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Classical Motion in Two-Dimensional Crystals

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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: $D(E) \sim \text{const} \cdot E^{3/2}$. This diffusion law is checked for a concrete crystal by numerically 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 the singularities and smooth elsewhere, Knauf[8] showed 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 Section 5 yields the result $D(E) \sim \text{const} \cdot E^{3/2}$ 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 path needs not be a straight path. In fact this is why the motion is diffusive (see Section 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

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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 numerical computations are related to a simple square lattice of Yukawa scatterers defined in Section 2. After introduction in Section 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 Section 4 the diffusion constant $D(E)$ is defined. Then I 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 Section 5 is compared with the Sinai billiard and the model of an egg-carton-like potential used by Geisel *et al.*[5]

In the following I call a path in configuration space a trajectory, whereas I call a path in phase space an orbit.

2. DEFINITIONS

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

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

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

Definition. We call a potential V an *$\mathscr{L}$-periodic Coulomb potential* (or sometimes briefly a Coulomb potential) if it satisfies three conditions:

(a) V is $\mathscr{L}$-periodic.

(b) Near a singularity $s \in \mathscr{S}$ the potential is *asymptotically Coulombic*, i.e.,

$$V(q-s) \sim -z\,|q-s|^{-1}, \qquad q \in M'_1 \tag{2}$$

where $z > 0$ is the charge of the nucleus situated as s.

(c) Elsewhere V is smooth.

For example, the class of attracting Yukawa potentials and specific $-1/r$ potentials of finite ranges[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':

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

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 $M_2' := M_1'/\mathscr{L}$. On the cotangent bundle T^*M_2' we have the Hamiltonian H_2':

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

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

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

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

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

where g' is the Euclidean metric on M_1' and E is the energy of the electron. So the Jacobian metric g_E' is conformal w.r.t. the Euclidean 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 Euclidean 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

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

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 (c)] outside of small circular neighborhoods 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 neighborhoods 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 $V^C(q) := -1/|q-s|$ 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 exists a threshold $h > 0$ so that for all energies $E \geqslant h$ the curvature $K_E'(q) < 0$. In fact the existence of h was proved in ref. 8 for Coulomb potentials of finite ranges and Coulomb potentials of Yukawa type. In Appendix D of ref. 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[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 $V^t := t \cdot V^1 + (1-t) \cdot V^0$, $0 \leqslant t \leqslant 1$, 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 behavior. (M'_1, g'_E) has negative curvature, but is neither compact nor geodesically complete. The problem of completion and compactification was solved in ref. 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 ref. 8, but is similar to the method presented in Chapter 2 of ref. 7. Notice that the motion in the punctured plane M'_1 is not complete. To see this, look at a particle moving toward the singularity s (for example, parallel to a symmetry axis of the crystal as in 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 trajectory, i.e., one simply reflects the trajectory at the scattering center $s \in \mathcal{S}$.

Consider now all trajectories (of fixed positive energy E) intersecting a small circular neighborhood 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 pericenter. The second number is the angle ϕ enclosed by any arbitrary fixed direction and the axis connecting the pericenter 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 $(E = \text{const} > 0)$ 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.

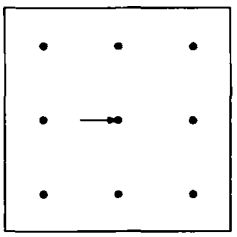

Fig. 1.

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

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

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

be these completions. The proof of Proposition 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 $(T^*M_1', \mathbf{d}p \wedge \mathbf{d}q, H_1')$ and $(T^*M_2', \mathbf{d}p \wedge \mathbf{d}q, H_2')$, respectively. In particular, $\omega_i|_{T^*M_i'} = d\mathbf{p} \wedge \mathbf{d}q$ and $H_i' = H_i|_{T^*M_i'}$, $i=1, 2$. Both 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 $E \geqslant h$.[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 $\langle \cdot\cdot \rangle_{\nu_E}$ is taken w.r.t. the probability measure ν_E. Let π: $P_1 \to P_2$ be 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 ref. 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 $E \geqslant h$.

Of course the value of the threshold h depends on the lattice $\mathscr{L}$ 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 $\mathscr{L}$ and the representative V^Y of the class of attracting Yukawa potentials.

The Coulomb potentials to which the proof in ref. 8 relates lead (for $E \geqslant h$) to negative curvature $K'_E(q)$ of the configuration spaces (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 Theorem 6.12 of ref. 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,

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

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 ith 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 $|p_0^i| := \{2[E - V(q_0^i)]\}^{1/2}$. The running time T was chosen sufficiently large, that is, the orbit was integrated over time steps $\tau, 2\tau, \ldots, 15\tau = T$ and T was considered to be large enough if the values $D_{\text{app}}^\tau(E)$ oscillated only in a small interval.

It might seem to be problematic to compute long orbits of an unstable flow Φ_t of Anošov 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 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

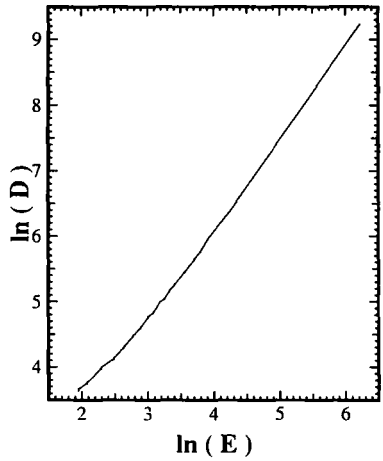

Fig. 2. Dependence of the diffusion constant D on the energy E.

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 behavior of the phase space flow.

The double logarithmic plot of the function $D(E)$ (Fig. 2) 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 $D(E) \sim \text{const} \cdot E^{3/2}$ for large E and a suitable positive constant. Up to numerical fluctuations Fig. 2 shows a convex function. The slope increases, but seems to be asymptotically constant. So the slope 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 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 ref. 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 $s \in \mathscr{S}$, whose radius scales with β/E, $\beta = \text{const}$ (see Lemma 5.5 of ref. 7 or Chapter 2.6 of ref. 11).

The meaning of the term macroscopic scattering is that the change of the direction of the electron after passing through a circular neighborhood 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 $\mathscr{L}$-periodic crystal a straight line f in a plane of randomly spread discs of the small radius r, $r \sim 1/E$. Suppose there are n singularities in the fundamental domain, whose area we normalize to 1. Then an area $\mathscr{A}$ of size A^2 will contain $A^2 \cdot n$ singularities in the mean, and the discs around the singularities will cover an area of $A^2 \cdot n \cdot \pi r^2 \sim 1/E^2$. The proability that a point in $\mathscr{A}$ lies on a disc is proportional to $1/E^2$. Consequently, the probability that a point of the line f is also contained in a disc is proportional to $1/E$ (this 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 goedesic 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 ref. 11].

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

$$D(E) = \lim_{T\to\infty} \frac{1}{T} \langle |q(T) - q_0|^2 \rangle_{\mu_E} = \lim_{T\to\infty} \frac{1}{T} \left\langle \left| \int_0^T \dot{q}(t)\, dt \right|^2 \right\rangle_{\mu_E}$$

$$= \lim_{T\to\infty} \frac{1}{T} \left\langle \int_0^T \int_0^T \dot{q}(s) \cdot \dot{q}(r)\, ds\, dr \right\rangle_{\mu_E}$$

$$= \lim_{T\to\infty} \frac{1}{T} \left\langle \int_0^T \int_{-T}^T \dot{q}(s) \cdot \dot{q}(s+t)\, dt\, ds \right\rangle_{\mu_E}$$

with $-T \leqslant t := r - s \leqslant T$. 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

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

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

$$D(E) \approx \lim_{T\to\infty} 2 \left\langle \int_0^T \dot{q}(0) \cdot \dot{q}(t)\, dt \right\rangle_{\mu_E}$$

$$= \lim_{T\to\infty} 2 \left\langle \{2[E - V(q_0)]\}^{1/2} \int_0^T \cos\phi(t)\, |\dot{q}(t)|\, dt \right\rangle_{\mu_E}$$

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:

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

Let $\delta \ll 1$; then in particular $\cos\phi(t) \approx 1$.

Remark. Exceptional initial values lead to unbounded τ. Consider as an example an electron moving on a symmetry axis of the potential (Fig. 3).

So one may write

$$D(E) \simeq 2\{2[E - \bar{V}]\}^{1/2} \left\langle \int_0^{\tau(\delta, q(0), \dot{q}(0))} \cos\phi(t)\, |\dot{q}(t)|\, dt \right.$$

$$\left. + \int_{\tau(\delta, q(0), \dot{q}(0))}^{\infty} \cos\phi(t)\, |\dot{q}(t)|\, dt \right\rangle_{\mu_E}$$

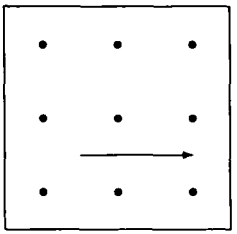

Fig. 3.

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 $D(E) \simeq [2(E-\bar{V})]^{1/2} \cdot \bar{s}(E)$, and with (8) $[\bar{s}(E) \sim c^{-1} \cdot E]$ it follows finally that for large E

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

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 mode 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 $\mathscr{L}$. Whereas the velocity stays constant between collisions, the particle is reflected elstically 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 centers of the discs, the horizon cannot be finite if the diameters of the discs are too 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 behavior; see Chapter 2.6 of ref. 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

(a)

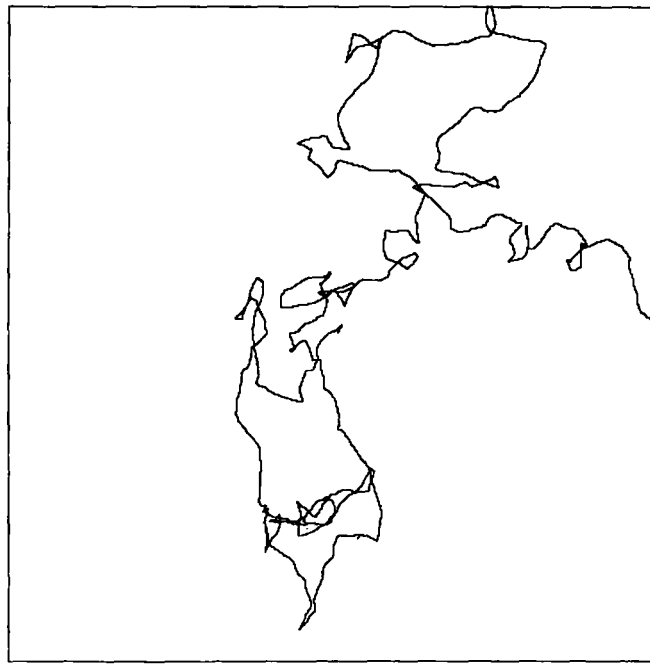

Fig. 4. (a) Energy $E = 80$, time $T = 270$, sizes 481×481; (b) energy $E = 160$, time $T = 360$, sizes 961×961.

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. 4a) and 4b, where trajectories corresponding to different energies are shown. Notice that the size 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.

7. SUMMARY

The Euclidean curvature decreases with E, but the *total Euclidean curvature* of a trajectory between two consecutive events of macroscopic scattering 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

(b)

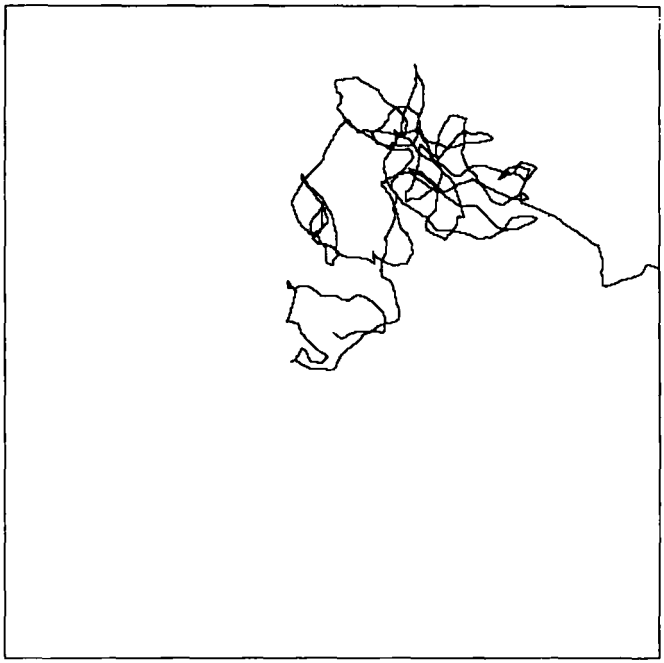

Fig. 4. *(Continued)*

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, see ref. 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 proprotional 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 $\sigma \sim \text{const} \cdot E^{1/2}$. I think this diffusion law is not yet in sharp contrast to the law $D(E) \sim \text{const} \cdot E^{3/2}$. 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 diameters scale with E^{-1} corresponding 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 energy E, the scattering discs become smaller than the critical diameter 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 *et al.* examined $1/f$ noise in such egg-carton-like potentials and also looked numerically for diffusive behavior. 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):

$$\lim_{t\to\infty}\left\langle\frac{q^2(t)}{t^2}\right\rangle_{\mathrm{QM}} = D_{\mathrm{QM}} > 0 \Leftrightarrow \langle q^2\rangle_{\mathrm{QM}} \sim D_{\mathrm{QM}}\cdot t^2$$

So it is qualitatively faster than the classical particle because of

$$\langle q^2\rangle_{\mathrm{CL}} \sim E^{3/2}\cdot t$$

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

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