim_{h\searrow 0} \int_{\mathbb{R}^{d+1}} f(x)\,\mathrm{d}\nu^h(x) = \int_{\mathbb{R}^{d+1}} f(x)\,\mathrm{d}\nu(x)$$

for continuous functions $f \in C_0^0(\mathbb{R}^{d+1}, \mathbb{R})$ of compact support).

As can already be seen from the one-dimensional case, the *supports* of the semiclassical measures ν^h are in general much larger than that of ν. If the bands do not touch, then $\mathbb{R} \times \{0\}$ belongs to $\mathrm{supp}(\nu^h)$ (since then by symmetry $\bar{v}_n^h(0) = 0$), whereas the classical motion is ballistic above $V_{\max}$.

In this section we draw conclusions from Birkhoff's ergodic theorem which for some potentials implies the truth of our conjecture.

We first show that the range of semiclassical asymptotic velocities is included in the *convex hull* of the classical ones. No assumption on the integrability or ergodicity of the classical system is made.

This involves a limit $T \to \infty$, $h \to 0$ which is controlled by the Birkhoff-type proposition 5.2.

Let X be a compact metric space, consider a continuous flow

$$\Phi^t : X \to X \qquad (t \in \mathbb{R})$$

and a continuous map

$$O : X \to \mathbb{R}^d.$$

Denote by $M(X)$ the set of Borel probability measures on X, $M(X,\Phi) \subset M(X)$ the set of flow invariant ones and

$$O_T(x) := \frac{1}{T}\int_0^T O \circ \Phi^t(x)\,\mathrm{d}t. \tag{23}$$

By Birkhoff's theorem the *good set*

$$G := \{x \in X \mid \lim_{T\to\pm\infty} O_T(x) \text{ exist and are equal}\}$$

has measure $\mu(G) = 1$ for all $\mu \in M(X,\Phi)$. We set $\bar{O} := \lim_{T\to\infty} O_T \restriction_G$.

The limit $\mathrm{dist}(O_T(x), \bar{O}(G)) \stackrel{T\to\infty}{\to} 0$ is in general not uniform in x. However this is true for the convex hull

$$\mathrm{conv}(\bar{O}(G)).$$

Denote for $\mathcal{C} \subset \mathbb{R}^d$ and for $\varepsilon > 0$ by $\mathcal{C}_\varepsilon \subset \mathbb{R}^d$ the ε-neighbourhood of $\mathcal{C}$.

Proposition 5.2. *For all* $\varepsilon > 0$ *there exists* $T_\varepsilon > 0$ *such that*

$$O_T(X) \subset \mathrm{conv}(\bar{O}(G))_\varepsilon \qquad (|T| > T_\varepsilon).$$

Proof of 5.2. By compactness of X and thus of $O(X)$ we could otherwise find an $\varepsilon > 0$, a sequence of points $x_n \in X$ and of times T_n with $T_n \to \pm\infty$ such that

$$z := \lim_{n\to\infty} O_{T_n}(x_n) \in \mathbb{R}^d$$

exists and $z \notin \mathcal{C}_\varepsilon$. Without loss of generality we assume that $T_n \to +\infty$.

Consider the sequence of probability measures $\mu_n \in M(X)$ given by

$$\mu_n(U) := \frac{1}{T_n} |\{t \in [0, T_n] | \Phi^t(x_n) \in U\}| \qquad (U \subset X \text{ Borel}).$$

We now use the following facts (see in Walters' book, [22, theorem 6.10]): $M(X)$ and $M(X, \Phi)$ are non-empty, convex, and compact in the weak-*-topology. The extreme points of $M(X, \Phi)$ coincide with the ergodic measures. By going to a subsequence, if necessary,

$$\mu := w^* - \lim_{n\to\infty} \mu_n \in M(X)$$

exists by compactness of $M(X)$. $\mu \in M(X, \Phi)$ and as $O_{T_n}(x_n) = \int O \, \mathrm{d}\mu_n$ the expectation $\int_X O \, \mathrm{d}\mu = z \notin \mathcal{C}_\varepsilon$. By Choquet decomposition of μ we would find an ergodic measure $\nu \in M(X, \Phi)$ with $\int_X O \, \mathrm{d}\nu \notin \mathcal{C}_\varepsilon$. On the other hand by ergodicity of ν there exists an $x \in X$ with $\bar{O}(x) = \int_X O \, \mathrm{d}\nu$, which is a contradiction. □

For $I \subset \mathbb{R}$ compact the phase-space region

$$\hat{P}_I := \{x \in \hat{P} | H(x) \in I\}$$

is compact and $\hat{\Phi}^t$-invariant so that we are in the situation of proposition 5.2.

The semiclassical analogue of the thickened energy shell $\hat{P}_I$ is

$$\hat{P}_I^h := \{(m, k) \in \hat{P}^h | E_m^h(k) \in I\}.$$

We equip them with the probability measures

$$\hat{\lambda}_I := \frac{\hat{\lambda}}{\hat{\lambda}(\hat{P}_I)} \qquad \text{on } \hat{P}_I$$

and (for h small)

$$\hat{\lambda}_I^h := \frac{\hat{\lambda}^h}{\hat{\lambda}^h(\hat{P}_I^h)} \qquad \text{on } \hat{P}_I^h.$$

These induce the image probability measures $\mu_I := \hat{\lambda}_I \bar{v}^{-1}$ and $\mu_I^h := \hat{\lambda}_I^h (\bar{v}^h)^{-1}$ on the space $\mathbb{R}^d$ of asymptotic velocities.

We shall now consider for $\varepsilon > 0$ intervals

$$I_\varepsilon := [E - \varepsilon, E + \varepsilon]$$

and show our semiclassical results on the group velocities.

Theorem 5.3. *Let $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ be $\mathcal{L}$-periodic, $E \in \mathbb{R}$, $\varepsilon > 0$.*

(1) Let $\mathcal{C} := \mathrm{conv}(\bar{v}(\hat{P}_{I_{2\varepsilon}}))$. Then for all $\eta > 0$, a.e. $k \in \mathbb{T}^*$ $\exists h_0$ $\forall h \leqslant h_0$

$$\bar{v}_j^h \in \mathcal{C}_\eta \qquad \text{if } E_j^h(k) \in I_\varepsilon$$

(2) let $\mathcal{S} := \mathrm{conv}(\mathrm{supp}(\mu_{I_{2\varepsilon}})) \subset \mathbb{R}^d$ be the convex hull of the support of $\mu_{I_{2\varepsilon}}$, then the semiclassical measures concentrate inside $\mathcal{S}$: For all $\eta > 0$

$$\lim_{h\searrow 0} \mu_{I_\varepsilon}^h(\mathcal{S}_\eta) = 1.$$

Remark 5.4. In general $\mathcal{S} \subset \overline{\mathcal{C}}$ is much smaller than $\overline{\mathcal{C}}$. As an example for ergodic motion one has by theorem 3.1(5) $\mathcal{S} = \{0\}$, whereas by theorem 3.1(2) $\overline{\mathcal{C}}$ contains a disk of radius $\frac{\sqrt{2}(E-V_{\max})}{\sqrt{E-V_{\mathrm{mean}}}}$.

Proof. The proof of (1) is based on theorem 5.2, whereas for (2) we use the almost everywhere convergence to the asymptotic velocity and a Shnirelman type argument. We shall freely use the semiclassical calculus as exposed in [20, 6] and references therein.

First we state a lemma about Bloch decomposition of anti-Wick quantization.

Lemma 5.5. *Let*

$$f \in C_b^\infty(\mathbb{R}^{2d}, \mathbb{R}) \qquad f(p, q+\ell) = f(p,q) \qquad (\ell \in \mathcal{L})$$
$$f^{\mathrm{AW}}\psi := \int_{\mathbb{R}^{2d}} f(p,q)\phi_{p,q}\langle\phi_{p,q}, \psi\rangle \frac{\mathrm{d}p\,\mathrm{d}q}{(2\pi h)^d} \qquad (\psi \in L^2(\mathbb{R}^d))$$

where

$$\phi_{p,q}(x) := \mathrm{e}^{-\frac{\mathrm{i}}{2h}pq}\mathrm{e}^{\frac{\mathrm{i}}{h}px}\phi(x-q) \qquad \phi(x) := (\pi h)^{-d/4}\mathrm{e}^{-\frac{x^2}{2h}}.$$

It holds

$$Uf^{\mathrm{AW}}U^{-1} = \int_{\mathbb{T}^*}^{\oplus} f^{\mathrm{AW}}(k)\frac{\mathrm{d}k}{|\mathbb{T}^*|}$$

with

$$f^{\mathrm{AW}}(k)\psi := \int_{\hat{P}} f(p,q)U\phi_{p,q}(k)\langle U\phi_{p,q}(k), \psi\rangle_{L^2(\mathbb{T})}\frac{\mathrm{d}p\,\mathrm{d}q}{(2\pi h)^d}.$$

Proof. By periodicity of f and unitarity of U we have

$$Uf^{\mathrm{AW}}\psi = \sum_{\ell\in\mathcal{L}}\int_{\hat{P}} f(p,q)U\phi_{p,q+\ell}\langle U\phi_{p,q+\ell}, U\psi\rangle\frac{\mathrm{d}p\,\mathrm{d}q}{(2\pi h)^d}.$$

Now

$$U\phi_{p,q+\ell}(k,x) = \mathrm{e}^{\mathrm{i}(p+hk)\ell/h}\mathrm{e}^{-\mathrm{i}/(2h)\ell p}U\phi_{p,q}(k,x)$$

so

$$Uf^{\mathrm{AW}}\psi(k) = \int_{\hat{P}} f(p,q)U\phi_{p,q}(k)\sum_{\ell\in\mathcal{L}}\int_{\mathbb{T}^*}\frac{\mathrm{d}k'}{|\mathbb{T}^*|}(\mathrm{e}^{\mathrm{i}(k-k')\ell}\langle U\phi_{p,q}(k'), U\psi(k')\rangle_{L^2(\mathbb{T})})\frac{\mathrm{d}p\,\mathrm{d}q}{(2\pi h)^d}$$

the claim follows now from Fourier inversion and the $\mathcal{L}^*$-periodicity of
$k' \mapsto \langle U\phi_{p,q}(k'), U\psi(k')\rangle$. □

A corollary of this lemma, the Egorov theorem and the Weyl–anti-Wick correspondence is:

$$\mathrm{e}^{\mathrm{i}H^h(k)t/h}f^{\mathrm{AW}}(k)\mathrm{e}^{-\mathrm{i}H^h(k)t/h} = (\hat{f}\circ\hat{\Phi}^t)^{\mathrm{AW}}(k) + \mathcal{O}_T(h).$$

Denote $\Lambda_\varepsilon^h(k) = \{j; E_j^h(k) \in I_\varepsilon\}$ and $\chi \in C_0^\infty(\mathbb{R},\mathbb{R})$, $\operatorname{supp}\chi \subset I_{2\varepsilon}$, $\chi \restriction_{I_\varepsilon} = 1$. For $j \in \Lambda_\varepsilon^h(k)$ consider the eigenfunction $\psi_{j,k}^h$ of $H^h(k)$ and its Husimi distribution $\rho_{j,k}^h : P \to \mathbb{R}$,

$$\rho_{j,k}^h(p,q) := (2\pi h)^{-d}|\langle U\phi_{p,q}(k), \psi_{j,k}^h\rangle_{L^2(\mathbb{T})}|^2.$$

We then have (using notation (23))

$$\bar{v}_j^h(k) = \int_{\hat{P}} (\chi(H)p)_T \, d\rho_{j,k}^h + \mathcal{O}_T(h).$$

We apply proposition 5.2 with $X = \hat{P}_{I_{2\varepsilon}}$. By time reversal symmetry $0 \in \operatorname{conv}(\bar{v}(X))$ so we find a T such that

$$(\chi(H)p)_T(X) \subset \operatorname{conv}(\bar{v}(X))_{\eta/2}$$

and an h such that $O_T(h) < \eta/2$. Thus (1) is proven.

Now we show that almost everywhere for k, for all $\eta > 0$

$$\lim_{h \searrow 0} \frac{\#\{m \in \Lambda_\varepsilon^h(k); |\bar{v}_m^h(k) - \int \chi(H)\bar{v} \, d\rho_{m,k}^h| < \eta\}}{\#\Lambda_\varepsilon^h(k)} = 1 \tag{24}$$

This implies (2) as $\int \chi(H)\bar{v} \, d\rho_{j,k}^h \subset \operatorname{conv}(\operatorname{supp} \mu_{I_{2\varepsilon}})$ by absolute continuity of $\chi(H) \, d\rho_{j,k}^h$ w.r.t. $\hat{\lambda}_{I_{2\varepsilon}}$, by time reversal symmetry and the bound 1 for the fraction.

By Birkhoff's theorem

$$\lim_{T \to \infty} \int_{\hat{P}} |\hat{v}_T(\hat{x}) - \bar{v}(\hat{x})| \, d\hat{\lambda}_{I_{2\varepsilon}} = 0.$$

So the set

$$B(T, \eta) := \left\{ \hat{x} \in \hat{P}_{I_{2\varepsilon}} \middle| |\hat{v}_T(\hat{x}) - \bar{v}(\hat{x})| \geqslant \frac{\eta}{4} \right\}$$

of phase-space points $\hat{x}$ eventually giving rise to $\hat{v}_T(\hat{x}) \notin \mathcal{S}_{\eta/2}$ can be made small:

$$\hat{\lambda}_{2\varepsilon}(B(T, \eta)) \leqslant \frac{\delta}{2} \qquad (T \geqslant T(\delta)).$$

On the other hand, by convergence on the h-independent $\hat{P}_{I_\varepsilon}$:

$$w^* - \lim_{h \searrow 0} \frac{1}{\#\Lambda_\varepsilon^h(k)} \sum_{m \in \Lambda_\varepsilon^h(k)} \rho_{m,k}^h = \hat{\lambda}_{I_\varepsilon}.$$

For $h \leqslant h(\delta)$ and $T \geqslant T(\delta)$ we thus have

$$\frac{1}{\#\Lambda_\varepsilon^h(k)} \sum_{m \in \Lambda_\varepsilon^h(k)} \rho_{m,k}^h(B(T, \eta)) \leqslant \delta.$$

By Tchebycheff's inequality

$$\#\{m \in \Lambda_\varepsilon^h(k) | \rho_{m,k}^h(B(T, \eta)) \geqslant \sqrt{\delta}\} \leqslant \sqrt{\delta} \#\Lambda_\varepsilon^h(k).$$

For m in the complementary set it holds:

$$\int_{\hat{P}} \chi(H)(p_T - \bar{v}) \, d\rho_{m,k}^h \leqslant \frac{\eta}{4} + 2\|\chi(H)\bar{v}\|_\infty \sqrt{\delta} < \frac{\eta}{2} \qquad (\delta < \delta(\eta))).$$

To summarize: for $\alpha > 0$ there is a T and a set $G_T^h \subset \Lambda_\varepsilon^h$ such that for h small enough $|\bar{v}_j^h - \int \chi(H)\bar{v} \, d\rho_{j,k}^h| < \eta$ for $j \in G_T^h$ and $\frac{\#G_T^h}{\#\Lambda_\varepsilon^h} \geqslant 1 - \alpha$. This finishes the proof of (2). $\square$

Corollary 5.6. *If the classical motion is non-ballistic with probability one on an energy interval I: $\mu_I = \delta_0$, then conjecture 5.1 holds true:*

$$w^* - \lim_{h \searrow 0} \nu^h = \nu.$$

For example, this is the case if the classical motion is ergodic.

6. Semiclassics: separable potentials

If the potential is separable, the distribution of semiclassical group velocities converges rapidly to the classical velocity distribution. We begin with the case of one dimension, and thus consider the operator $H := -h^2 \frac{d^2}{dx^2} + V(x)$ with potential $V \in C^r(\mathbb{R}, \mathbb{R})$, assuming w.l.o.g. that $V(x+1) = V(x)$. The band function of the nth band for the quasimomentum $k \in [-\pi, \pi]$ is denoted by $E_n(k) \equiv E_n^h(k)$. Of course $\frac{dE_n}{dk}(k) = 0$ or the band functions touch at the band edges $k = 0$ or $\pm\pi$. However, apart from small neighbourhoods of these values of the quasimomentum it holds:

Proposition 6.1. *Assume that the periodic potential $V \in C^r(\mathbb{R}, \mathbb{R})$, $r \geqslant 2$.*

(1) Then all bands in the energy interval $[V_{\max} + \varepsilon, \infty)$ meet the following uniform estimate. If the quasimomentum $|k| \in [h^{(r-1)/2}, \pi - h^{(r-1)/2}]$, then

$$\left| \operatorname{sign}(k) \cdot h^{-1} \frac{dE_n}{dk}(k) - (-1)^n v_{\mathrm{cl}}(E_n(k)) \right| \leqslant ch$$

for some $c = c(\varepsilon) > 0$,

$$v_{\mathrm{cl}}(E) = \frac{1}{2} \left(\int_0^1 \frac{1}{\sqrt{E - V(t)}} \, dt \right)^{-1} \qquad (E > V_{\max})$$

$v_{\mathrm{cl}}(E) = 0$ $(E \leqslant V_{\max})$ being the absolute value of the classical velocity.

(2) In the energy range $[V_{\min}, V_{\max} - \varepsilon]$ and for all $k \in [-\pi, \pi]$

$$\frac{dE_n}{dk}(k) = \mathcal{O}(h^\infty).$$

(3)

$$w^* - \lim_{h \searrow 0} \nu^h = \nu. \tag{25}$$

Proof.

(1) We first consider the energy interval $[V_{\max} + \varepsilon, \infty)$. For the k values under consideration, the Bloch eigenfunctions have no zeroes. So we are looking for zero-free solutions $\varphi : \mathbb{R} \to \mathbb{C}$ of the differential equation

$$H\varphi = E\varphi. \tag{26}$$

The complex phase $S := \frac{h}{i} \ln(\varphi)$ of such a solution solves the differential equation

$$(S')^2 - ihS'' - W = 0 \tag{27}$$

with $W := E - V$. We solve this equation, using the ansatz

$$S(x) = \tilde{S}_r(x) + h^{r+1} R(x, h) \qquad \text{with } \tilde{S}_r(x) := \sum_{n=0}^{r} h^n S_n(x).$$

With

$$S_0(x) := \int_0^x \sqrt{W(t)} \, dt$$

the recursion equation

$$iS''_{n-1} - \sum_{l=0}^{n} S'_l S'_{n-l} = 0 \qquad (n = 1, \ldots, r) \tag{28}$$

has the continuous solution

$$S_n(x) = \frac{1}{2}\int_0^x \frac{\mathrm{i}S''_{n-1}(t) - \sum_{l=1}^{n-1} S'_l(t)S'_{n-l}(t)}{\sqrt{W(t)}}\,\mathrm{d}t \qquad (n = 1, \ldots, r)$$

since $S'_0 = \sqrt{W} > 0$.

In particular we have $S_1(x) = \mathrm{i}\ln(\sqrt[4]{W(x)}) + c$. We set $c := 0$. Then on bounded intervals

$$\varphi(x) = \frac{1}{\sqrt[4]{W(x)}}\exp\left(\mathrm{i}\int_0^x \sqrt{W(t)}\,\mathrm{d}t/h\right) + \mathcal{O}(h^1).$$

As a consequence of (28) S_n is real if n is even and imaginary if N is odd. $\tilde{S}'_r$ is one-periodic.

However, unlike the real part of $\tilde{S}_r$ the imaginary part is always one-periodic. This can be seen, e.g. by considering the formal power series $\tilde{S}_\infty$ in h. By (27) the real part $R := \mathrm{Re}(\tilde{S}'_\infty)$ of the derivative is related to the imaginary part $I := \mathrm{Im}(\tilde{S}'_\infty)$ by

$$hR' = 2IR$$

so that $I = \frac{1}{2}h(\ln(R))'$. Thus the formal power series $\mathrm{Re}(\tilde{S}_\infty)$ is one-periodic, which implies the same periodicity for its coefficients S_{2n+1}.

Of course this argument is even valid if (by finite differentiability of V) only finitely many coefficients S_n are defined.

Thus for $E > V_{\max}$

$$\tilde{\varphi}_r := \exp\left(\frac{\mathrm{i}}{h}\tilde{S}_r\right) = A_r \exp\left(\frac{\mathrm{i}}{h}U_r\right) : \mathbb{R} \to \mathbb{C}$$

is a function with periodic modulus $A_r > 0$ and phase $U_r = \mathrm{Re}(\tilde{S}_r)$. We compare this with the solution φ of (26) with the initial values

$$\varphi(0) := \tilde{\varphi}_r(0) \qquad \varphi'(0) := \tilde{\varphi}'_r(0).$$

On bounded spatial intervals one has the estimate uniform in x and E

$$\varphi(x) = \tilde{\varphi}_r(x) + \mathcal{O}(h^r) \qquad \varphi'(x) = \tilde{\varphi}'_r(x) + \mathcal{O}(h^r).$$

The same is true for the matrix

$$M(x) := \begin{pmatrix} \varphi(x) & \bar{\varphi}(x) \\ \varphi'(x) & \bar{\varphi}'(x) \end{pmatrix}$$

of the corresponding fundamental system ($\bar{\varphi}$ is linearly independent of φ). The monodromy matrix $T := M(1) \cdot M(0)^{-1}$ has determinant one and trace

$$\mathrm{Tr}(T) = 2\,\mathrm{Re}(\tilde{\varphi}_r(1)/\tilde{\varphi}_r(0)) + \mathcal{O}(h^r) = 2\cos(U_r(1)/h) + \mathcal{O}(h^r).$$

Now we consider those quasimomenta k for which

$$\mathrm{dist}(U_r(1)/h, \pi \cdot \mathbb{Z}) > h^{(r-1)/2}.$$

For them $|\mathrm{Tr}(T)| < 2$ if $h < h_0$ so that the quasiperiodic function $x \mapsto \varphi(x)$ is bounded. Thus φ is a Bloch function with quasimomentum k,

$$\cos(k) = \tfrac{1}{2}\,\mathrm{Tr}(T).$$

Differentiating both sides w.r.t. k yields

$$\sin(k) = \sin(U_r(1)/h)\frac{\mathrm{d}U_r(1)}{\mathrm{d}E}h^{-1}\frac{\mathrm{d}E}{\mathrm{d}k} + \mathcal{O}(h^r). \tag{29}$$

On the other hand

$$\sin(k) = \sqrt{1 - (\tfrac{1}{2}\,\mathrm{Tr}(T))^2} = \pm\sin(U_r(1)/h)(1 + \mathcal{O}(h^1))$$

so that (29) implies the relation

$$h^{-1}\frac{\mathrm{d}E}{\mathrm{d}k} = \pm\left(\frac{\mathrm{d}U_r(1)}{\mathrm{d}E}\right)^{-1} + \mathcal{O}(h^1) \tag{30}$$

for the group velocity. By $U_r(1) = \int_0^1 \sqrt{W(t)}\,\mathrm{d}t + \mathcal{O}(h^1)$ we get the estimate

$$h^{-1}\frac{\mathrm{d}E}{\mathrm{d}k} = \pm\tfrac{1}{2}\left(\int_0^1 \frac{1}{\sqrt{E - V(t)}}\,\mathrm{d}t\right)^{-1} + \mathcal{O}(h^1)$$

for quasimomenta $|k| \in [h^{(r-1)/2}, \pi - h^{(r-1)/2}]$.

(2) For $E \leqslant V_{\max} - \varepsilon$ we have $v_{\mathrm{cl}}(E) = 0$. Quantum mechanically it is well known that the wavefunction and its derivatives are exponentially decreasing w.r.t. h well inside the potential well, say, for $V(x) \leqslant \varepsilon/2$. This implies exponential decay of the group velocity.

Namely

$$h^{-1}\frac{\mathrm{d}E_n}{\mathrm{d}k}(k) = \int_0^1 j_n(x)\,\mathrm{d}x = j_n(x)$$

for the current $j_n(x) = -\mathrm{i}h\,\mathrm{Im}(\bar{\varphi}_n(k)(x)\frac{\mathrm{d}}{\mathrm{d}x}\varphi_n(k)(x))$ of the eigenfunction $\varphi_n(k)$ with eigenvalue $E_n(k) \leqslant V_{\max} - \varepsilon$, since the divergence of the current of eigenfunction vanishes.

If we evaluate j at x inside the potential well, then we see that it is exponentially small. For more precise estimates valid in the multidimensional case we refer to Outassourt [15].

(3) The convergence of the semiclassical measures ν^h to ν follows from the following reasoning.

By a Weyl estimate we have weak-*-convergence in energy distribution:

$$w^* - \lim_{h\searrow 0} \hat{\lambda}^h (E^h)^{-1} = \hat{\lambda} H^{-1}$$

with $E^h : \hat{P}^h \to \mathbb{R}$, $E^h(m,k) := E^h_m(k)$ being the energy function on the Fermi surface. The first two parts of the proposition exclude the energy interval $(V_{\max} - \varepsilon, V_{\max} + \varepsilon)$. However, as $h \searrow 0$, we can let $\varepsilon \equiv \varepsilon(h) \searrow 0$, too. By the above Weyl estimate we do not lose anything of ν^h in the semiclassical limit, since

$$\lim_{h\searrow 0} \sum_{m\in\mathbb{N}} (2\pi h)|\{k \in \mathbb{T}^* \,|\, |E^h_m(k) - V_{\max}| < \varepsilon(h)\}| = 0.$$

Then (25) follows from (1) and (2). □

Corollary 6.2. *Let $V \in C^2(\mathbb{R}^d, \mathbb{R})$ be a separable periodic potential. Then Conjecture 5.1 holds true:*

$$w^* - \lim_{h\searrow 0} \nu^h = \nu.$$

Proof. By our assumption the potential is of the form

$$V(q) = \sum_{j=1}^{d} V_j(q_j)$$

with $V_j \in C^2(\mathbb{R}, \mathbb{R})$ of some period $l_j > 0$. Let ν_j^h and ν_j denote the (semi)classical measures for the one-dimensional potential V_j. Then

$$\nu = (\nu_1, \ldots, \nu_d)L^{-1} \qquad \text{and} \qquad \nu^h = (\nu_1^h, \ldots, \nu_d^h)L^{-1}$$

for the linear map $L : (\mathbb{R}^2)^d \to \mathbb{R}^{d+1}$,

$$L(h_1, v_1, h_2, v_2, \ldots, h_d, v_d) \mapsto (h_1 + \cdots + h_d, v_1, \ldots, v_d).$$

Although for $d > 1$ the linear map L is not injective and thus not proper, its restriction to

$$\times_{j=1}^{d}([V_{j,\min}, \infty) \times \mathbb{R}) \tag{31}$$

has this property, so that pre-images of compactly supported functions are still compactly supported. We may restrict L to (31), since the support of $(\nu_1, \ldots, \nu_d)$ is contained in (31), the spectrum of H_j being contained in $[V_{j,\min}, \infty)$

So multidimensional convergence follows from the one-dimensional one. □

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