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Sources of quantum waves

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Abstract
Due to the space and time dependence of the wavefunction in the time-dependent Schrödinger equation, different boundary conditions are possible. The equation is usually solved as an 'initial-value problem', by fixing the value of the wavefunction in all space at a given instant. We compare this standard approach to 'source boundary conditions' that fix the wave at all times in a given region, in particular at a point in one dimension. In contrast to the well known physical interpretation of the initial-value-problem approach, the interpretation of the source approach has remained unclear, since it introduces negative energy components, even for 'free motion', and a time-dependent norm. This work provides physical meaning to the source method by finding the link with equivalent initial-value problems.

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1. Introduction

The time-dependent Schrödinger equation is commonly solved as an 'initial-value problem'. In one dimension this means that the wavefunction $\psi(x,t)$ is fixed for all x at a reference time, usually $t=0$. However, it is also possible to use different boundary conditions by fixing $\psi(x,t)$ at a space point, say $x=0$, at all times. This 'source' approach has been followed to study the arrival time in quantum mechanics [1], or characteristic propagation velocities and times ('tunnelling times') in evanescent conditions [2–8]. In all of these applications the wavefunction is assumed to vanish for $x \geqslant 0$ and $t<0$,

$$\psi_s(x,t) = 0 \qquad x \geqslant 0 \quad t < 0 \tag{1}$$

the potential is zero or constant for $x \geqslant 0$ and $t>0$, and the solution of the Schrödinger equation is sought for the positive half-line and positive times, $\psi_s(x \geqslant 0, t > 0)$. We shall also limit the present discussion to these premises, and use the subscript s to denote the solutions that obey (1), computed for the spacetime domain $D_+ \equiv \{x \geqslant 0; t > 0\}$. They have been invariably written, up to constant factors and notational changes, as

$$\psi_s(x,t) = \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}E\, \mathrm{e}^{\mathrm{i}xp_+/\hbar - \mathrm{i}Et/\hbar} \chi_s(E) \tag{2}$$

where

$$\chi_s(E) = \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}t\, \psi_s(x=0,t)\, \mathrm{e}^{\mathrm{i}Et/\hbar} \tag{3}$$

is the energy Fourier transform of the given 'source signal' $\psi_s(x=0,t)$ and $p_+ = (2mE)^{1/2}$, with the branch cut taken along the negative imaginary axis of E. Because of (1), $\chi_s(E)$ is an analytical function of E for $\mathrm{Im}\, E > 0$; however, this does not guarantee the absence of singularities of $\chi_s(E)$ for real E, additional to the branch point. In fact, the integral over E is to be understood as going above the real axis; alternatively, $E \to E + \mathrm{i}0$ is to be substituted in the expressions above.

It is easy to check by substitution that (2) satisfies the Schrödinger equation. Actually, Allcock derived (2) as the most general form compatible with (1) [1]. However, its physical interpretation has remained unclear. For instance, a 'source signal' such as [2–8]

$$\psi_s(x=0,t) = \mathrm{e}^{-\mathrm{i}\omega_0 t}\Theta(t) \tag{4}$$

leads to an infinite norm as $t \to \infty$ for $\omega_0 > 0$. An interpretation of such an infinite norm might only be possible by invoking a multi-particle approach which we shall not pursue here. Instead, if we keep within the one-particle picture, it becomes clear that not all 'signals' $\psi_s(x=0,t)$ may be allowed physically. This does not mean that the results obtained with (4) are meaningless. This signal may be an idealized approximation during a certain time interval of an actual signal, and it is also an elementary component of an arbitrary physical signal. Our basic philosophy here is that the physical interpretation of (2) must rest on a process where a wavepacket located in the left half-line is liberated at $t = 0$ and crosses, in general only partially, to the right half-line. This was the point of view of Allcock too [1], although our scope will differ from his work. There must be a link between a physically valid ψ_s and some initial-value problem, and the objective of this paper is to find and discuss such a link and the meaning of the negative energies in (2). The consequences on the possibility to define time-of-arrival distributions in quantum mechanics are also examined.

2. Equivalence between initial-value and source boundary conditions

2.1. Free motion on the full line

In this section we shall solve the initial-value problem corresponding to a wave restricted fully to the left half-line up to $t = 0$, in the interval $[a, b]$, with $a < b < 0$, by an appropriate time-dependent potential that vanishes for $t \geqslant 0$. The resulting wave ψ_{iv} is only free from $t = 0$ onwards. It is also useful to introduce a related wave ψ_f which evolves freely *at all times*, positive and negative, and is equal to ψ_{iv} for $t \geqslant 0$,

$$\psi_f(x,t) = \int_a^b \mathrm{d}x'\, \langle x|U(t,t'=0)|x'\rangle \psi_{iv}(x',t'=0) \qquad \forall t. \tag{5}$$

Here $U(t,t') = \exp[-\mathrm{i}H_0(t-t')/\hbar]$ is the unitary evolution operator for the free-motion Hamiltonian H_0,

$$\langle x|U(t,t')|x'\rangle = \left[\frac{m}{\mathrm{i}h(t-t')}\right]^{1/2} \mathrm{e}^{\mathrm{i}m(x-x')^2/2\hbar(t-t')}. \tag{6}$$

By setting the following source signal:

$$\psi_s(x=0,t) = \psi_{iv}(x=0,t)\Theta(t) = \psi_f(x=0,t)\Theta(t) \tag{7}$$

the corresponding $\psi_s(x,t)$ is obtained via (2). We shall now establish the equality between ψ_s and ψ_f for positive times and positions when the 'boundary condition' of (7) is imposed on ψ_s. $\psi_f(x,t)$ may also be written as a momentum integral,

$$\psi_f(x,t) = \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}p \, \mathrm{e}^{\mathrm{i}xp/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \tilde{\psi}_f(p) \tag{8}$$

where $E = p^2/2m$, and

$$\tilde{\psi}_f(p) = \frac{1}{h^{1/2}} \int_a^b \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}px/\hbar} \psi_f(x, t=0). \tag{9}$$

It can be separated into positive and negative momentum components, $\psi_f(x,t) = \psi_{f,+}(x,t) + \psi_{f,-}(x,t)$. The positive momentum integral is now rewritten in terms of the energy variable $E = p^2/2m$,

$$\psi_{f,+}(x,t) = \frac{1}{h^{1/2}} \int_0^{\infty} \mathrm{d}E \, \mathrm{e}^{\mathrm{i}px/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \left(\frac{m}{2E}\right)^{1/2} \tilde{\psi}_f(\sqrt{2mE}). \tag{10}$$

To put $\psi_{f,-}$ in a similar form, note that, because of the restriction of the initial state within the left half-line at $t = 0$, its momentum representation $\tilde{\psi}_f(p)$, equation (9), is analytical in the complex plane p, and decays to zero as $|p| \to \infty$ in the upper half-plane. These two properties and the decaying behaviour of the exponentials of (8) in the second quadrant allow the substitution of the integral along the negative real axis by an integral along the positive imaginary axis (there are no poles and the integral along a large arc at infinity is zero), which under a suitable reparametrization can be rewritten as

$$\psi_{f,-}(x,t) = -\frac{\mathrm{i}}{h^{1/2}} \int_{-\infty}^{0} \mathrm{d}E \, \mathrm{e}^{\mathrm{i}xp_+/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \left(\frac{m}{-2E}\right)^{1/2} \tilde{\psi}_f \left[\mathrm{i}(-2mE)^{1/2}\right] \qquad x \geqslant 0 \quad t > 0. \tag{11}$$

Explicitly, the reparametrization of the integral is achieved by writing p as $\mathrm{i}\gamma$, with positive γ, for the integral along the imaginary axis, and then making the change of variables $E = -\gamma^2/2m$. Adding (10) and (11) we can now write $\psi_f(x,t)$ for $x \geqslant 0$, $t > 0$ in the form of the right-hand side of (2), with

$$\chi_f(E) = (m/2E)^{1/2} \tilde{\psi}_f \left[(2mE)^{1/2}\right] \tag{12}$$

in place of $\chi_s(E)$.

As before, the cut defining the square root branch is taken at the negative imaginary axis of E, so that the square roots are positive imaginary numbers for negative energies. It is also useful to write $\psi_f(x,t)$ as an integral in the momentum plane,

$$\psi_f(x,t) = \frac{1}{h^{1/2}} \int_L \mathrm{d}p \, \mathrm{e}^{\mathrm{i}px/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \tilde{\psi}_f(p) \qquad x \geqslant 0 \quad t > 0 \tag{13}$$

where the contour is an L-shaped line that goes downwards along the positive imaginary axis and rightwards along the positive real axis. Let us now *define* the function ϕ by the integral in (13) without any restriction on x or t,

$$\phi(x,t) \equiv \frac{1}{h^{1/2}} \int_L \mathrm{d}p \, \mathrm{e}^{\mathrm{i}px/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \tilde{\psi}_f(p) \tag{14}$$

and analyse its behaviour for $x \geqslant 0$ and $t < 0$. The contour L can be closed by a large arc in the first quadrant which does not contribute to the integral. By Cauchy's theorem, $\phi(x,t)$ is zero for $x \geqslant 0$ and $t < 0$. In particular, this means that $\phi(x=0,t) = \psi_s(x=0,t)$.

By writing (14) as an integral along the real energy axis, $\chi_f(E)$ is shown to be given by the Fourier transform,

$$\chi_f(E) = \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}Et/\hbar} \phi(x=0,t). \tag{15}$$

However, $\phi(x = 0, t) = \psi_s(x = 0, t)$, so that $\chi_f(E) = \chi_s(E)$, and therefore $\psi_s(x, t) = \psi_f(x, t)$ in the spacetime domain D_+ when the boundary condition specified in (7) is satisfied at $x = 0$, and the state is initially localized as indicated above.

Since in many instances the given function is the signal $\psi_s(x = 0, t)$ rather than its Fourier transform, it is also convenient to express (2) as an integral over time in terms of the signal. By inserting (3) and changing the order of integration, we find the appealing expression

$$\psi_s(x,t) = \int_0^t \mathrm{d}t'\, K_+(t,x;t',x'=0)\psi_s(x'=0,t') \tag{16}$$

where the kernel is given by

$$\begin{aligned} K_+(t,x;t',0) &= \frac{1}{h}\int_{-\infty}^{\infty} \mathrm{d}E\, \mathrm{e}^{\mathrm{i}p_+x/\hbar}\mathrm{e}^{\mathrm{i}E(t'-t)/\hbar} \\ &= \frac{1}{hm}\int_L \mathrm{d}p\, p\, \mathrm{e}^{-\mathrm{i}p^2(t-t')/(2m\hbar)}\mathrm{e}^{\mathrm{i}px/\hbar}. \end{aligned} \tag{17}$$

Note that $K_+(t, 0; t', 0) = \delta(t'-t)$. Let us evaluate (17) for $x \geqslant 0$ along the L-shaped contour in the momentum plane. For $(t - t') < 0$ the contour may be closed by a large arc at ∞ in the first quadrant, which does not contribute to the integral. Since no pole is enclosed, the integral is zero. This explains the upper limit t in (16).

For $(t - t') > 0$ the part of the contour in the imaginary axis may be deformed into the negative real axis. This allows the identification of K_+ with the derivative of the ordinary propagator,

$$\begin{aligned} K_+(t,x;t',0) &= \int_{-\infty}^{\infty} \mathrm{d}p\, \frac{p}{hm}\mathrm{e}^{\mathrm{i}p^2(t'-t)/(2m\hbar)}\mathrm{e}^{\mathrm{i}px/\hbar} \\ &= \frac{\hbar}{m\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\langle x|U(t,t')|0\rangle \\ &= \left[\frac{m}{\mathrm{i}h(t-t')^3}\right]^{1/2} x\mathrm{e}^{\mathrm{i}mx^2/2\hbar(t-t')} \qquad (t > t', x \geqslant 0). \end{aligned} \tag{18}$$

A related result was obtained by Allcock on his way to (2) [1], by considering the retarded free propagator. The expression of Allcock associates the source wavefunction to a time integral of the wavefunction *at* the source point times the free propagator, with a double-sided spatial derivative in between. It can be shown that it is equivalent to (16). An analogous relation is also obtained in three dimensions, with similar techniques but rather different objectives, by Mangin-Brinet *et al* [9], relating the wavefunction in one region of spacetime with the convolution over that region of the initial wavefunction with the propagator, plus a surface term with a double-sided gradient.

The relation found between ψ_s and ψ_f, and (12) are the main results of this section. They provide a physical interpretation of the source wavefunction in terms of an initial-value problem when there is free motion after the initial state is released at $t = 0$. Note that the knowledge of the signal $\psi_s(x = 0, t)$, or of its Fourier transform $\chi_s(E)$, allows one to recover the negative momentum part of the initial state $\psi_{iv}(t = 0)$ for the corresponding initial-value problem only insofar as the amplitude $\tilde{\psi}_f(p)$, known in principle along the positive real and imaginary axis, can be analytically continued into the negative real axis.

In this way, the normalizability required of ψ_f (or ψ_{iv}, for that matter), is carried over to ψ_s, which thus acquires the usual meaning of a wavefunction in quantum mechanics, that is, as a probability amplitude. It should be observed that not all functions of the form of (2) can have this meaning: only those that are indeed related to a given ψ_{iv} or ψ_f can be thus understood.

We may now see the origin of the negative energies in ψ_s: the contribution of the evanescent waves in the source solution, (2), is exactly equal to the contribution of negative momenta in the corresponding freely moving wavepacket ψ_f, (8). The change of variable and the shift in the path of integration lead to what could be termed apparent evanescent waves, which, in fact, can be understood as an artefact of the Fourier–Laplace transformation in time. It may be surprising from a classical perspective that such a negative momentum contribution exists at positive times and positions, considering that the wavepacket is entirely localized on the left at $t = 0$. In quantum mechanics, however, the negative momentum (equivalently, evanescent or negative energy) contribution is always present, since $\tilde{\psi}_{f,-}(p)$ is restricted to a half-line in momentum space and therefore $\psi_{f,-}(x)$ is necessarily different from zero from $-\infty$ to $+\infty$ except possibly at a finite number of points. It is true, however, that the influence of $\psi_{f,-}$ at $x > 0$ diminishes with the distance to the origin. This is illustrated in figures 1 and 2, that show the probability densities $|\psi_f(x,t)|^2$ and $|\psi_{f,\pm}(x,t)|^2$ versus x at two different instants. The state is initially (at $t = 0$) the ground state of an infinite well between a and b, $a < b < 0$, and has zero average momentum, $\langle p \rangle = 0$. Its time evolution may be expressed in terms of known functions, by using the results of Moshinsky [10], or, alternatively, Brouard and Muga [11]. Note the long tails of $|\psi_{f,\pm}(x, t = 0)|^2$ beyond $[a, b]$ in figure 1, and the important interference pattern between $\psi_{f,+}$ and $\psi_{f,-}$ in figure 2.

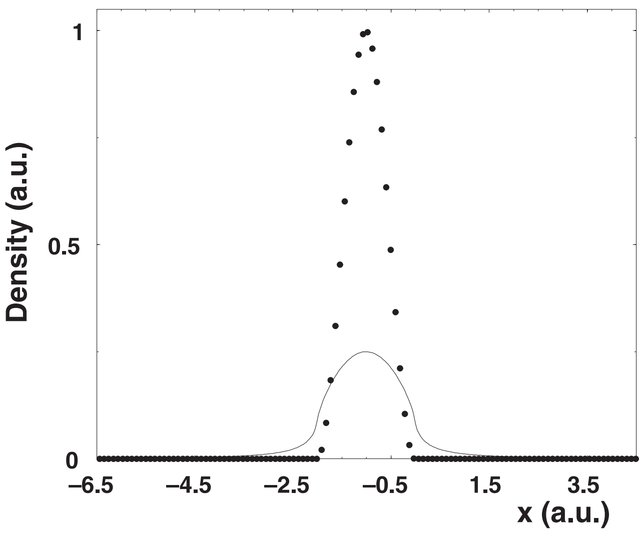

Figure 1. $|\psi_f(x,t)|^2$ (dotted curve), $|\psi_{f,+}(x,t)|^2$ (full curve), and $|\psi_{f,-}(x,t)|^2$ (broken curve, indistinguishable from the full curve) versus x for $t = 0$. The initial state is the ground state of an infinite well between $a = -2.01$ and $b = -0.01$, i.e. $\psi_{iv}(x, t = 0) = \left(\frac{2}{b-a}\right)^{1/2} \sin[(x - a)\pi/(b-a)]$ for $a \leqslant x \leqslant b$. Here and in figure 2, atomic units (au) are used, $m = 1, \hbar = 1$.

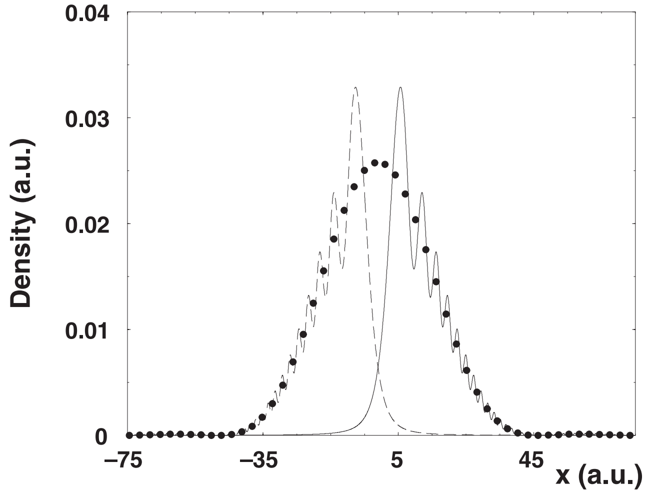

Figure 2. Same as figure 1, but for $t = 10$.

2.2. Generalization for potentials that vanish outside an interval

The above results can be generalized for an arbitrary cut-off potential profile that vanishes outside an interval $[c, d]$, located between the initial state and the source point $x = 0$, i.e. such that $a < b \leqslant c \leqslant d \leqslant 0$. The time evolution of the wave, ψ_b, for $x \geqslant d$ is given by [11, 12]

$$\psi_b(x, t) = \frac{1}{h^{1/2}} \int_\Omega \mathrm{d}p\, \mathrm{e}^{\mathrm{i}px/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} T(p) \tilde{\psi}_b(p) \qquad x \geqslant d \tag{19}$$

(to be compared with (8)), where $T(p)$ is, for $p > 0$, the transmission amplitude, and its analytical continuation elsewhere; similarly to (9), $\tilde{\psi}_b(p) = h^{-1/2} \int_a^b \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar} \psi_b(x, t = 0)$. The contour Ω goes from $-\infty$ to ∞. If there are bound states it passes above the corresponding poles of $T(p)$ in the positive imaginary axis. $T(p)$ is analytical in the upper half-plane except in these points. Moreover, it tends to one as[3] $|p| \to \infty$ [13–15]. This means that the same manipulations done for the free motion wavefunction to write it in the form of ψ_s can now be performed, but instead of $\tilde{\psi}\left[(2mE)^{1/2}\right]$ in (12) one must write $T[(2mE)^{1/2}]\tilde{\psi}\left[(2mE)^{1/2}\right]$ in the more general case. The same arguments that have enabled us to identify ψ_f and ψ_s in D_+ when the boundary condition of (7) is satisfied are now applicable to identify $\psi_s(x, t)$ and $\psi_b(x, t)$ in the same domain when

$$\psi_s(x = 0, t) = \psi_b(x = 0, t)\Theta(t) \tag{20}$$

is imposed as the signal at the source point $x = 0$.

In any case free motion or motion with a localized potential barrier in the full curve do not easily allow one to construct source signals dominated by negative energy components. But these are precisely the signals of interest to study propagation velocities and characteristic times for evanescent conditions [2–8]. The way to construct them and their relation to initial-value problems is through the use of potentials with different asymptotics for positive and negative positions, which are examined in the next subsection. Moreover, the full evolution

[3] The cut-off condition is not strictly necessary for the left-hand edge of the potential. The analyticity of $T(p)$ (except possibly at simple bound state poles on the imaginary axis) and the limit $T(p) \to 1$ as $|p| \to 1$ in the upper half-plane hold for potentials that satisfy $\int_{-\infty}^{\infty} \mathrm{d}x\, (1 + x^2)|V(x)| < \infty$ [13].

of the wavefunction in those cases cannot be reduced to the formulae above, thus requiring further analysis.

2.3. 'Step potentials' with different asymptotic levels

Here we shall show the connection between source wavefunctions and initial-value problems for the simple step potential,

$$V(x) = \Theta(x)V_0 \qquad V_0 > 0 \tag{21}$$

as well as any other cut-off 'step' potentials between c and d, such that $V(x > d) = V_0$ and $V(x < c) = 0$. As before, we assume that the initial state is localized between a and b, with $a < b \leqslant c \leqslant d \leqslant 0$. Following the method used in [11] to write (19), it is possible to write the wavefunction for $x > 0$ as [12]

$$\psi_{step}(x,t) = \frac{1}{h^{1/2}} \int_\Omega \mathrm{d}p\, \mathrm{e}^{-\mathrm{i}Et/\hbar} \mathrm{e}^{\mathrm{i}qx/\hbar} T^l(p) \tilde{\psi}_{step}(p) \tag{22}$$

where $\tilde{\psi}_{step}(p) = h^{-1/2} \int_a^b \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar} \psi_{step}(x, t = 0)$. This is an exact expression, where $E = p^2/2m$, and q, for real p, is given by

$$q = \begin{cases} -(p^2 - p_0^2)^{1/2} & p < -p_0 \\ \mathrm{i}(p_0^2 - p^2)^{1/2} & -p_0 < p < p_0 \\ (p^2 - p_0^2)^{1/2} & p > p_0. \end{cases} \tag{23}$$

Here and in the following p_0 equals $(2mV_0)^{1/2}$. For arbitrary values of p in the complex plane, $q = (p^2 - p_0^2)^{1/2}$ with the understanding that the two branch points at $p = \pm p_0$ are joined by the shortest branch cut, slightly displaced below the real axis. In particular, for a point $p = \mathrm{i}\gamma$ ($\gamma > 0$) the corresponding q is $\mathrm{i}(\gamma^2 + p_0^2)^{1/2}$. $T^l(p)$ is, for $p > p_0$, the transmission amplitude for left incidence, and its analytical continuation elsewhere. As in the previous subsection, the contour Ω goes from $-\infty$ to ∞ passing above the branch cut and possible bound-state poles of $T^l(p)$ on the imaginary axis. The integrand in equation (22) is formally similar to that of equation (19), but note the change in the exponent and the different character of the transmission amplitude.

The integral in (22) may also be written in the q-plane as

$$\psi_{step}(x,t) = \frac{1}{h^{1/2}} \int_{C,L} \mathrm{d}q\, \mathrm{e}^{\mathrm{i}qx/\hbar} \mathrm{e}^{-\mathrm{i}Et/\hbar} \frac{q}{p} T^l(p) \tilde{\psi}_{step}(p) \tag{24}$$

where now $p = (q^2 + p_0^2)^{1/2}$ has two branch points at $q = \pm \mathrm{i}p_0$ joined by a branch cut. The contour C goes from $-\infty$ to $+\infty$, passing above the part of branch cut in the positive imaginary axis and above the poles of $T^l(p)$. (Note that whenever there are bound-state poles they are above the branch point at $q = \mathrm{i}p_0$.) The alternative contour L goes from $\mathrm{i}\infty$ to ∞ in the q-plane, as shown in figure 3.

Finally, we set the zero of energy at the upper level of the potential profile using the change of variable $E' = E - V_0 = q^2/2m$, and define the wave that satisfies the Schrödinger equation for this new level in terms of the wavefunction written for the lower level, $\psi'_{step}(x,t) = \mathrm{e}^{\mathrm{i}V_0 t/\hbar} \psi_{step}(x,t)$,

$$\begin{aligned} \psi'_{step}(x,t) &= \frac{1}{h^{1/2}} \int_L \mathrm{d}q\, \mathrm{e}^{\mathrm{i}qx/\hbar} \mathrm{e}^{-\mathrm{i}E't/\hbar} \frac{q}{p} T^l(p) \tilde{\psi}'_{step}(p) \\ &= \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}E'\, \mathrm{e}^{\mathrm{i}qx/\hbar} \mathrm{e}^{-\mathrm{i}E't/\hbar} \frac{m}{p} T^l(p) \tilde{\psi}'_{step}(p). \end{aligned} \tag{25}$$

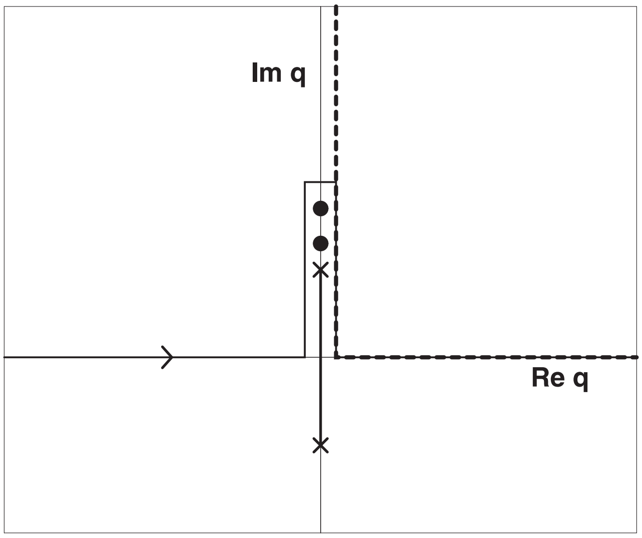

Figure 3. Integration contours C (full line) and L (broken line) in the q-plane. The crosses represent branch points joined by a branch cut. The circles on the imaginary axis are bound states.

We have thus expressed ψ'_{step} in the form of the source wavefunction ψ_s. The same arguments used to find the equality of ψ_f and ψ_s in D_+ may now be applied to identify ψ_s and ψ_{step}. In particular,

$$\chi_s(E') = \frac{m}{p} T^l(p) \tilde{\psi}'_{step}(p) \tag{26}$$

where $p = \left[2m\left(E' + V_0\right)\right]^{1/2}$, when

$$\psi_s(x=0,t) = \psi_{step}(x=0,t)\Theta(t). \tag{27}$$

All the connections made in this section between the momentum amplitude $\tilde{\psi}_f(p)$ and the energy Fourier transform of the source signal at $x = 0$ have required a wavepacket strictly localized between a and b, in order to perform contour deformations. It is intuitively clear, however, that relaxing this condition cannot lead to a completely different behaviour in the relevant energy region, and our numerical tests indicate that the deviations, if any, are to be found in the region of very negative values of E'.

3. Application to the arrival time

Allcock obtained (2) by assuming that (1) was satisfied, and that $V(x) = 0$ for $x > 0$, without any further specification of the potential after the initial state is released [1]. But each experimental set-up will involve a particular potential profile, and we have seen that the interpretation of the source solutions in terms of an initial-value problem depends on the particular potential that determines the dynamics. We shall, in particular, choose the simplest case of free motion to analyse Allcock's objection to the possibility of defining an ideal (apparatus-independent) arrival-time concept in quantum mechanics based on (2). This section is an elaboration of the arguments given in [16].

Allcock's motivation for studying quantum mechanics with sources was the fact that the expression for the wavefunction, (2), involves an integral over energy from $-\infty$ to ∞. This suggested a possible way out of Pauli's argument against the existence of self-adjoint time operators conjugate to a semi-bounded Hamiltonian[4].

The core of Allcock's objection rests on the identification of the total arrival probability at a point $X > 0$, $P(\infty)$, with the total amount of norm to the right of X as $t \to \infty$,

$$P(\infty) \equiv \lim_{t\to\infty} \int_X^\infty \mathrm{d}x\, |\psi_s(x,t)|^2 = \int_0^\infty \mathrm{d}E\, |\langle E|\psi_s\rangle|^2. \tag{28}$$

Here

$$\langle E|\psi_s\rangle \equiv \chi_s(E)(2E/m)^{1/4} \tag{29}$$

where, as before, the branch cut for the fourth root is set at the negative imaginary axis. For free motion the second equality in (28) is to be expected since $\langle E|\psi_s\rangle(2E/m)^{1/4}$, with $E > 0$, is nothing but the amplitude for positive momentum p, so that we recover from (28) the known result

$$\lim_{t\to\infty} \int_X^\infty \mathrm{d}x\, |\psi_s(x,t)|^2 = \int_0^\infty \mathrm{d}p\, |\tilde{\psi}_f(p)|^2. \tag{30}$$

Using two other independent routes Allcock arrives at integral expressions for a hypothetical total arrival time probability in contradiction with (28) because they have contributions from $E < 0$; the simplest one is $\int_{-\infty}^{\infty} \mathrm{d}E\, |\langle E|\psi_s\rangle|^2$. He therefore concludes '*unequivocally that an ideal concept of arrival time cannot be established for the problem with sources* $(-\infty < E < \infty)$'. In the light of the identification between $\psi_s(x,t)$ and $\psi_f(x,t)$ in D_+ made in section 2, the flaw in Allcock's argument is that he is overlooking the contribution of negative momenta. According to classical prejudice one would not expect that negative momenta play any role for $t > 0$ at $X > 0$, if the initial state is confined within the left half-line. But quantum mechanics works otherwise, as figures 1 and 2 clearly show. Since the negative energy part of $\psi_s(x,t)$ is equal to $\psi_{f,-}(x,t)$, we may equivalently think of the contribution of the negative momenta to a time-of-arrival probability in terms of evanescent waves. The negative energy components penetrate the positive coordinate region for some time before finally abandoning it. But Allcock's definition of $P(\infty)$ disregards this contribution entirely. Note that our criticism of the validity of $P(\infty)$ is rather independent of the theory chosen for defining an arrival time distribution. However, we cannot fail to point out that the equality between ψ_s and ψ_f in the spacetime domain D_+ immediately allows one to associate Kijowski's distribution Π_K [16, 21] to the source problem for free motion. This arrival time distribution has been discussed extensively elsewhere [22–24]. Similarly, for a general potential profile the generalization of Π_K proposed in [23] is applicable.

4. Discussion

The physical meaning of source boundary conditions used for the one-dimensional, time-dependent, single-particle Schrödinger equation has been clarified by showing the equivalence of the corresponding solution ψ_s, see (2), with standard initial-value problems for positive times and positions. We have first shown the connection between (2) and the ordinary initial-value-problem integral expression for a free motion wavepacket, and then have extended this result for other potential profiles, in particular for the step barriers, which allow one to inject waves dominated by evanescent energies into the right half-line.

[4] In fact, Pauli's argument is not as fierce as it seems. Apart from the technical flaws emphasized by Galapon [17, 18], time observables may be associated with positive operator-valued measures (POVMs), without requiring that the first moment operator of the POVM be self-adjoint [16], see also [19, 20].

Each of the potential profiles may correspond to a different experimental arrangement. Depending on the potential the origin of the evanescent waves in the source solution may be traced back to either negative momentum components (which are present in all cases, and become the only source of negative energies for free motion), or 'true' evanescent components, namely energy components which are already negative in the associated initial-value problem, relative to the region of positive x. This occurs in the step potentials, for example, where positive momenta with respect to the lower level become imaginary momenta in the upper level region. In addition to scattering contributions to the negative energies, we have also allowed for the possibility of bound state contributions, that may become important if the initial state overlaps with the normalized eigenstates of the Hamiltonian.

Apart from elucidating the physical content of previous works that have made use of source boundary conditions, our results have also served to analyse critically Allcock's negative statements about the possibility to define an ideal probability distribution of time of arrival for quantum waves with sources. We argue that Allcock's postulated expression for a total arrival probability is flawed since it ignores the quantum contribution of negative momenta at positive positions and times.

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