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Velocity and Entropy of Motion in Periodic Potentials

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Abstract

This is a report on recent joint work with J. Asch, and with T. Hudetz and F. Benatti.

We consider classical, quantum and semiclassical motion in periodic potentials and prove various results on the distribution of asymptotic velocities.

The Kolmogorov-Sinai entropy and its quantum generalization, the Connes-Narnhofer-Thirring entropy, of the single particle and of a gas of noninteracting particles are related.

After the mathematical proof [10], [9] of Bloch's Theorem for a large class of periodic potentials the focus of interest shifted towards other subjects like motion in quasiperiodic or random potentials.

However, the relation between the KdV equation and the one-dimensional Schrödinger operator with a periodic potential showed an unexpected richness of the latter subject, the generalization to the multi-dimensional case being a current subject of research.

Here we give a short survey on a complementary aspect: The *dynamics* generated by that Schrödinger operator

$$H^{\hbar} = -\frac{\hbar^2}{2}\Delta + V(q) \tag{1}$$

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and the corresponding Hamiltonian function.

This is mainly done by analyzing the (asymptotic) velocity of the motion, and its dynamical entropy.

1 Ballistic and Non-Ballistic Motion

In the paper [1] we consider the qualitative aspects of the distribution of asymptotic velocity.

Our starting point is to provide a proof of a folk conjecture according to which the quantum mechanical motion for (1) is ballistic.

Thus 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 it descends to a function on the unit cell $\mathbb{T} := \mathbb{R}^d/\mathcal{L}$), and denote its Fourier transform by $\mathcal{F}V$.

The symmetries of $H^\hbar$ 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

$$U : L^2(\mathbb{R}^d) \to \int_{\mathbb{T}^*}^{\oplus} L^2(\mathbb{T}, dq) \frac{dk}{|\mathbb{T}^*|}$$

the unitary operator defined by extension from Schwarz space of

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

Our assumption on the regularity of the potential is:

$d = 2$: $V \in L^p(\mathbb{T})$ with $p > 1$,

$d = 3$: $V \in L^2(\mathbb{T})$ and

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

Under this assumption $UHU^{-1} = \int_\oplus H(k) \frac{dk}{|\mathbb{T}^*|}$ with an analytic family $H(k)$ of operators with compact resolvent. So we may write $H(k) = \sum_{n=1}^\infty E_n(k) P_n(k)$ where $E_n(k)$ are the eigenvalues in ascending order, $P_n(k)$ the eigenprojections.

Theorem 1 *If* $\psi \in L^2(\mathbb{R}^d)$ *meets*

$$(D\psi, D\psi) + (q\psi, q\psi) < \infty,$$

then the asymptotic velocity of this wave function is given by

$$\lim_{t\to\infty} \frac{q(t)\psi}{t} = U^{-1}\left(\int_{\mathbb{T}^*}^{\oplus} \sum_{n=1}^{\infty} \hbar^{-1}\nabla_k E_n(k) P_n(k)\ \frac{dk}{|\mathbb{T}^*|}\right) U\psi,$$

and

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

See also the paper [4] by Gerard and Nier.

So the quantity which determines the motion of the particle is the *semi-classical asymptotic velocity*, given by

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

In order to understand the distribution of that quantity, we consider its classical counterpart.

The classical motion in a $\mathcal{L}$-periodic potential V on $\mathbb{R}^d$ is described by Hamilton's equations on phase space $P := T^*\mathbb{R}^d$ for

$$H : P \to \mathbb{R}, \qquad H(p,q) = \tfrac{1}{2}p^2 + V(q).$$

If $V \in C^2(\mathbb{R}^d, \mathbb{R})$ (as we assume here), the flow $\Phi^t : P \to P$ exists uniquely for all times $t \in \mathbb{R}$.

We will analyze its restrictions $\Phi_E^t := \Phi^t|_{\Sigma_E}$ 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. 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 $\hat{\Phi}_E^t := \hat{\Phi}^t|_{\hat{\Sigma}_E}$.

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.

Minimum $V_{\min}$, mean value V_{mean} and maximum $V_{\max}$ of the potential are relevant energy scales.

As a consequence of Birkhoff's Ergodic Theorem for $\hat{\lambda}$-almost all $\hat{x}_0 \in \hat{P}$

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

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 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 asymptotic velocity and thus introduce the *energy-velocity map*

$$A := (\hat{H}, \bar{v}) : \hat{P} \to \mathbb{R}^{d+1}. \tag{2}$$

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

ν is invariant under $(h, v) \mapsto (h, -v)$, since the motion is reversible, and $|\bar{v}(x)| \leq \sqrt{2(H(x) - V_{\min})}$.

For regular values E of the energy 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 $\sqrt{E - V_{\min}}$.

Theorem 2 *1. For $d = 1$ the motion is ballistic at $x = (p, q) \in P$ iff $E := H(x) > V_{\max}$, with asymptotic velocity*

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

($l > 0$ 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*

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

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

$$\frac{\sqrt{2}(E - V_{\max})}{\sqrt{E - V_{\text{mean}}}} \le \|\bar{v}(x)\| \le \sqrt{2(E - V_{\min})}, \qquad (x \in B_E). \tag{3}$$

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

   E_{th} is given by the following condition. For $E > E_{\text{th}}$ 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 exist a threshold energy $E_{\text{th}} \ge V_{\max}$ and for $E > E_{\text{th}}$ subsets $\hat{B}_E \subset \hat{\Sigma}_E$ of measures*

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

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 $\bar{v}_E = 0$ with probability one. However, if in addition $E > V_{\max}$, the trajectories are unbounded with probability one:*

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

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

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

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

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

However, by linearization of the flow near the collision orbits and addition of cylinders $\mathbb{R} \times S^1$ (parametrizing energy and direction of the collision points) one may regularize the motion, see [5].

One thus obtains a smooth extension (P, ω, H) of the incomplete Hamiltonian system, P being a four-dim. manifold with Hamiltonian function $H : P \to \mathbb{R}$ and symplectic form ω. The smooth flow $\Phi^t : P \to P$ generated by H is complete, and one can proceed like in the former case.

It is known [6] that under mild additional conditions the flow of energy $E \geq E_{\text{th}}$ in the plane is diffusive, and that its restriction to the configuration torus $\mathbb{R}^2/\mathcal{L}$ is ergodic. In particular Them. 2.5 holds true.

However, there is an exceptional set of fast orbits:

Theorem 3 *If $\Delta \ln(E_{\text{th}} - V) > 0$, then for all $E \geq E_{\text{th}}$ 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*

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

is dense.

This statement can be thought of as a 'very large deviation' result

It is known [6] that under the same conditions the Coulombic periodic potentials generate a motion which is of Anosov type.

To the contrary we show

Theorem 4 *If $d \geq 2$, and $V \in C^2(\mathbb{R}^d, \mathbb{R})$, then there is no energy E for which Φ^t_E is an Anosov flow.*

A geometric version of that theorem is: Geodesic flows on a torus $(\mathbb{T}, g)$ are never Anosov.

As the example of $d = 2$ dimensions shows, this is not merely a consequence of the topological form of the energy shell (which is then a three-torus for $E > V_{\max}$, the simplest example of an Anosov flow having phase space $\mathbb{T}^3$).

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 $k \cdot d$-dimensional torus. Thus the theorem implies that it will be very hard to show ergodicity of gases if the interparticle forces are smooth.

The proof of the Theorem 4 is based on a somewhat converse statement in [8], which says for $d > 1$ that existence of a single energy surface which is completely foliated by invariant Lagrangean tori implies constancy of the potential.

Similar to (2) we introduce the *energy-velocity map*

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

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

Conjecture 5 *For all $\mathcal{L}$-periodic potentials $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$*

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

(which means $\lim_{\hbar \searrow 0} \int_{\mathbb{R}^d} f(x) d\nu^\hbar(x) = \int_{\mathbb{R}^d} f(x) d\nu^\hbar(x)$ for continuous functions $f \in C_0^0(\mathbb{R}^{d+1}, \mathbb{R})$ of compact support).

We shall now consider for $\varepsilon > 0$ intervals $I_n := [E - n\varepsilon, E + n\varepsilon]$ and deduce that the group velocities for energies in $I = I_1$ are included in a thickened convex hull of the classical ones with energies in I_2, provided $\hbar$ is small.

Theorem 6 *Let the $\mathcal{L}$-periodic potential $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$, $E \in \mathbb{R}$, $\varepsilon > 0$. Then $\exists\, \hbar_0 \; \forall\, \hbar < \hbar_0$*

$$\bar{v}_m^\hbar(k) \in \Big(\mathrm{conv}(\bar{v}(\hat{P}_{I_2}))\Big)_\varepsilon \qquad \text{if } E_m^\hbar(k) \in I.$$

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

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

We equip them with the probability measures

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

and (for $\hbar$ small)

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

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

Theorem 7 *Let $\mathcal{S} := \mathrm{conv}(\mathrm{supp}(\mu_I)) \subset \mathbb{R}^d$ be the convex hull of the support of μ_I, then the semiclassical measures concentrate inside $\mathcal{S}$: For all $\varepsilon > 0$*

$$\lim_{\hbar \searrow 0} \mu_I^\hbar(\mathbb{R}^d - \mathcal{S}_\varepsilon) = 0.$$

Remark 8 *In general $\mathcal{S} \subset \overline{\mathcal{C}}$ is much smaller than $\overline{\mathcal{C}}$. As an example for ergodic motion one has by Thm. 2.5 $\mathcal{S} = \{0\}$, whereas by Thm. 2.2 $\overline{\mathcal{C}}$ contains a disk of radius $\frac{\sqrt{2}(E-V_{\mathrm{max}})}{\sqrt{E-V_{\mathrm{mean}}}}$.*

Corollary 9 *If the classical motion is non-ballistic with probability one on an energy interval I ($\mu_I = \delta_0$), then Conjecture 5 holds true.*

For example, this is the case if the classical motion is ergodic. Then the group velocity is only a quantum floctuation vanishing in the semiclassical limit. This is also true in the case of Coulombic potentials [7].

Theorem 10 *Let $V \in C^2(\mathbb{R}^d, \mathbb{R})$ be a separable periodic potential. Then Conjecture 5 holds true.*

In fact, assuming V to be C^∞, we show that one has fast convergence to the classical measure.

2 Classical and Quantum Dynamical Entropy

In the first part of [2] we give a self-contained introduction into the notion of CNT entropy. This entropy, introduced by Connes, Narnhofer and Thirring in [3], generalizes the Kolmogorov-Sinai-entropy of an automorphism of a probabilility space.

Then we apply these notions to the case of motion in a periodic potential. For lack of space we do not formulate here our technical assumptions and precise results, but refer the interested reader to [2].

One Particle (Classical). The notion of measure theoretic entropy is not directly applicable to the description of a classical particle in a periodic potential, since Liouville measure is invariant under lattice translation and thus infinite. However one may divide by the lattice $\mathcal{L}$ and thus consider motion on the configuration torus $\mathbb{T} = \mathbb{R}^d/\mathcal{L}$, using Liouville measure.

In that case the KS entropy is zero if the potential is separable, and should be positive in the generic case. If the potential is smooth, it is of order $1/\sqrt{E}$ as the energy E of the particle goes to infinity (Prop. 5.6 of [2]).

The generalization, due to Bowen, of topological entropy to non–compact phase spaces is directly applicable to the motion in the crystal, but coincides with the topological entropy of the motion on the configuration torus. The topological entropy of smooth potentials has an E–independent upper bound, and for ≥ 3 freedoms there exist smooth potentials with a similar E–independent lower bound (Prop. 5.5 of [2]).

For Coulombic periodic potentials the topological entropy is a smooth increasing function asymptotic to $c\sqrt{E}$ (Prop. 5.8 of [2]).

One Particle (Quantal). The CNT entopy is undefined for the motion in configuration space and zero for motion on the configuration torus. This is one motivation to consider the noninteracting gas.

Classical Gas. Although second quantization (or Poisson construction, as it is called in the case of classical dynamical systems) is a purely functorial construction, the consideration of a gas of non–interacting particles sheds new light on the single–particle dynamics.

Classically the unbounded system is now described by a *probability* measure. As noted by Goldstein, the total entropy of an ideal gas is infinite. This was a motivation for him to introduce space time entropy which, as he showed, equals entropy density. This is a finite quantity for the motion in a periodic potential, since it equals the entropy per particle multiplied by the density of particles (Thm. 5.14 of [2]).

However, if one considers only a *bounded* configuration space region B, then for large energies and smooth potentials the local entropy associated with that region is infinite, since every incoming particle carries an infinite amount of information.

For energies below the delocalization threshold that entropy is finite (Thm. 5.14 of [2]).

Above an energy threshold, the gas of classical particles in a Coulombic periodic potential forms a space-time $\mathbb{K}$-system with strictly positive entropy densities (Prop. 5.15 of [2]). Thus it has extremely good ergodic properties.

Fermi Gas. Last we consider a noninteracting Fermi gas in $\mathbb{R}^d$ with a lattice-invariant quasi-free state.

We prove that for a *shift* by a lattice vector v the local CNT entropy in region B is finite and for large B asymptotically proportional to the surface area of ∂B in the v direction times the speed $|v|$ (Thm. 5.19 of [2]).

The finiteness of local CNT entropy is a consequence of coarse–graining of phase space with cells of volume $(2\pi\hbar)^d$. So each particle carries only a finite amount of information.

In a forthcoming paper we will apply these techniques to the motion of the noninteracting quantum electron gas in a periodic potential. This needs phase space microlocalization, and we indicate in an appendix the usefulness of local algebras of Wannier functions in this context.

The growth of the local CNT entropy with the surface area instead with the volume is a clear sign of the fact that quantum chaos is less chaotic than classical chaos. For it is not the dynamics of the particles in the bulk, but the information carried by the electron entering the region, that leads to that growth of entropy.

In the case of the Coulombic potential the above-mentioned vanishing of speed in the semiclassical limit has the curious consequence that, apart from a 'kinematical factor' $(2\pi\hbar)^{-d}$ corresponding to coarse-graining of phase space, the local CNT entropy associated with B *decreases* as Planck's constant goes to zero. The physical reason is simply that less particles enter B per unit time.

References

[1] Asch, J., Knauf, A.: *Motion in Periodic Potentials.* Preprint (1997)

[2] Benatti, F., Hudetz, T., Knauf, A.: *Quantum Chaos and Dynamical Entropy.* Preprint (1997)

[3] Connes, A., Narnhofer, H., Thirring, W.: *Dynamical Entropy for C* algebras and von Neumann Algebras.* Commun. Math. Phys. **112**, 691 (1987).

[4] Gérard, Ch., Nier, F.: *Scattering Theory for the Perturbations of Periodic Schrödinger Operators.* Preprint Ecole Polytechnique (1997)

[5] Klein, M., Knauf, A.: *Classical Planar Scattering by Coulombic Potentials.* Lecture Notes in Physics m 13. Berlin, Heidelberg, New York: Springer; 1993

[6] Knauf, A.: *Ergodic and Topological Properties of Coulombic Periodic Potentials.* Commun. Math. Phys. **110**, 89–112 (1987)

[7] Knauf, A.: *Coulombic Periodic Potentials: The Quantum Case.* Annals of Physics **191**, 205–240 (1989)

[8] Knauf, A.: *Closed orbits and converse* KAM *theory.* Nonlinearity **3**, 961–973 (1990)

[9] Reed, M., Simon, B.: *Methods in Mathematical Physics, Vol. IV: Analysis of Operators.* New York: Academic Press 1978

[10] Thomas, L.E.: *Time Dependent Approach to Scattering from Impurities in a Crystal.* Commun. Math. Phys **33**, 335–343 (1973)