Classical motion in two-dimensional crystals

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Abstract

The classical motion of an electron of high enough energy in a two-dimensional crystal is diffusive for many potentials with Coulomb singularities. A simple model of the dynamics is developed, which predicts the dependence of the diffusion constant D on the particle energy E in the high energy limit: $D(E) \sim const \cdot E^{3/2}$.
This diffusion law is checked for a concrete crystal, by numerical integrating the Hamilton equations for an ensemble of initial conditions. Finally this method is compared with other models of the classical dynamics in a crystal, especially the Sinai billiard.
Key Words: Two-dimensional diffusion, Jacobi metric, geodesic flow, negative curvature, Anosov, mean free path length, Sinai billiard.

1 Introduction

For many two-dimensional periodic potentials which are asymptotically negative coulombic near to the singularities and smooth elsewhere, Knauf showed in [8] the diffusivity of the motion of a classical electron. Diffusion takes place for energies E exceeding a positive threshold h. In the mean a fast particle departs farther than a slower one. The diffusion constant $D = D(E)$ increases with the energy E. But how does D depend on the energy E ? The model introduced in Sect. 5 yields the result $D(E) \sim const \cdot E^{\frac{3}{2}}$, as $E \nearrow \infty$. A crucial role in the derivation is played by the mean free path length $\bar{s}$, which is the mean path length between two consecutive distinct changes of the direction of the electron. I demand a 'distinct change' because a free

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path needs not be a straight path. In fact this is why the motion is diffusive (see Sect. 6).
One might at first be tempted to expect the Lorentz gas (Sinai billiard) with infinite horizon to describe the dynamics for high energies, but the Lorentz gas of infinite horizon is not diffusive. Trajectories calculated by the computer show clearly that a path of an electron does not look like the path of a billiard ball, but is curved, even in the case of high energy.
The polynomial dependence of the diffusion constant D predicted by the model introduced in this paper was checked numerically. All numerically computations are related to a simple square lattice of Yukawa scatterers defined in (Sect. 2). After introduction (in Sect. 3) of the Jacobi metric g'_E in configuration space and some operations for compactifying and completing the phase space, the problem of classical motion in a crystal is translated into the problem of finding a geodesic flow on closed (i.e., compact and without boundary) Riemannian manifolds of negative curvature. By this reformulation of the problem I also succeed in calculating a threshold h for diffusion. In Sect. 4 the diffusion constant $D(E)$ is defined. Then I will describe the numerical method for calculating $D(E)$. A critical discussion of the method of integrating such long orbits of an unstable flow follows. Then the model introduced in Sect. 5, will be compared with the Sinai billiard and the model of an egg-carton-like potential used by Geisel, Zacherl and Radons.
In the following I call a path in configuration space a trajectory, whereas I call a path in phase space an orbit.
At this point I would like to thank my adviser Andreas Knauf for helpful discussions.

2 Definitions

Let the lattice $\mathcal{L}$ be generated by the linear independent vectors $v_1, v_2 \in \mathbf{R}^2$.

$$\mathcal{L} := \{kv_1 + lv_2 | (k,l) \in \mathbf{Z}^2\}. \tag{1}$$

Let $\mathcal{S} \subset \mathbf{R}^2$ be the $\mathcal{L}-$invariant discrete set (i.e. every translation with respect to $v \in \mathcal{L}$ is onto on the set $\mathcal{S}$) of all positions of the nuclei. Now the punctured plane $M'_1 := \mathbf{R}^2 \backslash \mathcal{S}$ is the configuration space. Consider the classical motion of a pointlike particle (the electron) of mass normalized to one in a $\mathcal{L}$-periodic Coulomb potential V.
Definition: We call a potential V a *$\mathcal{L}$-periodic Coulomb potential* (or some-

times shortly Coulomb potential), if it satisfies the three conditions:
a) V is $\mathcal{L}$-periodic,
b) near a singularity $s \in \mathcal{S}$ the potential is *asymptotically Coulombic*, i.e.

$$V(q-s) \sim -z|q-s|^{-1},\ q \in M_1', \tag{2}$$

where $z > 0$ is the charge of the nucleus situated at s,
c) elsewhere V is smooth.
For example the class of attracting Yukawa potentials and specific $-\frac{1}{r}$-potentials of finite ranges (see [8]) meet these conditions.
The motion is described by the Hamilton function H_1', which is defined on the cotangent bundle T^*M_1' of the punctured plane M_1':

$$H_1'(p,q) := \frac{p^2}{2} + V(q),\ (p,q) \in T^*M_1'. \tag{3}$$

Observe that the motion in the crystal is determined by the motion in a fundamental domain. After identification of opposite sides this domain becomes the punctured torus $M_2' := M_1'/\mathcal{L}$. On the cotangent bundle T^*M_2' we have the Hamiltonian H_2':

$$H_2'(p,q) := \frac{p^2}{2} + V(q),\ (p,q) \in T^*M_2' \tag{4}$$

Remark: For the concrete numerical computation of the diffusion constant D (defined in Sect. 4) I have used a simple square lattice $\mathcal{L}^s$, where $v_1 := (1,0)$ and $v_2 := (0,1)$ in Euclidian coordinates. Furthermore every cell contains one nucleus (Yukawa scatterer): $\mathcal{S} = \mathcal{L}^s$. The field of the nuclei gives rise to the potential $V(q)$, consisting of Yukawa potentials
$V^Y(q) := -\frac{1}{|q|}e^{-|q|};\ q \in M_1'$. We have

$$V(q) := \sum_{s \in \mathcal{S}} V^Y(q-s),\ q \in M_1'. \tag{5}$$

Because of the exponential terms the sum $V(q)$ and all its derivatives converge absolutely.
Of course the potential V^Y is a special representative in the class of attracting Yukawa potentials.

3 Jacobi metric and negative curvature

For $E > \max(0, V_{\max})$, $V_{\max} := \sup_{q \in M_1'} V(q)$, the Jacobi metric g_E' on M_1' is defined by:

$$g_E'(q) := (1 - \frac{V(q)}{E})\, g'(q),\ q \in M_1',$$

where g' is the Euclidian metric on M_1' and E is the energy of the electron. So the Jacobian metric g_E' is conformal w.r.t. the Euclidian metric g' (see for example Abraham and Marsden [1]) Chapter 3.7). Up to a time reparametrization any trajectory in (M_1', g') that solves the Hamilton differential equations is a geodesic in (M_1', g_E') and vice versa. So we may as well examine the geodesic motion in (M_1', g_E'). Whereas the punctured plane (M_1', g') is flat, the Gaussian curvature K_E' of (M_1', g_E') is given by

$$K_E'(q) := \frac{(1 - V(q)/E)\Delta V(q)/E + |\nabla V(q)|^2/E^2}{2(1 - V(q)/E)^3}, \tag{6}$$

with Euclidian gradient ∇ and Laplacian Δ. It is revealing to discuss (6) for the specific case of the lattice of Yukawa potentials (5). Then the Laplacian is given by

$$\Delta V(q) = \sum_{s \in \mathcal{S}} (1 + \frac{1}{|s-q|} + \frac{1}{|s-q|^2})\, V^Y(q-s),$$

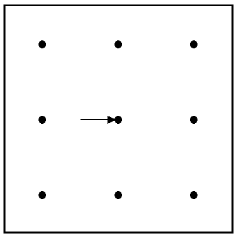
and $\Delta V(q) < 0$. For positive energy $E > 0$ the only negative contribution to the curvature (6) comes from the term $\Delta V(q)$. Now it should be clear that, given the smoothness of the periodic potential (condition 1.c) outside of small circular neighbourhoods of the singularities, one can find a value $E > 0$, so that the term $|\nabla V(q)/E|^2$ is absolutely dominated by the term $\Delta V(q)/E$ because of the square exponent in the first term. Therefore $K_E'(q)$ is negative outside of these neighbourhoods for high enough energy E. Furthermore, one observes that for $q \to s$ the Yukawa potential behaves asymptotically Coulombic (corresponding to condition 1.a). But for a simple Coulomb potential $V^C(q) := -\frac{1}{|q-s|}$ of only one nucleus (at s) the curvature

$$K_E'(q) = -\frac{1}{2E(|q-s| + 1/E)^3} < 0$$

is smaller than zero for positive energy E and $q \neq s$. The absolute value of $K_E'(q)$ even increases as $q \to s$. These arguments motivate the assumption

that there exist a threshold $h > 0$, so that for all energies $E \geq h$ the curvature $K'_E(q) < 0$. In fact the existence of h was proved in [8] for Coulomb potentials of finite ranges and Coulomb potentials of Yukawa type. In appendix D of [11] I computed analytically $h = 5.17$ as the threshold for the potential (5) of the simple square lattice consisting of Yukawa scatterers.
It is obvious that a small perturbation of the potential does not destroy the property of negative curvature because it is an open property defined by an inequality. Furthermore it has been shown in [7] that the set of potentials leading to strictly negative curvature $K'_E(q)$ is a convex set. This means that given two potentials V^0, V^1 for which $K'_E(q)$ becomes strictly negative for all energies E exceeding some threshold $h > 0$, then we have immediately a class of potentials $V^t := t \cdot V^1 + (1-t) \cdot V^0, 0 \leq t \leq 1$, for which $K'_E < 0$ holds true.
On the other hand, the negative curvature condition is obviously violated if $\Delta V(q) > 0$ for any point $q \in M'_1$.
Geodesic flows on closed Riemannian manifolds are the standard examples for mixing behaviour. (M'_1, g'_E) has negative curvature but is neither compact nor geodesically complete. The problem of completion and compactification was solved in [8]. There Knauf proved that the motion in the plane (M'_1, g'_E) obeys a diffusion law. Before defining the diffusion constant D one needs a complete flow Φ_t on phase space. The regularization scheme used here differs from that used in [8], but is similar to the method presented in Chapter 2 of [7]. Notice that the motion in the punctured plane M'_1 is not complete. To see this, look at a particle moving towards the singularity s (for example parallel to a symmetry axis of the crystal as in Figure 1).

Fig.1



Such a trajectory leads to s in finite time. One obtains a complete flow by continuing the motion by backward scattering of those particles (as in Fig.1) which are on a collision trajecyory, i.e. one simply reflects the trajectory at the scattering centre $s \in \mathcal{S}$.
Consider now all trajectories (of fixed positive energy E) intersecting a small

circular neighbourhood U_s centered at $s \in \mathcal{S}$. They may be parametrized by two numbers:
The first number is the angular momentum L of the corresponding particle w.r.t. the nucleus at s, measured at the pericentre. The second number is the angle ϕ enclosed by any arbitrary fixed direction and the axis connecting the pericentre and the singularity s. (One may choose (L, ϕ, E, t) as coordinates in the Kepler problem. Consequently all hyperbolas as solutions of the unbounded ($E = const > 0$) Kepler problem may be parametrized by L and ϕ.) This set of trajectories is even a manifold. Call it $\mathcal{O}(U_s)$.
Remark: Every collision trajectory may be considered as a limit of trajectories of identical angle ϕ and decreasing angular momentum L. So the angle ϕ is well defined for collision trajectories, too.
Collision trajectories are characterized by the condition $L = 0$. So they are a submanifold of codimension one in the manifold $\mathcal{O}(U_s)$ and they are therefore of measure zero in the manifold $\mathcal{O}(U_s)$. Consequently all collision trajectories are completely described by their direction ϕ and their energy E. So it is clear that one obtains a topological completion P_1 of phase space T^*M_1' by adding one cylinder $S^1 \times \mathbf{R}$ (direction, energy) per singularity $s \in \mathcal{S}$ of the punctured plane M_1'. The completion P_2 of T^*M_2' is analogous. So let

$$P_1 := T^*M_1' \cup (\bigcup_{s \in \mathcal{S}} S^1 \times \mathbf{R}),$$

$$P_2 := T^*M_2' \cup (\bigcup_{s \in \mathcal{S}/\mathcal{L}} S^1 \times \mathbf{R})$$

be these completions. The proof of Prop. 2.3 in Klein and Knauf [7] implies that P_1 and P_2 are not only topological manifolds. (P_1, ω_1, H_1) and (P_2, ω_2, H_2) are unique smooth extensions of the Hamilton systems $(T^*M_1', \vec{dp} \wedge \vec{dq}, H_1')$ and $(T^*M_2', \vec{dp} \wedge \vec{dq}, H_2')$, respectively. In particular $\omega_i|_{T^*M_i'} = \vec{dp} \wedge \vec{dq}$ and $H_i' = H_i|_{T^*M_i'}, i = 1, 2$. P_1 and P_2 are smooth four-dimensional manifolds and every $E > V_{\max}$ is a regular value of the smooth Hamiltonians H_1 and H_2. So the energy shells $\Sigma_E^i := H_i^{-1}(E), i = 1, 2$ are smooth three-dimensional manifolds (Regular Value Theorem). Furthermore, the shell Σ_E^2 is compact and the flow Φ_t^2 on Σ_E^2 generated by H_2 is mixing, Anosov and Bernoulli for all $E \geq h$ [8].

4 Definition of the diffusion constant $D(E)$

Notice that the Liouville measure μ on P_1 splits into two factors (depending on the phase point $(p,q) \in P_1$), let μ_E be the factor acting on the submanifold Σ_E^1 of P_1 and let ν_E be a probability measure which is absolutely continuous w.r.t. μ_E $(\nu_E \ll \mu_E)$. Then we define the diffusion constant

$$D(E) := \lim_{T\to\infty} \frac{\langle |q(T,(p_0,q_0)) - q_0|^2\rangle_{\nu_E}}{T}. \tag{7}$$

The expectation value $\langle ..\rangle_{\nu_E}$ is taken w.r.t. the probability measure ν_E. Let $\pi : P_1 \to P_2$ the canonical projection. Because $\nu_E \ll \mu_E$ also $\nu_E \circ \pi^{-1} \ll \mu_E^2$ holds true, where μ_E^2 is the factor of the Liouville measure μ^2 on P_2 acting on Σ_E^2.
By the definition (7) it is clear that if $D(E)$ exists, then it is nonnegative, because the time T is positive and the numerator is nonnegative. We call the motion in the crystal *diffusive*, if a finite and positive limit $D(E)$ exists.
In [8] the following was proved for attracting Yukawa potentials and specific potentials of finite ranges:
There exists a threshold h, so that the motion is diffusive for all energies $E \geq h$.
Of course the value of the threshold h depends on the lattice $\mathcal{L}$ defined in (1) and on the potential $V(q)$. In the case of the attracting Yukawa potentials the existence of h does not depend on the lattice $\mathcal{L}$ and the representative V^Y of the class of attracting Yukawa potentials.
The Coulomb potentials to which the proof in [8] relates to lead (for $E \geq h$) to negative curvature $K_E'(q)$ of the configuration space (M_1', g_E'). Then they give rise to a (complete) geodesic flow which is Anosov and Bernoulli and finally they lead to diffusion. So one can understand that the threshold $h = 5.17$ guaranteeing negative curvature $K_E'(q)$ for the potential (5), also guarantees diffusion in the field of the potential (5), i.e. diffusion in the lattice of Yukawa scatterers.
The three conditions of absolute continuity $\nu_E \circ \pi^{-1} \ll \mu_E^2$, the compactness of Σ_E^2 and the strong mixing property of the measure preserving flow Φ_t^2, guarantee (by Thm. 6.12 of [13]) the independence of the diffusion constant $D(E)$ of the choice of the absolutely continuous probability measure ν_E on the energy shell Σ_E^1.

In the case of the special Yukawa potential (5) $D(E)$ is approximated by numerical computation of finite time trajectories.

$$D_{app}^T(E) := \frac{1}{N}\sum_{i=1}^{N}\frac{|q(T,(p_0^i,q_0^i)) - q_0^i|^2}{T},$$

where the energy $E > h$ is fixed, N is the number of trajectories and (p_0^i, q_0^i) is the initial value of the i-th trajectory. The values of q_0^i and $p_0^i/|p_0^i|$ are chosen randomly w.r.t. the uniform distributions on M_2' and S^1. Here $|p_0^i| := \sqrt{2\ (E - V(q_0^i))}$. The running time T was chosen sufficently large, that is, the orbit was integrated over time steps $\tau, 2\tau, ...\ 15\tau = T$ and T was considered to be large enough if the values $D_{app}^\tau(E)$ oscillated only in a small interval.

It might seem to be problematic to compute long orbits of an unstable flow Φ_t of Anosov type, because the used Runge-Kutta method of fourth order entails small errors and these errors preclude approximating a true orbit associated to the initial value (p_0^i, q_0^i) by a computed orbit (of course in a bounded integration time). Because of the exponential instability, the error increases exponentially, too. But here the Shadowing Lemma of R. Bowen [2] comes into play (which is essentially based on the Anosov property, too). It deals with discrete Anosov systems and says that for an infinite sequence of phase space points $\{x_i\}_{i\in\mathbf{Z}}$ with $d(\Phi(x_i), x_{i+1}) < \alpha$ (the 'α-orbit', a computed orbit is such a sequence, although a finite one) one can find a true orbit $\{y_i\}_{i\in\mathbf{Z}}$ ('β-orbit') with $d(\Phi_i(y), x_i) < \beta$ for all $i \in \mathbf{Z}$. Here d is the distance on Σ_E^2 induced by the metric g_E'. Therefore, a computed orbit is as good as a true orbit for examining the statistical behaviour of the phase space flow.

The double logarithmic plot of the function $D(E)$ (Fig. 4) indicates a polynomial dependence of D on E in the limit of large energy E. A two-parameter χ^2-confidence and fitting test statistically confirms the assumption of polynomial dependence. For example, the three points associated to the highest energies $E \in \{100, 200, 500\}$ lie on a straight line g with probability of 71%. The slope of that fitted line is $m = 1.45$. One has to compare this numerical result with that of the simple model presented below, which predicts that $D(E) \sim const\ E^{\frac{3}{2}}$ for large E and a suitable positive constant. Up to numerical fluctuations Fig. 4 shows a convex function. The slope increases but seems to be asymptotically constant. So the slope $\frac{3}{2}$ is not only confirmed by the small difference from the number 1.45, but by the form of the graph $D(E)$ as a whole, too.

5 A model for the dependence of the diffusion constant D on the energy E

The intention of this section is to give an idea about the structure which generates the exponent $\frac{3}{2}$ in the diffusion law.
This is no proof of the diffusion law. The existence of a finite and positive constant ($D(E)$ was proved in ([8]), but not the diffusion law (7) itself (the proof is not yet finished).
The increase of the diffusion constant $D(E)$ with the energy E follows from a rise of the mean free path length $\bar{s}(E)$ and a faster covering of this length by the electron. In the development of this model it is fundamental to notice that macroscopic scattering of the electron takes place only inside of small circles centered at $s \in \mathcal{S}$, whose radius scales with β/E, $\beta = const$ (see Lemma 5.5 of [7] or Chapter 2.6 of [11]).
The meaning of the term macroscopic scattering is that the change of the direction of the electron after passing through a circular neighbourhood of a nucleus exceeds a given angle δ. This observation motivates the examination of the energy dependence of the mean path length $\bar{s}(E)$.
For that purpose consider now instead of a typical trajectory of the electronic odyssey in the $\mathcal{L}$-periodic crystal a straight line f in a plane of randomly spread discs of the small radius $r, r \sim \frac{1}{E}$. Suppose there are n singularities in the fundamental domain, whose area we normalize to 1. Then an area $\mathcal{A}$ of size A^2 will contain $A^2 \cdot n$ singularities in the mean, and the discs around the singularties wil cover an area of $A^2 \cdot n \cdot \pi r^2 \sim \frac{1}{E^2}$. The probability that a point in $\mathcal{A}$ lies on a disc is proportional to $\frac{1}{E^2}$. Consequently the probability that a point of the line f is also contained in a disc is proportional to $\frac{1}{E}$, (that means that there is a good chance that a line of length E is intersected at least once by a disc). Therefore a segment of length A of the straight line f will be intersected (in the mean) by $c \cdot A/E$ discs and the mean distance between two intersections is of the order E/c, where c is constant, because $c \cdot A/E \cdot E/c = A$. So it follows that

$$\bar{s}(E) \sim c^{-1} \cdot E \tag{8}$$

and the approximation becomes better with large E, since then one may neglect the place covered by the discs on f.
The justification of this derivation of $\bar{s}(E)$ may be this: What we used to call a periodic lattice does in a sense not look periodic if one takes the perspective of an electron in that plane, since the electron moves in general not on

a straight line (the geodesic in the Euclidean metric), but on the geodesics w.r.t. the Jacobian metric g'_E. This implies that equidistant points (w.r.t. the Euclidean metric) in the crystal have in general different distances w.r.t the Jacobian metric g'_E (for a more physical deduction of $\bar{s}(E)$ see Chapter 2.6 of [11]).

With a dot symbolizing the standard scalar product in $\mathbf{R}^2$ write again (7)

$$\begin{aligned} D(E) &= \lim_{T\to\infty} \frac{1}{T}\langle\, |q(T)-q_0|^2\,\rangle_{\mu_E} = \lim_{T\to\infty}\frac{1}{T}\langle\, |\int_0^T \dot{q}(t)\; dt|^2\rangle_{\mu_E} \\ &= \lim_{T\to\infty}\frac{1}{T}\langle \int_0^T\int_0^T \dot{q}(s)\cdot\dot{q}(r)\; dsdr\rangle_{\mu_E} \\ &= \lim_{T\to\infty}\frac{1}{T}\langle \int_0^T\int_{-T}^T \dot{q}(s)\cdot\dot{q}(s+t)\; dtds\rangle_{\mu_E} \end{aligned}$$

with $-T \leq t := r-s \leq T$. For large T the inner integral should not depend on s (so the outer integration will only produce the factor T). Let $s=0$. We have

$$D(E) \;\approx\; \lim_{T\to\infty}\langle \int_{-T}^T \dot{q}(0)\cdot\dot{q}(t)\; dt\rangle_{\mu_E}$$

By assumption of symmetry of the integral (for large T) we get a Green-Kubo formula [10]:

$$\begin{aligned} D(E) &\approx \lim_{T\to\infty} 2\langle \int_0^T \dot{q}(0)\cdot\dot{q}(t)\; dt\rangle_{\mu_E} \\ &= \lim_{T\to\infty} 2\langle\sqrt{2(E-V(q_0))}\int_0^T \cos\phi(t)\; |\dot{q}(t)|\; dt\rangle_{\mu_E} \end{aligned}$$

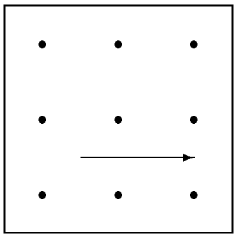
where $\phi(t)$ is the angle between the two vectors $\dot{q}(0)$ and $\dot{q}(t)$. Let $\bar{V}$ be the mean w.r.t. the measure $dq_1\wedge dq_2$ of $V(q)$. Now divide the interval $[0,T]$ into the parts $[0,\tau]$ and $[\tau,T]$, where τ is the time of the first macroscopic scattering of the electron. That is, during the time τ the angle $\phi(t)$ is bounded by a small positive δ. So the time τ depends besides the initial values $q(0),\dot{q}(0)$ on δ:

$$\tau\,(\delta;\,(q(0),\dot{q}(0)) := \sup\{\tilde{\tau}\in\mathbf{R}^+ \mid \quad |\phi\,(t,q(0),\dot{q}(0))| < \delta\;\forall\, t\;\in\;\; [0,\tilde{\tau}]\,\}$$

Let $\delta \ll 1$, then in particular holds $\cos\phi(t)\approx 1$.
Remark: Exceptional initial values lead to unbounded τ. Consider as an

example an electron moving on a symmetry axis of the potential (Fig. 2).

Fig.2



So one may write

$$D(E) \simeq 2\sqrt{2(E-\bar{V})}\langle \int_0^{\tau(\delta,q(0),\dot{q}(0))} \cos\phi(t)\ |\dot{q}(t)|dt + \int_{\tau(\delta,q(0),\dot{q}(0))}^{\infty} \cos\phi(t)\ |\dot{q}(t)|dt\rangle_{\mu_E}$$

For simplicity we assume that $\cos\phi(t)$ and $|\dot{q}(t)|$ are not correlated and that after collision time τ the values of $\cos\phi(t)$ are uniformly distributed. Under this assumption the second integral will disappear in the mean. The first integral is exactly the *mean free path length* $\bar{s}(E)$. So $D(E) \simeq \sqrt{2(E-\bar{V})}\cdot \bar{s}(E)$, and with (8) ($\bar{s}(E) \sim c^{-1}\cdot E$) it follows finally that for large E:

$$D(E) \sim const \cdot E^{\frac{3}{2}}. \tag{9}$$

6 Comparison with similar models

The deduction of the diffusion law (9) uses the existence of the mean free path length $\bar{s}(E)$. Its existence is not trivial, but it is possible to show it.

In contrast to this model (classical motion in a Coulomb crystal), the mean free path length does not exist in the model of the two-dimensional periodic *Lorentz gas* [3, 12] of *infinite horizon*, so it is not surprising that it is not diffusive. The well known Lorentz gas consists of a particle freely moving in the plane between a discrete set of disjoint discs. This discrete set is invariant under a lattice $\mathcal{L}$. Whereas the velocity stays constant between collisions, the particle is reflected elastically from the boundaries of the scatterers like a billiard ball. The particle has *infinite horizon* if there

exists a trajectory which passes through the crystal without touching any scatterer. An important property of this model is the following: Fixing the centres of the discs, the horizon cannot be finite if the diametres of the discs are to small. This is the case if there is, for example, only one disc per unit cell which touches no side of the cell. The nonexistence of the mean free path length may be derived from the existence of trajectories staying for a sufficiently long time in 'channels' formed by parallel unscattered trajectories (channeling behaviour, see Chapter 2.6 [11]).
It might be surprising that the described Lorentz gas is qualitatively different even from the high-energy classical motion in the Coulomb crystal, because the Euclidean curvature of a trajectory in the Coulomb crystal decreases with the energy E. Of course, if one looks at segments of fixed length the segments become more and more straight with increasing energy E. But consider at Fig. 3a) and Fig. 3b), where trajectories corresponding to different energies are shown. Notice that the sizes of the considered part of the crystal is enlarged proportional to E (corresponding to the energy dependence of $\bar{s}$). One observes that the trajectory even of a particle of high energy does *not* look like the trajectory of a billiard ball, but is curved. Without entering any circle of macroscopic scattering the electron is able to change its direction by sufficiently many 'weak' scatterings.
Summary: The Euclidean curvature decreases with E but the *total Euclidean curvature* of a trajectory between two consecutive events of macroscopic scatterings does not vanish in general, because the mean free path length $\bar{s}$ increases in E. (The total curvature of a path is the curvature integrated over this path, i.e., the 'historically' measured change of the direction of the tangent). This nonvanishing of the total curvature generated by 'weak' scattering is responsible for diffusion.
Diffusion takes place independently of the arrangement of the scatterers in a crystal of Yukawa scatterers. On the other hand the finiteness of the horizon is essential in the model of the Lorentz gas. The Lorentz gas of finite horizon is diffusive. One may compare the diffusion constant σ defined in that model (for example look at [4]) with the diffusion constant D defined in (7). One way to take the dependence of diffusion processes on the energy into account in the model of the Lorentz gas is, to increase the velocity of the particle. But the law of reflection does not depend on the energy (because the angles of incidence do not). So the particle covers its trajectory with a speed propotional to the square root of the energy (apart from the moments of reflection, the particle sees no potential and it has only kinetic energy). The length covered in a fixed interval of time will be proportional

to the square root of the energy, too. Consequently the diffusion constant $\sigma(E)$ would increase like: $\sigma \sim const \cdot E^{\frac{1}{2}}$. I think this diffusion law is not yet in sharp contrast to the law $D(E) \sim const \cdot E^{3/2}$. Recall that the faster covering of the mean free path length $\bar{s}(E)$ in the Coulomb model gives asymptotically the factor $E^{1/2}$, too. So it seems to be more natural to compare the Coulomb model with the Lorentz gas of finite horizon with scattering discs, whose diametres scale with E^{-1} correponding to the scaling of the circles of macroscopic scattering in the Coulomb case. The diffusion law, one would obtain by that reflection of the Lorentz model, would have to be compared with the $E^{3/2}$-law (7). Then the main qualitative difference would be the following: With increasing the energy E, the scattering discs become smaller than the critical diametre of finiteness of the horizon. Diffusion no longer takes place for high energy.
A further difference between the two models is that phase space is in fact smooth for the Coulomb crystal, whereas any hard core potential like the Lorentz gas shows edges in phase space.
Another way of modeling the classical motion in a crystal is to consider a real analytic (and not only differentiable) periodic potential. But KAM theory predicts, apart from the fact that the motion becomes ballistic for high energy, the existence of elliptical orbits (on condition that the particle is able to leave the unit cell) already for low energies. So the set of orbits channeling 'nearly unscattered' through the crystal has positive measure. The motion is therefore not diffusive. Geisel, Radons and Zacherl examined $1/f$-noise in such egg-carton like potentials they also looked numerically for diffusive behaviour. However, they neglected exactly the 'channeling orbits'.
Last remark: No answer without questions! Remember that the motion of the quantum mechanical wave packet is always ballistic (Bloch theorem):

$$\lim_{t\to\infty} \langle \frac{q^2(t)}{t^2} \rangle_{QM} = D_{QM} > 0$$

$$\Leftrightarrow \langle q^2 \rangle_{QM} \sim D_{QM} \cdot t^2.$$

So it is qualitatively faster than the classical particle because of

$$\langle q^2 \rangle_{CL} \sim E^{\frac{3}{2}} \cdot t.$$

If a quantum particle behaves more and more classically in the high energy range it has also to get slower. This question arises in [9], where Knauf treats the quantum case of periodic Coulombic potentials.

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