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Bohmian trajectories and Klein's paradox

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Abstract

We compute the Bohmian trajectories of the incoming scattering plane waves for Klein's potential step in explicit form. For finite norm incoming scattering solutions we derive their asymptotic space–time localization and we compute some Bohmian trajectories numerically. The paradox, which appears in the traditional treatments of the problem based on the outgoing scattering asymptotics, is absent.

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1. Introduction

Bohmian mechanics [1, 2] attempts to reconcile quantum mechanics first with the notion of observation-independent properties of physical systems ('realism') and second with strictly deterministic basic laws connecting these properties ('determinism'). While in standard quantum mechanics a system acquires a specific property only upon measurement by random quantum jumps, within Bohmian mechanics each individual system has all its possible properties completely specified independently of any measurement. This is achieved by completing the quantum states through 'hidden variables', which determine all outcomes of experiments with individual systems. Whether the laws, which connect hidden variables, can be tested experimentally, is still under debate [3, 4]. In any case the basic aim of Bohmian mechanics has been appreciated by a growing community [5], and apart from all fundamental controversies, Bohmian trajectories undoubtedly help to visualize the time evolution of wavefunctions.

While the main bulk of work within Bohmian mechanics has been devoted to the Schrödinger dynamics, there exist some results concerning relativistic quantum mechanics. Among these is Holland's work on the Klein paradox [6]. In this paper the Bohmian trajectories are computed, which follow from the treatment of Klein's Paradox as it is given by Bjorken and Drell [7]. Bjorken and Drell present a plane wave solution of the Dirac equation for an electron, which is exposed to a sufficiently high, one-dimensional potential step. They talk about the various parts of their solution as incoming, transmitted and reflected waves. The paradox then arises because the reflected probability current is greater than the incoming current and the

transition current is directed towards the potential step. Holland [6] determined the Bohmian trajectories associated with the plane wave solution of Bjorken and Drell. He showed that they are time like, future directed and do not intersect. Furthermore they do not begin or end at finite time. Thus there is no indication for the production or annihilation of electron–positron pairs in these trajectories. However, there is something strange about them. They emerge from the region with nonzero potential instead of moving into this region in the course of time. Furthermore the trajectories of the physically interpretable finite norm wavepackets have not been considered at all in [6].

A long time ago Bongaarts and Ruijsenaars [8] had already pointed out the reason for the paradoxically directed transition current of Bjorken and Drell's treatment: the chosen sign for the momentum parameter in the region with nonzero potential. As a consequence, the plane waves of Bjorken and Drell obey the boundary condition of an outgoing scattering solution instead of an incoming one: a wavepacket superposition of these waves is localized within the potential-free half space and propagates away from the potential step at large positive times. At large negative times the wavepacket approaches the potential step from both sides. Thus the surrounding talk of 'incoming', 'transmitted', and 'reflected' waves, which was used by Bjorken and Drell, is mathematically unjustified and misleading.

In contrast to these outgoing wavepackets, a wavepacket superposition of the corresponding incoming plane wave solutions, is localized within the potential-free half space and propagates towards the potential step at large negative times. At large positive times it moves away from the potential step in both directions. Thus, in this case the picture of an incoming, transmitted and reflected wave is based on mathematical facts. Elaborate numerical studies of the evolution of Gaussian wavepackets have been made in order to confirm the completely different behaviour of the two types of wavepackets [9]. As a result, the paradox of a negative transition current, as formulated by Bjorken and Drell and investigated by Holland, disappears, if the incoming scattering solutions are used in place of the outgoing ones.

In this paper we first discuss the Bohmian mechanics, associated with the incoming scattering solutions of Klein's paradox, which initially move in the potential-free region towards the potential step. For the building block plane waves we prove that all Bohmian trajectories move into the region with nonzero potential. Second, we consider the finite norm wavepackets. We derive their asymptotic space–time localization properties and compute some trajectories numerically. We find that at large negative times, all trajectories, which carry a substantial part of the total norm, are located in the region with zero potential and are directed towards the potential step, where some of them are reflected and some are transmitted. At large positive times these trajectories move away from the potential step. No indication for pair creation at the step can be found. There remains, however, as will be shown here, a physically questionable acceleration of slow packets upon passing the potential step.

2. The two-dimensional Dirac equation

The set of space–time points is assumed to be $M := \mathbb{R}^2$. Let $\mathrm{i}d_M =: (x^0, x^1)$ denote the standard chart of M. The associated tangent frame is $\underline{\partial} := (\partial_0, \partial_1)$. A Minkowskian metric on M is defined by $G_p(\partial_\mu, \partial_\nu) := \delta^0_\mu\delta^0_\nu - \delta^1_\mu\delta^1_\nu$ for each $p \in M$. Let $\underline{e} = (e_1, e_2)$ be an orthonormal basis of a two-dimensional $\mathbb{C}$-vector space W with scalar product $S : W \times W \to \mathbb{C}$. The linear mappings $\gamma^\mu : W \to W$ are defined by $\gamma^0(e_0) = e_1$, $\gamma^0(e_1) = e_0$ and $\gamma^1(e_0) = e_1$, $\gamma^1(e_1) = -e_0$. A differentiable function $\psi : M \to W$ with

$$\mathrm{i}\gamma^\mu \left(\partial_\mu - \mathrm{i}\frac{e}{\hbar c}A_\mu\right)\psi = \kappa\psi \quad (\text{on } M) \tag{1}$$

is called a classical solution of the Dirac equation with continuous external potential $A = A_\mu \mathrm{d}x^\mu \equiv (A_\mu)$ and Compton length $\kappa^{-1} \in \mathbb{R}_{>0}$. The differential geometric notation is as in [10].

Let ψ^1 and $\psi^2 : M \to \mathbb{C}$ denote the (spinor-) component functions of the function $\psi : M \to W$ with respect to the basis $\underline{e}$, i.e. $\psi =: e_1\psi^1 + e_2\psi^2$. The (Lorentz invariant) indefinite inner product L of the spinor space W in terms of its scalar product S reads $L(v, w) := S\left(v, \gamma^0 w\right) = v^{2*}w^1 + v^{1*}w^2$. The current vector field $j_\psi := j^0_\psi \partial_0 + j^1_\psi \partial_1 \equiv (j^\mu_\psi)$ of a function $\psi : M \to W$ is defined by $j_\psi := L(\psi, \gamma^\mu \psi)\partial_\mu = \left(\left|\psi^1\right|^2 + \left|\psi^2\right|^2\right)\partial_0 + \left(\left|\psi^1\right|^2 - \left|\psi^2\right|^2\right)\partial_1$. Due to $G(j_\psi, j_\psi) = 4\left|\psi^1\psi^2\right|^2 \geqslant 0$, the current is nowhere space like. Where j_ψ is nonzero, it is future oriented. If ψ is a classical solution of the Dirac equation (1), then $\mathrm{div}(j_\psi) = 0$.

For sufficiently regular potential, [11] from $\mathrm{div}(j_\psi) = 0$ and $j^0_\psi \geqslant 0$ a probability structure for the spaces $\Sigma_\tau := \left\{p \in M : x^0(p) = \tau\right\}$ with $\tau \in \mathbb{R}$ can be established as follows. The norm of the restriction ψ_τ of a classical solution ψ to Σ_τ for any $\tau \in \mathbb{R}$ is defined by

$$\|\psi_\tau\| := \left(\int_{-\infty}^{\infty} j^0_\psi(\tau, \xi) d\xi\right)^{\frac{1}{2}}.$$

For solutions with $\|\psi_0\| < \infty$ the equation $\|\psi_\tau\| = \|\psi_0\|$ holds for any $\tau \in \mathbb{R}$. Therefore the density

$$\rho_{\psi,\tau} := \frac{j^0_\psi(\tau, \xi)}{\|\psi_0\|^2} |\mathrm{d}\xi| \qquad \text{with} \quad \xi := x^1\big|_{\Sigma_\tau}$$

is a probability density on Σ_τ.

It has been suggested in section 12.2 of [1], and in section 12.2 of [2], that, due to $\mathrm{div}(j_\psi) = 0$, the density $\rho_{\psi,\tau}$ is the transport of $\rho_{\psi,0}$ from Σ_0 to Σ_τ along the flow lines of j_ψ. The phenomenon may be visualized as the evolution of the mass distribution of a cloud of dust along the individual particle trajectories. In consequence, the set of flow lines of j_ψ, the Bohmian trajectories, have been taken seriously as the possible particle world lines, i.e. each (one particle) system in the quantum state represented by ψ is supposed to realize one of the flow lines of j_ψ in the course of time.

A general set of potentials and initial conditions (including singular ones) seems to be unknown such that the global Bohmian trajectories densely fibre $\mathrm{supp}(j_\psi)$. (A global trajectory is one which extends both unboundedly into the past and into the future. A dense fibration is such that the set $X \subset \mathrm{supp}(j_\psi)$ of points, which lie on a global Bohmian trajectory, obeys $\rho_{\psi,\tau}(X \cap \Sigma_\tau) = 1$ for any $\tau \in \mathbb{R}$.) The analogous problem in the Schrödinger case has been described by Berndl in [5] and resolved in [12] for a wide class of potentials.

Lacking such general results for the Dirac equation we confine ourselves to the very specific case of a discontinuous potential step. Let $0 \leqslant V \in \mathbb{R}$ and $\Theta : \mathbb{R} \to \mathbb{R}$ denote the step function $\Theta(x \geqslant 0) := 1$ and $\Theta(x < 0) := 0$. Then the differential 1-form $A := A_0 \mathrm{d}x^0$ with $-\frac{e}{\hbar c} A_0 := V \cdot \left(\Theta \circ x^1\right)$, defined on $U := \left\{p : x^1(p) \neq 0\right\}$, is introduced as an external potential into the restriction of (1) to the domain U. Only classical solutions of the restricted equation with a continuous extension to M are taken into consideration. This yields the following system of partial differential equations for differentiable component functions $\psi^i : U \to \mathbb{C}$ with continuous extension to M:

$$\mathrm{i}\partial_0 \begin{pmatrix} \psi^1 \\ \psi^2 \end{pmatrix} = \begin{pmatrix} -\mathrm{i}\partial_1 + V\Theta(x^1) & \kappa \\ \kappa & \mathrm{i}\partial_1 + V\Theta(x^1) \end{pmatrix} \begin{pmatrix} \psi^1 \\ \psi^2 \end{pmatrix} \qquad (\text{on } U) \qquad (2)$$

For any such solution ψ, the current j_ψ is continuous on M and differentiable on U. On U the continuity equation $\mathrm{div}(j_\psi) = 0$ holds.

3. Localization of free wavepackets

The finite norm solutions of (2) with $V > 0$ will be constructed from the plane wave solutions of (1) in the case $A = 0$. Thus this case is summarized first. See e.g. [13].

Notation 1. *Let* $\overline{\omega} : \mathbb{R} \to \mathbb{R}_{>0}$ *with* $\overline{\omega}(k) := \sqrt{\kappa^2 + k^2}$ *and* $\Omega : \mathbb{R} \to \mathbb{R}_{>0}$ *with* $\Omega(k) := \sqrt{\overline{\omega}(k) + k}$. *Then* $u : \mathbb{R} \to W$, $v : \mathbb{R} \to W$ *with*

$$u(k) := \underline{e} \cdot \begin{pmatrix} \Omega(k) \\ \Omega(-k) \end{pmatrix} \qquad v(k) := \underline{e} \cdot \begin{pmatrix} -\Omega(k) \\ \Omega(-k) \end{pmatrix}.$$

Remark 2. For $k \neq 0$ both $(u(k), u(-k))$ and $(v(k), v(-k))$ is a basis of W. The following relations hold:

$$\begin{aligned} S(u(k), u(k)) &= 2\overline{\omega}(k) & S(v(k), v(k)) &= 2\overline{\omega}(k) \\ S(u(k), u(-k)) &= 2\kappa & S(v(k), v(-k)) &= 2\kappa \\ L(u(k), \gamma^1 u(k)) &= 2k & L(v(k), \gamma^1 v(k)) &= 2k \\ L(u(k), \gamma^1 u(-k)) &= 0 & L(v(k), \gamma^1 v(-k)) &= 0. \end{aligned}$$

Lemma 3. *Let* $k \in \mathbb{R} \setminus 0$ *and let the function* $f : \mathbb{R} \to W$ *be differentiable. Then (a) and (b) hold.*

(a) $\exp(-\mathrm{i}\overline{\omega}(k)x^0) f(x^1) : M \to W$ *solves the Dirac equation (1) with* $A = 0$ *if and only if for some* $\alpha, \beta \in \mathbb{C}$

$$f\left(x^1\right) = \alpha \exp(\mathrm{i}kx^1)u(k) + \beta \exp(-\mathrm{i}kx^1)u(-k).$$

(b) $\exp(\mathrm{i}\overline{\omega}(k)x^0) f\left(x^1\right) : M \to W$ *solves the free Dirac equation (1) with* $A = 0$ *if and only if for some* $\alpha, \beta \in \mathbb{C}$

$$f\left(x^1\right) = \alpha \exp(-\mathrm{i}kx^1)v(k) + \beta \exp(\mathrm{i}kx^1)v(-k).$$

Notation 4. *For* $k \in \mathbb{R}$ *we denote* $\sqrt{2\pi}U_k := \exp(-\mathrm{i}(\overline{\omega}(k)x^0 - kx^1)u(k)$, *and* $\sqrt{2\pi}V_k := \exp(\mathrm{i}(\overline{\omega}(k)x^0 - kx^1)v(k)$.

The frequency of these plane wave solutions belongs to $(-\infty, -\kappa) \cup (\kappa, \infty)$. To each frequency within this range a two-dimensional subspace of single-frequency solutions to (1) exists. The space of solutions with frequency $\overline{\omega}(k) > \kappa$ is spanned by (U_k, U_{-k}) and the space of solutions with frequency $-\overline{\omega}(k) < -\kappa$ is spanned by (V_k, V_{-k}). Both U_k and V_k are constant along the space-like phase velocity vector field $f := \partial_0 + \frac{\overline{\omega}(k)}{k}\partial_1$. The current vector field, associated with both U_k and V_k, is future oriented, time like, and constant:

$$j_{U_k} = j_{V_k} = \frac{1}{\pi}(\overline{\omega}(k)\partial_0 + k\partial_1).$$

From the plane wave solutions U_k and V_k of (1) finite norm wavepackets are formed by superposition. Let $I \subset \mathbb{R}$ be a compact interval and let the function $a : I \to \mathbb{C}$ be continuous. Then the functions from $I \times M$ into W, with either $(k, p) \mapsto a(k)U_k(p)$ or $(k, p) \mapsto a(k)V_k(p)$, first are continuous and second have continuous partial derivatives with respect to x^μ. Therefore the functions from M into W with either $p \mapsto \int_I a(k)U_k(p)\,\mathrm{d}k$ or $p \mapsto \int_I a(k)V_k(p)\,\mathrm{d}k$ are differentiable and the differentiation may be interchanged with the integration and these functions are solutions of (1) with $A = 0$.

Notation 5. *For a continuous function $a : I \to \mathbb{C}$, defined on a compact real interval I, wavepacket solutions $U[a]$ and $V[a]$ of (1) are defined by*

$$U[a] := \int_I \mathrm{d}\mu(k) a(k) U_k \qquad \text{and}$$

$$V[a] := \int_I \mathrm{d}\mu(k) a(k) V_k \qquad \text{with} \quad \mathrm{d}\mu(k) := \frac{\mathrm{d}k}{2\overline{\omega}(k)}.$$

$U[a]$ is called the positive-frequency packet, $V[a]$ is called the negative-frequency packet.

The movement of 'narrow' wavepackets $U[a]$ and $V[a]$ can be made plausible by replacing the function $\overline{\omega}$ in the factor $\exp(-\mathrm{i}x^0\overline{\omega})$ by its tangent approximation at a point k_0 from the domain I. This yields $U[a] \simeq P_+[a]\, U_{k_0}$ and $V[a] \simeq P_-[a]\, V_{k_0}$, with $v_g^0 := \frac{k_0}{\overline{\omega}(k_0)}$ and

$$P_\pm[a] := \int_I \mathrm{d}\mu(k) a(k) \exp\big[\mp \mathrm{i}(k-k_0)\cdot(v_g^0 x^0 - x^1)\big].$$

The functions $P_\pm[a]$, which modulate the plane waves U_{k_0} and V_{k_0}, are constant along the (future directed, time like) group velocity vector field $g := \partial_0 + v_g^0 \cdot \partial_1$ on M. Thus the sign of k_0 determines the direction of propagation of $P_\pm[a]$ and in case of $k_0 > 0$ the approximations to both $U[a]$ and $V[a]$ propagate towards growing x^1.

A more conclusive derivation of the space–time localization of the wavepackets $U[a]$ and $V[a]$ follows from proposition (3.1) of [14]. In the present case of one space dimension this proposition reads as follows.

Proposition 6. *Let $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ denote the Fourier transformation, formally given by*

$$\mathcal{F}(f) : k \mapsto \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-\mathrm{i}kx) f(x)\, \mathrm{d}x.$$

Let $\omega : \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable. The first derivative of ω is denoted as ω'. Define for any $t \in \mathbb{R}$ the unitary time evolution operator $u_t : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ through $u_t(f) := \mathcal{F}^{-1}(\exp(-\mathrm{i}\omega t)\mathcal{F}(f))$. Let $f \in L^2(\mathbb{R})$ and $v_1, v_2 \in \mathbb{R}$ be such that $v_1 < \omega'(k) < v_2$ for all $k \in \mathrm{supp}\mathcal{F}(f)$. Then

$$\lim_{t\to\infty} \int_{-\infty}^{tv_1} |u_t(f)(x)|^2\, \mathrm{d}x = \lim_{t\to\infty} \int_{tv_2}^{\infty} |u_t(f)(x)|^2\, \mathrm{d}x = 0.$$

Remark 7. Since $\|f\|_{L^2}^2 = \|u_t(f)\|_{L^2}^2$ for all $t \in \mathbb{R}$, the above statement is equivalent to

$$\lim_{t\to\infty} \int_{tv_1}^{tv_2} |u_t(f)(x)|^2\, \mathrm{d}x = \|f\|_{L^2}^2 .$$

$u_t(f)$ localizes for $t \to \infty$ within the interval $t \cdot [v_1, v_2]$.

Remark 8. The localization of $u_t(f)$ for $t \to -\infty$ can be obtained from the limit $t \to \infty$ of the evolution $\widetilde{u}_t := u_{-t}$, which has the frequency function $\tilde{\omega} := -\omega$. In this case $-v_2 < \tilde{\omega}'(k) < -v_1$. Thus

$$\|f\|_{L^2}^2 = \lim_{t\to\infty} \int_{-tv_2}^{-tv_1} |\widetilde{u}_t(f)(x)|^2\, \mathrm{d}x = \lim_{t\to-\infty} \int_{tv_2}^{tv_1} |u_t(f)(x)|^2\, \mathrm{d}x$$

follows. Both limits are covered by

$$\|f\|_{L^2}^2 = \lim_{t\to\pm\infty} \int_{t\cdot[v_1,v_2]} |u_t(f)(x)|^2\, \mathrm{d}x.$$

An application of proposition (6) to the component functions of $U[a]$ and $V[a]$ yields the following localization for $\rho_{\psi,\tau}$.

Proposition 9. *$v_g := \overline{\omega}' : \mathbb{R} \to \mathbb{R}$, $k \mapsto \frac{k}{\overline{\omega}(k)}$ denotes the group velocity of $\overline{\omega}$. The function $a : [k_1, k_2] \to \mathbb{C}$ be continuous. The real numbers v_1 and v_2 are chosen such that $v_1 < v_g(k_1)$ and $v_g(k_2) < v_2$. For $\psi \in \{U[a], V[a]\}$ then*

$$\lim_{\tau\to\pm\infty} \int_{\tau[v_1,v_2]} \rho_{\psi,\tau} = 1.$$

Proof. We shall check first that the assumptions of proposition (6) hold for the component functions of our wavepackets. Consider the positive frequency case. Since the functions Ω and $\overline{\omega}$ are continuous and since $\frac{1}{\overline{\omega}}$ is bounded, the function

$$g^i : \mathbb{R} \to \mathbb{C} \qquad k \mapsto \begin{cases} \dfrac{a(k)\Omega(-(-1)^i k)}{2\overline{\omega}(k)} & \text{for} \quad k_1 < k < k_2 \\ 0 & \text{otherwise} \end{cases}$$

belongs to $L^2(\mathbb{R})$. Now $U[a]^i$ is given by $U[a]^i_\tau = \mathcal{F}^{-1}\left(\exp(-\mathrm{i}\overline{\omega}\tau) g^i\right)$. As $\overline{\omega}$ has continuous derivatives of arbitrary order, the evolution is of the type of proposition (6). The second derivative $\overline{\omega}''(k) = \frac{\kappa^2}{\overline{\omega}(k)^3} > 0$ implies that the group velocity function $k \mapsto \overline{\omega}'(k) = \frac{k}{\overline{\omega}'(k)}$ is strictly increasing. From this one obtains the bounds $v_1 < \overline{\omega}'(k) < v_2$ for any $k \in [k_1, k_2]$. Thus proposition (6) yields

$$\left\| U[a]^i\big|_{\Sigma_\tau} \right\|^2_{L^2} = \lim_{\tau\to\pm\infty} \int_{\tau\cdot[v_1,v_2]} \left|U[a]^i(\tau, x)\right|^2 \mathrm{d}x.$$

From this and $\|U[a]_\tau\|^2 = \left\|U[a]^1_\tau\right\|^2_{L^2} + \left\|U[a]^2_\tau\right\|^2_{L^2}$ the statement follows. The case of negative-frequency packets is analogous. □

Remark 10. Proposition (9) states that the probability density $\rho_{\psi,\tau}$ is localized within the x^1 interval $\tau \cdot [v_1, v_2]$ for $\tau \to \pm\infty$. In case of $0 < k_1 < k_2$ it is localized in the half space $x^1 < 0$ for $\tau \to -\infty$ and in the half space $x^1 > 0$ for $\tau \to \infty$. The localization is right moving. In the case of $k_1 < k_2 < 0$ it is localized in the half space $x^1 > 0$ for $\tau \to -\infty$ and in the half space $x^1 < 0$ for $\tau \to \infty$. It is left moving.

4. Plane waves for $V > 2\kappa$

Let $\psi = \exp(-\mathrm{i}\omega x^0) f(x^1)$ with $f : \mathbb{R} \to W$ be a single-frequency solution of (2) with the frequency $\omega > \kappa$. With some $\alpha, \beta \in \mathbb{C}$ the equation $\psi = \alpha U_k + \beta U_{-k}$ holds on $M_- := \left\{p \in M : x^1(p) < 0\right\}$. Here $k > 0$ is determined by $\overline{\omega}(k) = \omega$. On $M_+ := \left\{p \in M : x^1(p) > 0\right\}$ the function $\exp(\mathrm{i}Vx^0)\psi$ equals a single-frequency solution of equation (1) with $A = 0$. Its frequency reads $\omega' := \omega - V$.

Klein's phenomenon occurs for $\omega' < -\kappa$. Thus we restrict our discussion to the case $\kappa < \omega < V - \kappa$. This implies $V > 2\kappa$. In that case

$$\psi = \exp(-\mathrm{i}Vx^0)\left[\gamma V_q + \delta V_{-q}\right] \qquad (\text{on } M_+)$$

with $\gamma, \delta \in \mathbb{C}$ and with $q > 0$ being determined by $-\overline{\omega}(q) = \omega' = \overline{\omega}(k) - V$. The constants $\alpha, \beta, \gamma, \delta$ are restricted by the condition that ψ is continuous, which is equivalent to

$$\alpha U_k(0,0) + \beta U_{-k}(0,0) = \gamma V_q(0,0) + \delta V_{-q}(0,0). \tag{3}$$

Since $U_k(0,0)$ and $U_{-k}(0,0)$ are linearly independent, this system of linear equations for $(\alpha, \beta, \gamma, \delta)$ is of rank 2. Thus the space of single-frequency solutions ψ to (2) is two

dimensional. Within this space there are several one-dimensional subspaces of particular physical importance.

One of these spaces comprises the single-frequency solutions with $\delta = 0$. Its relevance emerges from the asymptotic behaviour in time of the wavepackets formed from these solutions. As will be discussed in the next section, the $x^0 = \tau$ restrictions of such wavepackets localize for $\tau \to -\infty$ within the half line $x^1 < 0$. Thus these packets have a right-moving incoming asymptotics. Similarly, the $\alpha = 0$ plane waves are the building blocks, from which incoming left-moving packets are formed through superposition. Wavepackets built from either $\alpha = 0$ or $\delta = 0$ plane waves correspond to the 'incoming' scattering solutions of the general quantum scattering theory [13]. They have a well defined half space localization and direction of movement for $\tau \to -\infty$. 'Outgoing' scattering solutions approaching a wavepacket which, for $\tau \to \infty$, moves out exclusively towards $x^1 \to -\infty$, are obtained from $\gamma = 0$. These are the solutions, on which [6,7] base their discussion of Klein's phenomenon. Finally, 'outgoing' solutions, which approach a wavepacket, that, for $\tau \to \infty$, exclusively moves out towards $x^1 \to \infty$, are obtained from $\beta = 0$.

Up to a constant factor the single-frequency solutions with $\delta = 0$ are given by the following lemma, which follows from the continuity condition (3) with $\alpha = 1$ and $\delta = 0$.

Lemma 11. *Let $V > 2\kappa > 0$ and $k > 0$ be such that $\overline{\omega}(k) < V - \kappa$ holds. Let the function $\psi : M \to W$ be continuous and such that for some $q > 0$ and some $r, t \in \mathbb{C}$*

$$\psi = \begin{cases} U_k + rU_{-k} & \text{on} \quad M_- \\ \exp(-\mathrm{i}Vx^0)tV_q & \text{on} \quad M_+ \end{cases}$$

holds. Then ψ is a solution of (2) if and only if (1)–(3) hold.

(1) q is the unique solution of $\overline{\omega}(k) + \overline{\omega}(q) = V$ in $\mathbb{R}_{>0}$,

(2) $r = r(k) := \frac{-2\kappa V}{V^2 - (k-q)^2}$,

(3) $t = t(k) := -2\frac{k}{\kappa}\frac{\Omega(k)\Omega(-q)}{V+k-q}$.

Notation 12. *The solution ψ of (2), which is given by lemma (11) is denoted by U_k^{in} in what follows.*

Remark 13. Observe that due to $V^2 - (k-q)^2 = 2(\kappa^2 + \overline{\omega}(k)\overline{\omega}(q) + kq) > 0$ and due to $V + k - q = \overline{\omega}(k) + k + \overline{\omega}(q) - q > \overline{\omega}(q) - q > 0$ the inequalities $r(k) < 0$ and $t(k) < 0$ hold.

Remark 14. The wavenumber q is given explicitly through $q = s(k)$, with the differentiable function

$$s : \left(0, \sqrt{V^2 - 2\kappa V}\right) \to \left(0, \sqrt{V^2 - 2\kappa V}\right) \qquad k \mapsto \sqrt{V^2 - 2V\overline{\omega}(k) + k^2}.$$

The function s is a monotonically decreasing bijection. It has the fixed point $k_0 = \frac{V}{2}\sqrt{1 - \left(\frac{2\kappa}{V}\right)^2}$. Thus if $k < k_0$ then $q > k_0$ and if $k > k_0$ then $q < k_0$. These inequalities will show up in the group velocity of narrow wavepackets through either an acceleration or a deceleration upon transition through the potential's singularity at $x^1 = 0$.

Proposition 15. *For the current vector field $j_{U_k^{\mathrm{in}}}$*

$$\pi j_{U_k^{\mathrm{in}}} = t(k)^2\left[\overline{\omega}(q)\partial_0 + q\partial_1\right] + 2\kappa r(k)\Theta(-x^1)\left[\cos(kx^1) - 1\right]\partial_0$$

holds. $j_{U_k^{\mathrm{in}}}$ is differentiable and $\mathrm{div}(j_{U_k^{\mathrm{in}}}) = 0$ everywhere on M.

Proof. From remark (2) one obtains by inserting the restrictions of U_k^{in} to $M_\pm$ into the current's definition the equations

$$\pi j_{U_k^{\text{in}}} = \begin{cases} \left[\overline{\omega}(k)\left(1+r(k)^2\right) + 2\kappa r(k)\cos(kx^1)\right]\partial_0 + k\left(1-r(k)^2\right)\partial_1 & \text{on} \quad M_- \\ t(k)^2\left\{\overline{\omega}(q)\partial_0 + q\,\partial_1\right\} & \text{on} \quad M_+. \end{cases}$$

The continuity of U_k^{in} implies the continuity of $j_{U_k^{\text{in}}}$, which in turn is equivalent to the equations

$$\overline{\omega}(k)\left(1+r(k)^2\right) + 2\kappa r(k) = \overline{\omega}(q)t(k)^2$$
$$k\left(1-r(k)^2\right) = qt(k)^2.$$

(They are easily checked by inserting the explicit expressions for $r(k)$ and $t(k)$.) From this the formula for $j_{U_k^{\text{in}}}$ follows on M. Though U_k^{in} is not differentiable where $x^1 = 0$, its current field is differentiable in every $p \in M$ because of $\left[\cos(kx^1) - 1\right](p) = 0$ and $\left(\partial_\mu\left[\cos(kx^1) - 1\right]\right)(p) = 0$ for $x^1(p) = 0$. Obviously, $\operatorname{div}(j_{U_k^{\text{in}}}) = 0$ holds on $M_+ \cup M_-$. Since $j_{U_k^{\text{in}}}$ is differentiable on M, it follows that $\operatorname{div}(j_{U_k^{\text{in}}}) = 0$ on M. □

Remark 16. From the j^1-continuity condition $\left(1 - r(k)^2\right) = \frac{qt(k)^2}{k} > 0$ and from $r(k) < 0$ the bounds $-1 < r(k) < 0$ follow.

Remark 17. Since the Lie bracket $\left[\partial_0, j_{U_k^{\text{in}}}\right] = 0$, the current vector field $j_{U_k^{\text{in}}}$ is x^0-shift invariant.

Definition 18. *Let j be a differentiable vector field on M. Let $\gamma_p : I \to M$ obey the differential equation $\dot{\gamma}_p = j \circ \gamma_p$ and the initial condition $\gamma(0) = p$. The open interval $I \subset \mathbb{R}$ is assumed to be maximal. Since j is differentiable, γ_p is unique. γ_p is called the maximal integral curve of j through $p \in M$ and the set $\gamma_p(I) \subset M$ is called the orbit of γ_p. If j is the current vector field of a solution ψ of the Dirac equation, then the orbit of γ_p is called the Bohmian trajectory of ψ through p.*

Remark 19. $j_{U_k^{\text{in}}}$ is a bounded and everywhere future directed time-like vector field with positive, constant component $j^1_{U_k^{\text{in}}}$. Thus along a Bohmian trajectory of U_k^{in} the function x^1 increases with x^0, i.e. the trajectories move towards the potential step from $x^1 < 0$. To be more specific: on M_+ the equation $j_{U_k^{\text{in}}} = t(k)^2 j_{U_q}$ holds. On M_- the current $j_{U_k^{\text{in}}}$ is the sum of $t(k)^2 j_{U_q}$ and the nonconstant ∂_0-directed, bounded vector field $\frac{2\kappa}{\pi} r(k)\left[\cos(kx^1) - 1\right]\partial_0$. Due to $r(k) < 0$ the additional term belongs to $R_{\geqslant 0} \cdot \partial_0$, which implies

$$0 < t(k)^2 j^0_{U_q} \leqslant j^0_{U_k^{\text{in}}} \leqslant t(k)^2 j^0_{U_q} + \frac{4\kappa}{\pi}\left|r(k)\right| \text{ on } \quad M_-.$$

From this and $j_{U_k^{\text{in}}} = t(k)^2 j_{U_q}$ (on M_+) it follows that, due to

$$G(j_{U_k^{\text{in}}}, j_{U_k^{\text{in}}}) \geqslant t(k)^2 G(j_{U_q}, j_{U_q}) = t(k)^2 \frac{\kappa^2}{\pi^2} > 0$$

$j_{U_k^{\text{in}}}$ is globally time like and future directed. Thus the current has no zeros and is nowhere light like.

Remark 20. The velocity vector field $v_{U_k^{\text{in}}} := \frac{j^1_{U_k^{\text{in}}}}{j^0_{U_k^{\text{in}}}}\partial_1$ of $j_{U_k^{\text{in}}}$ relative to the inertial frame (∂_0, ∂_1) is given by

$$v_{U_k^{\text{in}}} = q\left[\overline{\omega}(q) - \frac{2\kappa r(k)}{t(k)^2}\Theta(-x^1)\left(1 - \cos(kx^1)\right)\right]^{-1}\partial_1.$$

On M_+ it is the constant field $\frac{q}{\overline{\omega}(q)}\partial_1$ and on M_- it oscillates between the positive bounds

$$\frac{q}{\overline{\omega}(q)+\frac{4\kappa|r(k)|}{t(k)^2}}\partial_1 \leqslant v_{U_k^{\text{in}}} \leqslant \frac{q}{\overline{\omega}(q)}\partial_1.$$

From the bounds of $v_{U_k^{\text{in}}}$ it is obvious that a Bohmian trajectory of U_k^{in} cannot have a higher velocity within the range M_- than it has within M_+, where its velocity is less than 1. An explicit formula for the Bohmian trajectories of U_k^{in} is given by the following proposition.

Proposition 21. *The Bohmian trajectory $\Gamma_{k,\tau}$ of U_k^{in} through $p_0 := (\tau, 0)$ is the set of all $p \in M$, on which*

$$x^0 - \tau = \frac{\overline{\omega}(q)}{q}x^1 - \frac{2\kappa r(k)}{kt(k)^2}\theta(-x^1)\big[kx^1 - \sin(kx^1)\big] \tag{4}$$

holds. $\{\Gamma_{k,\tau}\}_{\tau\in\mathbb{R}}$ is a disjoint covering of M and $\Gamma_{k,\tau} \cap \{p \in M : x^1(p) = 0\} = p_0$.

Proof. The current $j := j_{U_k^{\text{in}}} = a\partial_0 + b\partial_1 + c\Theta(-x^1)(1-\cos(kx^1))\partial_0$ with $\pi a := \overline{\omega}(q)t(k)^2$, $\pi b := qt(k)^2$, $\pi c := -2\kappa r(k)$ is differentiable on M. With $\gamma^\mu := x^\mu \circ \gamma$ the differential equation $\dot\gamma = j \circ \gamma$ decomposes into $\dot\gamma^1 = b$ and

$$\dot\gamma^0 = \begin{cases} a & \text{for} \quad \gamma^1 > 0 \\ a + c(1-\cos(k\gamma^1)) & \text{for} \quad \gamma^1 < 0. \end{cases}$$

The initial condition $\gamma^1(0) = 0$ thus implies $\gamma^1(\lambda) = b\lambda$ for all $\lambda \in \mathbb{R}$. Inserting this into the equation for the component γ^0 one obtains from $\gamma^0(0) = \tau$

$$\gamma^0(\lambda) = \begin{cases} a\lambda + \tau & \text{for} \quad \lambda > 0 \\ (a+c)\,\lambda - \dfrac{c}{kb}\sin(kb\lambda) + \tau & \text{for} \quad \lambda < 0. \end{cases}$$

Thus the maximal integral curve γ_{p_0} of j through p_0 reads

$$\gamma_{p_0} : \mathbb{R} \to M \qquad \gamma_{p_0}(\lambda) = (\tau, 0) + \lambda\cdot(a, b) + \Theta(-\lambda)\left(c\cdot\left(\lambda - \frac{\sin(kb\lambda)}{kb}\right), 0\right).$$

Its orbit is the set $\Gamma_{k,\tau}$ of points $p \in M$, on which

$$x^0 - \tau = \frac{a}{b}x^1 + \frac{c}{kb}\theta(-x^1)\big[kx^1 - \sin(kx^1)\big]$$

holds. Obviously $\Gamma_{k,\tau} = (\tau, 0) + \Gamma_{k,0}$ holds. As $x^0\big|_{\Gamma_{k,\tau}}$ is expressed in terms of $x^1\big|_{\Gamma_{k,\tau}}$, the trajectories $\Gamma_{k,\tau}$ and $\Gamma_{k,0}$ therefore do not intersect for $\tau \neq 0$. In particular, $\Gamma_{k,0}$ intersects $\{p \in M : x^1(p) = 0\}$ only at the single point $(0, 0)$. Because $x^1\big|_{\Gamma_{k,\tau}} \to \mathbb{R}$ is a bijection, the Bohmian trajectory of j through an arbitrary point p is obtained by the proper choice of τ. Thus $\{\Gamma_{k,\tau}\}_{\tau\in\mathbb{R}}$ is a disjoint covering, a fibration of M. □

Figure 1 shows the trajectory $\Gamma_{k,0}$ for $V = 2.25\kappa$ and $k = \frac{\kappa}{2}$ within the space–time region where $-600 < \kappa x^0 < 200$ and $-50 < \kappa x^1 < 50$.

5. Incoming localized solutions for $V > 2\kappa$

Notation 22. *Let $a : I \to \mathbb{C}$ be continuous on a closed interval $I = [k_1, k_2] \subset \mathbb{R}_{>0}$ of positive real numbers such that on I the inequality $\overline{\omega} < V - \kappa$ holds. The constants V and κ obey $V > 2\kappa$. Then $U^{\text{in}}[a] : M \to W$ denotes the wavepacket $U^{\text{in}}[a] := \int_I \mathrm{d}\mu\,(k)a(k)U_k^{\text{in}}$.*

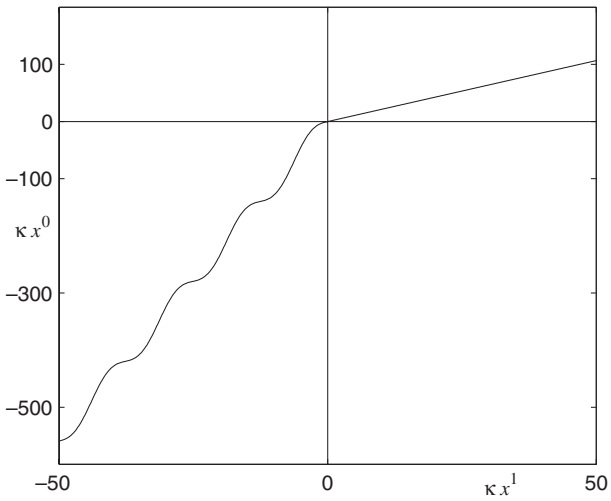

Figure 1. $\Gamma_{k,0}$ for $k = \kappa/2$ and $V = 2.25\kappa$.

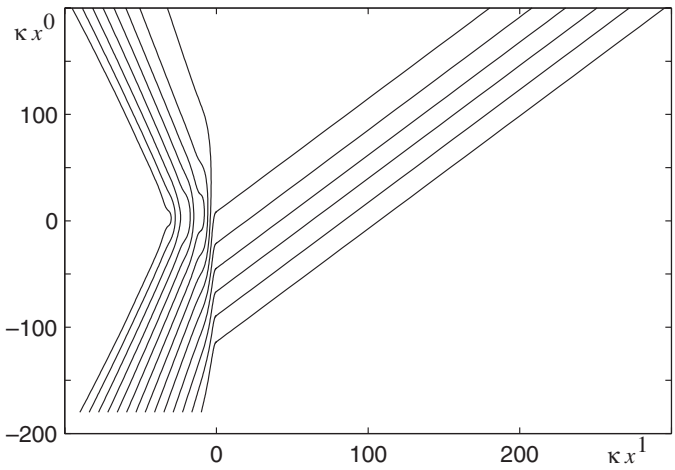

Figure 2. Trajectories for $\Delta = 0.1\kappa$ and $K = 0.3\kappa$.

Proposition 23. *$U^{\mathrm{in}}[a]$ is continuous on M and differentiable on U. It is a solution of equation (2). Let $a_r : [-k_2, -k_1] \to \mathbb{C}$ and $a_t : [s(k_2), s(k_1)] \to \mathbb{C}$ be defined by $a_r(k) := r(-k)a(-k)$, $a_t(q) := \frac{q}{k}t(k)a(k)$ with $k = \sqrt{V^2 - 2V\overline{\omega}(q) + q^2}$. Then the equations $U^{\mathrm{in}}[a] = U[a] + U[a_r]$ on M_- and $U^{\mathrm{in}}[a] = \exp(-\mathrm{i}Vx^0)V[a_t]$ on M_+ hold.*

Proof. From $U_k^{\mathrm{in}} = U_k + r(k)U_{-k}$ (on M_-) there follows on M_-

$$\int_{k_1}^{k_2} \mathrm{d}\mu(k)a(k)U_k^{\mathrm{in}} = \int_{k_1}^{k_2} \mathrm{d}\mu(k)a(k)U_k + \int_{-k_2}^{-k_1} \mathrm{d}\mu(k)a(-k)r(-k)U_k.$$

This proves $U^{\mathrm{in}}[a] = U[a] + U[a_r]$ on M_-.

Similarly, with $q = s(k) := \sqrt{V^2 - 2V\overline{\omega}(k) + k^2}$ there follows on M_+

$$\int_{k_1}^{k_2} \mathrm{d}\mu(k)a(k)U_k^{\mathrm{in}} = \exp(-\mathrm{i}Vx^0)\int_{k_1}^{k_2} \mathrm{d}\mu(k)a(k)t(k)V_{s(k)}.$$

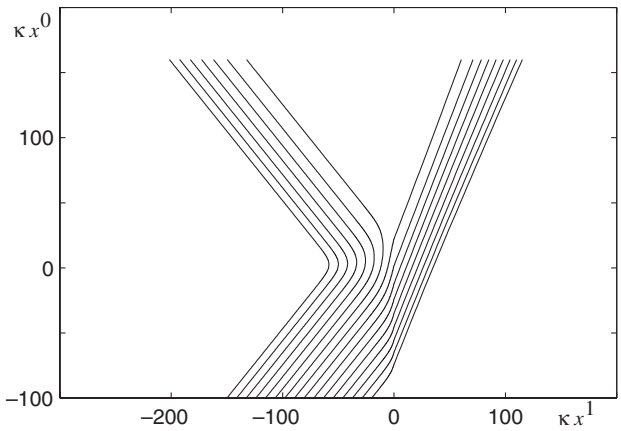

Figure 3. Trajectories for $\Delta = 0.05\kappa$ and $K = 2.7\kappa$.

The function s is defined implicitly by $\overline{\omega} + \overline{\omega} \circ s = V$. This implies first $s = s^{-1}$ and second $\mathrm{d}\overline{\omega} = -\mathrm{d}\,(\overline{\omega} \circ s)$. Substitution of the integration variable k by $q = s(k)$ then yields

$$\begin{aligned}\int_{k_1}^{k_2} \frac{\mathrm{d}k}{2\overline{\omega}(k)} a(k)t(k)V_{s(k)} &= \int_{k_1}^{k_2} \frac{\mathrm{d}\overline{\omega}\,(k)}{2k} a(k)t(k)V_{s(k)} \\ &= -\int_{s(k_1)}^{s(k_2)} \frac{\mathrm{d}\overline{\omega}\,(q)}{2q} \frac{q}{s(q)} a(s(q))t(s(q))V_q \\ &= \int_{s(k_2)}^{s(k_1)} \mathrm{d}\mu\,(q) \frac{q}{s(q)} a(s(q))t(s(q))V_q.\end{aligned}$$

This proves $U^{\mathrm{in}}[a] = \exp(-\mathrm{i}Vx^0)V[a_t]$ on M_+. The statements about the continuity and differentiability follow from the continuity of a_r and a_t through application of elementary analysis theorems. □

Remark 24. The localization of $U^{\mathrm{in}}[a]$ for $\tau \to \pm\infty$ is immediate from proposition (23). Since a_r has its domain within $\mathbb{R}_{<0}$ and a and a_t have their domains within $\mathbb{R}_{>0}$, the wavepacket $U[a_r]$ is left moving, while $U[a]$ and $U[a_t]$ are right moving. At large negative times $U^{\mathrm{in}}[a]$ approximates $U[a]$, which moves in through M_- towards $x^1 = 0$. At large positive times $U^{\mathrm{in}}[a]$ approximates $U[a_t] + U[a_r]$. The transmitted wave $U[a_t]$ moves away from $x^1 = 0$ through M_+ and the reflected one, $U[a_r]$, moves away from $x^1 = 0$ through M_-.

Rigorous analysis of whether the Bohmian trajectories of $U^{\mathrm{in}}[a]\big|_{M_-}$ may be connected with the trajectories of $U^{\mathrm{in}}[a]\big|_{M_+}$ across $x^1 = 0$ in a unique way is left to further investigation. As an indication that this should be possible, we present some trajectories, computed numerically.

For $V = 4\kappa$ we choose for several values of the constants $\Delta > 0$ and $K > 0$ the Fourier amplitude

$$a : [k_1, k_2] \to \mathbb{R} \qquad a(k) := \exp\left(\frac{-(k-K)^2}{\Delta^2}\right)$$

with $k_1 = K - 2\Delta, k_2 = K + 2\Delta$. The domain of the function s of remark (14) is $0 < k < \sqrt{8}\kappa$ and its fixed point is $k_0 = \sqrt{3}\kappa$. Clearly, the constants K and Δ have to be chosen such that $[k_1, k_2]$ is contained in the domain of s. First the wavepacket $U^{\mathrm{in}}[a]$ is computed numerically

in that space–time region, where it hits the potential step. Second from the associated current field some Bohmian trajectories are computed by numerical integration. The starting points are chosen within Σ_τ around the centre of localization of $\rho_{U^{\text{in}}[a],\tau}$. The initial time τ is such that the main bulk of the probability distribution $\rho_{U^{\text{in}}[a],\tau}$ has not yet arrived at the potential step.

Figure 2 shows some trajectories for $\Delta = 0.1\kappa$ and $K = 0.3\kappa$ within the space–time region where $-180 < \kappa x^0 < 200$ and $-100 < \kappa x^1 < 300$. Since the wavenumbers k from the domain of a obey $k < k_0$ the domain of a is mapped into $k > k_0$ by s such that the transmitted packet is faster than the incoming one. This might be considered as what is left over from Klein's paradox.

Figure 3 shows some trajectories for $\Delta = 0.05\kappa$ and $K = 2.7\kappa$ within the space–time region where $-100 < \kappa x^0 < 160$ and $-300 < \kappa x^1 < 200$. Since the wavenumbers k from the domain of a obey $k > k_0$ the transmitted packet is slower than the incoming one. Many more pictures for related situations are contained in [15].

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