Scattering theory from microscopic first principles

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Abstract

We sketch a derivation of abstract scattering theory from the microscopic first principles defined by Bohmian mechanics. We emphasize the importance of the flux-across-surfaces theorem for the derivation, and of randomness in the impact parameter of the initial wave function—even for an, inevitably inadequate, orthodox derivation.

[1] Dedicated to Joel Lebowitz, with love and admiration, for his 70th birthday. Supported in part by the DFG, by NSF Grant No. DMS95–04556, and by the INFN.

1 Introduction

Abstract scattering theory, or the S-matrix formalism, can be regarded as a phenomenological description analogous to thermodynamics. And like thermodynamics, it should be derivable from microscopic first principles. It is somewhat surprising that while this was done long ago for thermodynamics, by Boltzmann and Gibbs using the methods of statistical mechanics, it has not yet been achieved for quantum scattering theory.

We believe there are two main sources of difficulty: (1) failure to pay sufficiently careful attention to the experimental conditions in scattering phenomena, and in particular to the fact that randomness in the initial wave function is an experimental reality that is crucial to an understanding of the emergence of the textbook formula for the differential cross section, involving the absolute square of the momentum matrix elements of the T-matrix; and (2) failure to pay sufficiently careful attention to precisely which microscopic first principles the derivation could conceivably be based upon.

We shall argue that while orthodox quantum theory is not up to the job, Bohmian mechanics is, and we shall sketch the derivation. Since scattering theory is at the heart of the experimental evidence for quantum theory, we believe that understanding how the formulas of scattering theory emerge from microscopic first principles should be of general interest.

2 The S-matrix

The basic formula of abstract scattering theory concerns the probability of finding a system in the *free state* g asymptotically in the future given that it was in the *free state* f asymptotically in the past. This is expressed in terms of the basic object of scattering theory, the scattering operator S, usually called the S-matrix. The probability $P(f \to g)$ for scattering from state f to state g is given by

$$P(f \to g) = |\langle g, Sf \rangle|^2 , \tag{1}$$

where f and g are members of some Hilbert space $\mathcal{H}$, the space of *free* states, with inner product $\langle \cdot, \cdot \rangle$.

This formula is often considered very appealing since it makes no reference to space-time processes, but directly relates experimental procedures: "preparation" in the distant past to "measurement" in the distant future. From (1) one computes, via formal manipulations, values for the experimentally relevant cross section, an issue which we shall take up in Section 4.

We first review how expression (1) is understood in mathematical physics as emerging from Hamiltonian quantum mechanics.

3 The Schrödinger evolution and the S-matrix

We shall be concerned here with the scattering of a single spinless quantum particle off of a "target," or, what amounts mathematically to more or less the same thing, of a pair of spinless particles off of each other. [2] We thus begin our analysis with the non-relativistic quantum mechanics for a single spinless particle in an external potential V.

The state of the system at time t is given by its wave function $\psi_t \in L^2(\mathbb{R}^3)$, which evolves according to Schrödinger's equation

$$\mathrm{i}\frac{\partial \psi_t}{\partial t} = H\psi_t\,, \tag{2}$$

where $H = H_0 + V$ with $H_0 = -\frac{1}{2}\Delta$ (in units for which $\hbar = 1$ and $m = 1$). A solution ψ_t is determined by a choice of the initial condition $\psi = \psi_0$ at time $t = 0$,

$$\psi_t = \mathrm{e}^{-\mathrm{i}Ht}\psi_0\,. \tag{3}$$

If the scattering potential V decays sufficiently rapidly at spatial infinity, one expects scattering states, i.e., states that eventually leave the influence of the potential, to evolve for large positive times according to the free dynamics given by H_0, i.e., that the motion is asymptotically free. In the following definition this free motion, defining the asymptotics, is invoked. We demand that for every scattering state ψ there exists a state ψ_{out} such that

$$\lim_{t\to\infty} \|\mathrm{e}^{-\mathrm{i}Ht}\psi - \mathrm{e}^{-\mathrm{i}H_0 t}\psi_{\text{out}}\| = 0\,. \tag{4}$$

[2] Recall that the scattering of two particles interacting via a translation invariant pair potential can be reduced to potential scattering of one particle by a change of variables to relative and center-of-mass coordinates. However, in quantum mechanics this is not as trivial as in classical mechanics, since one also must assume for this that the wave function is a product wave function in the new coordinates. This will not be the case in general, but one can easily convince oneself that this condition is satisfied, for example, in the case of two particles both described by plane waves.

Thus, one is interested in the existence and the range of the wave operator

$$\Omega_+ := \lim_{t\to\infty} \mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0 t}\,, \tag{5}$$

where the limit is in the strong sense. If the wave operator exists,[3] every state in its range eventually moves freely in the sense of (4), since Ω_+ maps every "free state" ψ_{out} to the corresponding "scattering state" ψ. One can repeat these considerations for the behavior of wave functions in the distant past and define analogously the wave operator

$$\Omega_- := \lim_{t\to-\infty} \mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0 t}\,. \tag{6}$$

It is well known and not difficult to see that the wave operators exist for short-range potentials.[4]

Whenever the wave operators exist, they obey the intertwining relations, which follow from a simple calculation:

$$\mathrm{e}^{-\mathrm{i}Ht}\Omega_\pm = \Omega_\pm \mathrm{e}^{-\mathrm{i}H_0 t}\,. \tag{7}$$

And thus, on the domain $D(H_0)$ of H_0, we have by differentiation

$$H\Omega_\pm = \Omega_\pm H_0\,. \tag{8}$$

As a consequence of this relation and the fact that $\Omega_\pm$ are partial isometries (i.e., that they act unitarily from their domain to their ranges $\mathrm{Ran}(\Omega_\pm)$) one concludes that the restrictions of H to $\mathrm{Ran}(\Omega_\pm)$ are unitarily equivalent to H_0. As such, they have the same spectrum, and we may conclude that $\mathrm{Ran}(\Omega_\pm) \subset \mathcal{H}_{\mathrm{ac}}(H)$, the absolutely continuous subspace of H, the set of all states having an absolutely continuous spectral measure for$H$. Thus scattering states are very much related to spectral theory.

[3] Note that it might appear physically natural to define the wave operator as the inverse of Ω_+, i.e., as the map from scattering states ψ to the corresponding future asymptotic states ψ_{out}. However, one does not know a priori which states are scattering states. Thus the domain of definition of that operator would be far from clear! In fact, the goal of the mathematical physics of scattering theory is precisely to clarify such issues. With the definition (5), this question is shifted to that of the range of Ω_+.

[4] Short-range potentials basically decay, as $x \to \infty$, like $|x|^{-1-\epsilon}$ for some $\epsilon > 0$. In the case of long-range potentials one must use, instead of $\mathrm{e}^{-\mathrm{i}H_0 t}$, a modified free dynamics to define the wave operators.

As we remarked in footnote 3, the task of determining the range of the wave operators is less simple. It was one of the main preoccupations of mathematical scattering theory for several decades. From a physical point of view one might expect that every state orthogonal to all bound states eventually leaves the influence of the potential and moves freely, and hence is in the range of the wave operators. Since the set of bound states of H is $\mathcal{H}_{\mathrm{pp}}(H)$, the spectral subspace of H spanned by its eigenvectors, this is mathematically expressed by

$$\mathrm{Ran}(\Omega_\pm) = \mathcal{H}_{\mathrm{cont}}(H)\,, \tag{9}$$

where $\mathcal{H} = \mathcal{H}_{\mathrm{pp}}(H) \oplus \mathcal{H}_{\mathrm{cont}}(H)$. Wave operators (and the corresponding Hamiltonians H) satisfying (9) are called *asymptotically complete*. When H is asymptotically complete the set of scattering states is precisely $\mathcal{H}_{\mathrm{cont}}$. Asymptotic completeness has been established for many different systems, including many-particle systems (see, e.g., [15,9,24] and the references therein).

The continuous part of the spectrum can in general be separated into two parts, the absolutely continuous part, supporting spectral measures absolutely continuous with respect to Lebesgue measure, and the singular continuous part, supporting singular continuous spectral measures. With what we already know from the existence of the wave operators, we may conclude that a Hamiltonian which is asymptotically complete has no singular continuous spectrum.

Assuming asymptotic completeness, as we shall for the rest of this paper, we turn to the standard description of the scattering experiment. A scattering state is a solution of (3) with $\psi \in \mathcal{H}_{\mathrm{ac}}$ and with $t = 0$ any time between preparation and detection. The preparation is done at a very large negative time and the detection at a very large positive time. The scattering state is expressed in terms of its asymptotic in-state $\psi_{\mathrm{in}} := \Omega_-^{-1}\psi$ $(= f)$, which is mapped by the scattering operator S to the asymptotic out-state $\psi_{\mathrm{out}} := \Omega_+^{-1}\psi = S\psi_{\mathrm{in}}$, so that

$$S := \Omega_+^{-1}\Omega_-\,. \tag{10}$$

Since $\Omega_- : L^2(\mathbb{R}^3) \to \mathcal{H}_{\mathrm{ac}}(H)$ and $\Omega_+^{-1} : \mathcal{H}_{\mathrm{ac}}(H) \to L^2(\mathbb{R}^3)$, the scattering operator S is well defined. In view of (4), the scattering state at the time of detection is close to ψ_{out} evolved forward in time via the free evolution and at the time of preparation it is close to ψ_{in} evolved backwards in time.

4 The scattering cross section and the scattering process

Textbook scattering theory is primarily concerned with transitions between plane waves, states of well defined momentum, and this also seems to be of primary interest to experimentalists. Roughly speaking, one tries to apply equation (1) with f and g momentum eigenstates. For a variety of reasons, this leads to many difficulties, some associated with the outgoing state (or the out-process) and some with the incoming state (the in-process). The treatment of outgoing plane waves is superficially straightforward from an orthodox perspective, and we shall focus in this section primarily on coping with the in-process. Later, in Sections 6–8, we shall argue that even with regard to the out-process, things are not as straightforward as they seem, that the framework of orthodox quantum theory does not, in fact, provide an adequate microscopic basis for scattering theory, and that Bohmian mechanics does.

Probabilities for transitions to plane waves correspond to the statistics for the results of a final momentum measurement. In abstract scattering theory, the scattering cross section is calculated as the probability that the momentum of the asymptotic state in the far future lies in the cone $C_\Sigma := \{k \in \mathbb{R}^3 : k/|k| \in \Sigma\}$, $\Sigma \subset S^2$, the unit sphere in $\mathbb{R}^3$. We shall assume that Σ is closed. According to the standard measurement formalism one integrates the modulus square of the Fourier transform of the state at the time of measurement (the momentum distribution) over the cone C_Σ. Since the state at a large time τ is approximately $\mathrm{e}^{-\mathrm{i}H_0\tau}S\psi_{\mathrm{in}}$ and the momentum is preserved by the free evolution, the relevant probability density is $|\langle k|S\psi_{\mathrm{in}}\rangle|^2 = |\widehat{S\psi_{\mathrm{in}}}(k)|^2$. Thus the scattering cross section is given, independently of τ, by

$$\sigma^\psi(\Sigma) := \int\limits_{C_\Sigma} |\widehat{\Omega_+^{-1}\psi}(k)|^2 \, \mathrm{d}^3k = \int\limits_{C_\Sigma} |\widehat{S\psi_{\mathrm{in}}}(k)|^2 \, \mathrm{d}^3k \tag{11}$$

for any scattering state ψ. This is the central formula of scattering theory.

Since in scattering theory one is interested in the *changes* that occur during the scattering process, it is convenient to replace S in (11) by $T := S - I$. We thus define

$$\sigma_T^\psi(\Sigma) := \int\limits_{C_\Sigma} \left|\widehat{T\psi}_{\mathrm{in}}(k)\right|^2 \mathrm{d}^3k \,. \tag{12}$$

For the case in which ψ_{in} is an (approximate) plane wave, σ_T corresponds to the genuine scattering events, in which a change in direction is detected; because most of the plane wave will never overlap the scattering region, these occur only rarely in this case. A (heuristically) straightforward computation yields that T is an integral operator with kernel $-2\pi\mathrm{i}\delta(k^2/2 - k'^2/2)T(k,k')$, so that

$$\widehat{T\psi}_{\mathrm{in}}(k) = -2\pi\mathrm{i} \int\limits_{|k'|=|k|} T(k,k')\widehat{\psi}_{\mathrm{in}}(k')|k'|\mathrm{d}\Omega(k') \tag{13}$$

We turn now to the in-process, the treatment of incoming plane waves. If we substitute a plane wave for ψ_{in} in (12), we obtain an infinite quantity, proportional to $\delta(0)$. This is not terribly astonishing since a plane wave is nonnormalizable and nonphysical. A plane wave is not a possible quantum state for a single particle. Rather, a plane wave is often regarded as describing a spatially homogeneous beam of particles.

Moreover, it is with a prepared beam of particles, of approximate momentum k_0, approximately spatially homogeneous prior to its reaching the scattering region, that real-world scattering experiments are mainly concerned. And the quantity of primary physical interest is such experiments is the differential cross section $\sigma_{\mathrm{diff}}^{k_0}(\Sigma)$, describing the rate at which particles are scattered into (i.e., measured in) the solid angle Σ when the beam has unit current (one particle per unit of time per unit of cross section area perpendicular to the beam).

The infinite quantity obtained from (12) by setting $\psi_{\mathrm{in}} \sim \mathrm{e}^{\mathrm{i}k_0\cdot x}$ must be suitably normalized to obtain the differential cross section. A theoretical physics type argument in which this is done can be found in [5,19]. Very loosely speaking, it is argued that by dividing with the quantum flux of the plane wave through a unit area integrated over all time, another infinite quantity, one cancels the $\delta(0)$ factor. It is claimed that the computation yields

$$\sigma_{\mathrm{diff}}^{k_0}(\Sigma) = 16\pi^4 \int\limits_{\Sigma} |T(\omega|k_0|, k_0)|^2 \,\mathrm{d}\Omega\,. \tag{14}$$

This formula—which is also suggested by naive scattering theory, see Section 5—is, as we shall argue, correct. But the argument in [5,19] is, too say the least, somewhat obscure. Moreover, even if it were in a sense crystal clear, it could not, as we shall also explain, be regarded as providing a derivation of (14) from microscopic first principles.

The point is that to the extent that the individual quantum particles in a beam have a wave function at all, that wave function must be normalizable, i.e., an element of the Hilbert space, and cannot be a plane wave. [5] Rather, the

[5] If the particles were in an entangled state, for example because of symmetry, then the individual particles would not described by a wave function at all. We shall assume here that we are dealing with situations for which this possibility can

particles in our homogeneous beam should be regarded as being, initially, at time $-\tau$, in approximate momentum eigenstates, described by wave functions $\psi_{-\tau}$ whose Fourier transform is supported in a small neighborhood of k_0, $|\widehat{\psi}_{-\tau}(k)|^2 \approx \delta(k-k_0)$. We must thus consider the limit in which the prepared wave functions, while remaining normalized, achieves zero momentum spread: $|\widehat{\psi}_{-\tau}(k)|^2 \to \delta(k-k_0)$.

The simplest way to model such a homogeneous beam is as follows: We consider as input a spatially homogeneous collection of particles, statistically and quantum mechanically independent and noninteracting (with each other), moving with momentum $\approx k_0$, where all particles have at preparation wave functions identical up to translation: the prepared wave functions are translates of a common wave function ϕ with $|\widehat{\phi}(k)|^2 \approx \delta(k-k_0)$. In such a beam the "centers" of the prepared wave functions are independently and uniformly distributed in a plane perpendicular to k_0, far from the scattering region and on the incoming side. More precisely, we model the beam by a Poisson system of points (y,t) corresponding to wave functions which are prepared at a rate uniform in time and with centers y uniformly distributed in a two dimensional plane $\Gamma_L = \{-L\frac{k_0}{|k_0|} + a \,|\, a \perp k_0\}$. The point (y,t) corresponds to a particle whose wave function at time t $(= -\tau)$ is ϕ_y, where the subscript indicates translation: ϕ_y is the translation of ϕ by y. If, as we shall assume, the Poisson system has unit density or intensity, then the beam it describes has unit current.

Since each particle (y,t) in the beam scatters into Σ with probability given by (12) with ψ_{in} replaced by ψ_{in}^y, the in-state corresponding to ϕ_y, [6] it follows that the rate at which the particles of the beam scatter into Σ is given by the integral of this over the plane Γ_L. Since in the limit $|\widehat{\phi}(k)|^2 \to \delta(k-k_0)$ the ϕ_y's will spread over the scattering region, we must first perform the limit $L \to \infty$. We thus obtain as the quantity that should yield the theoretical differential cross section

$$\sigma_{\text{diff}}^{k_0}(\Sigma) = \lim_{|\widehat{\phi}(k)|^2 \to \delta(k-k_0)} \lim_{L\to\infty} \int_{C_\Sigma} \int_{y\in\Gamma_L} \left|\widehat{T\psi_{\text{in}}^y}(k)\right|^2 \mathrm{d}^2 y \, \mathrm{d}^3 k \,, \tag{15}$$

be ignored.

[6] More precisely, $\psi_{\text{in}}^y = \Omega_-^{-1}\phi_y$, the in-state corresponding to $(y,0)$. Clearly, by time-translation invariance, the scattering probability is independent of t. This corresponds to the fact that the in-state associated with (y,t) is $e^{-iH_0 t}\psi_{\text{in}}^y$; the outgoing momentum distribution corresponding to (y,t) is thus independent of t, since the free evolution commutes with S.

or, somewhat more explicitly,

$$\sigma^{k_0}_{\text{diff}}(\Sigma) = \lim_{|\widehat{\phi}(k)|^2 \Rightarrow \delta(k-k_0)} \lim_{L\to\infty} \int_{C_\Sigma} \int_{y\in\Gamma_L} \left|\widehat{\Omega_+^{-1}\phi_y}(k)\right|^2 \mathrm{d}^2y\,\mathrm{d}^3k\,, \tag{16}$$

provided $k_0 \notin C_\Sigma$.[7] The $\Rightarrow$ in (16) means that the limit is such that $\widehat{\phi}(k)$ is *strictly* supported on a neighborhood of k_0 that shrinks to k_0 (which is perhaps unrealistic as an assumption on the prepared state). (15) and (16) need not agree, even for $k_0 \notin C_\Sigma$, if the first limit in (16) were understood as allowing a tail on $\widehat{\phi}(k)$. This is because the unscattered tail of $\widehat{\phi}(k)$ could contribute as much to scattering into C_Σ as genuine scattering from near k_0. Such pathological events correspond to situations in which the particle would typically not be aimed at the target and in fact would not be detected at all. The use of T in (15), and $\Rightarrow$ in (16), has the desirable effect of not counting such events.

It is shown by Amrein, Jauch, and Sinha [1] that

$$\lim_{|\widehat{\psi}_{\text{in}}(k)|^2\to\delta(k-k_0)} \int_{C_\Sigma}\int_{y\in\Gamma_L} \left|\widehat{T\psi_{\text{in},y}}(k)\right|^2 \mathrm{d}^2y\,\mathrm{d}^3k = 16\pi^4 \int_\Sigma |T(\omega|k_0|,k_0)|^2\,\mathrm{d}\Omega\,. \tag{17}$$

They compute

$$\begin{aligned}\int_{a\perp k_0} \left|\widehat{T\psi_{\text{in},a}}(k)\right|^2 \mathrm{d}^2a &= 4\pi^2 \int_{a\perp k_0} \left| \int_{|k'|=|k|} T(k,k')\mathrm{e}^{\mathrm{i}a\cdot k'}\widehat{\psi}_{\text{in}}(k')|k'|\mathrm{d}\Omega' \right|^2 \mathrm{d}^2a \\ &= 16\pi^4 \int_{|k'|=|k|} (\cos\theta')^{-1}\,|T(k,k')|^2 \left|\widehat{\psi}_{\text{in}}(k')\right|^2 \mathrm{d}\Omega'\,, \end{aligned} \tag{18}$$

where θ' is the angle between k_0 and k'. For the second equality one uses that the a-integration over $\mathrm{e}^{\mathrm{i}a\cdot(k'-k'')}$ produces $(2\pi)^2\delta(k'_\perp - k''_\perp)$, $k_\perp$ being the projection of k on the plane perpendicular to k_0. This in turn yields effectively a $\delta(\omega' - \omega'')$ if one assumes that $\widehat{\psi}_{\text{in}}$ is supported in a neighborhood of k_0 that is contained in the half space $P_{k_0} := \{k \in \mathbb{R}^3 : k\cdot k_0 \geq 0\}$. Then in the limit $|\widehat{\psi}_{\text{in}}(k)|^2 \to \delta(k-k_0)$ the r.h.s. of (18) becomes $16\pi^4\,|T(k,k_0)|^2\,\delta(|k|-|k_0|)$, and integrating this over C_Σ yields (17). (It is clear from the right hand side of (18) that (18) is invariant under translations of ψ_{in}, so that (17) is independent of L.)

[7] If V has bound states, ϕ_y typically will not be in $\mathcal{H}_{\text{ac}}$. In this case, ϕ_y in (16) should be replaced by $P_{\mathcal{H}_{\text{ac}}}\phi_y$ and ψ^y_{in} in (15) by $\Omega_-^{-1}P_{\mathcal{H}_{\text{ac}}}\phi_y$. The analysis sketched here would then have to be replaced by a somewhat more complicated one. We ignore this possibility here.

Writing for $\Omega_+^{-1}\phi_y$ in (16)

$$\Omega_+^{-1}\phi_y = S\phi_y + \Omega_+^{-1}\phi_y - \Omega_+^{-1}\Omega_-\phi_y = T\phi_y + \phi_y + \Omega_+^{-1}(\phi_y - \Omega_-\phi_y) \quad (19)$$

we see that (14) then follows from the condition

$$\lim_{L\to\infty} \int\limits_{y\in\Gamma_L} \|T(\phi_y - \Omega_-^{-1}\phi_y)\|^2 \, \mathrm{d}^2 y = 0, \quad (20)$$

which is presumably typically satisfied, although we are aware of no proof of this. With (20), we need only invoke (17) with $\psi_{\mathrm{in}} = \phi$.

We remark that (20) is considerably weaker than the simpler-looking sufficient condition $\lim_{L\to\infty} \int_{y\in\Gamma_L} \|\Omega_-\phi_y - \phi_y\|^2 \, \mathrm{d}^2 y = 0$: The application of T may drastically diminish $\phi_y - \Omega_-^{-1}\phi_y$. To appreciate this, note that as $L \to \infty$, $T\psi_{\mathrm{in}}^y$ itself becomes very small. As you translate ϕ away from the scattering region, it has further to go before it gets there. Thus, since wave functions spread under the (free) time evolution, in all directions, when the wave function begins very far away, it develops a large lateral spread by the time the scattering region is approached and hence, since the scattering region is more or less localized, most of the wave function does not scatter. We note also that it is shown in [27] that for a quite general class of short-range potentials $\lim_{L\to\infty} \|\Omega_-\phi_y - \phi_y\| = 0$ if $|\widehat{\phi}(k)|^2 \approx \delta(k - k_0)$. [8]

We wish to emphasize that the integration over the impact parameter, i.e., over y, is crucial not merely for the proof of (14) but for the result itself. If all of the particles in the beam had the very same initial wave function ϕ_L, the total cross section—the integral of the differential cross section over S^2—would then depend on detailed geometrical characteristics of ϕ_L such as the impact parameter and the distance L to the target. Even if ϕ_L were an approximate plane wave, with more or less constant modulus over most of its support, by the time it had approached the target it would have developed a slowly varying profile whose spread and whose position relative to the target would be crucial for the total cross section. Experimenters don't have to worry much about such details because they work with homogeneous beams having a random impact parameter.

[8] More generally, it is shown [27] that this result holds whenever ϕ is such that $\widehat{\phi}$ is supported in the half space P_{k_0}. The proof of this is very similar to the proof of the well known fact that the analogous result holds for $\psi_L := \mathrm{e}^{\mathrm{i}LH_0}\psi$, i.e., when one moves the state sufficiently far backwards in time according to the free time evolution (see, e.g., [22]).

5 Naive scattering theory and the naive cross section

The formula (12) is not very concrete. How does one actually compute T? Using heuristic stationary methods, this was first done by Max Born [7] in the first paper on quantum mechanical scattering theory, in which also the statistical law $\rho = |\psi|^2$ first appeared! We shall review here how "stationary scattering theory" can be exploited to rigorously obtain a formula for T linking the stationary and the time-dependent methods.

Consider solutions ψ of the stationary Schrödinger equation with the asymptotics

$$\psi(x) \approx \mathrm{e}^{\mathrm{i}k_0\cdot x} + f^{k_0}(\omega)\frac{\mathrm{e}^{\mathrm{i}|k_0||x|}}{|x|} \quad \text{for } |x| \text{ large}\,. \tag{21}$$

In naive scattering theory (cf., e.g., Notes to Chapter XI.6 in [23]) the first term is regarded as representing an incoming plane wave and the second the outgoing scattered wave with angle-dependent amplitude.

Such wave functions can be obtained as solutions of the Lippmann-Schwinger equation

$$\psi(x,k) = \mathrm{e}^{\mathrm{i}k\cdot x} - \frac{1}{2\pi}\int \frac{\mathrm{e}^{\mathrm{i}|k||x-y|}}{|x-y|}V(y)\psi(y,k)\,\mathrm{d}^3y\,. \tag{22}$$

These solutions form a complete set, in the sense that an expansion in terms of these generalized eigenfunctions, a so-called generalized Fourier transformation, diagonalizes the continuous spectral part of H. (In fact from the intertwining relation (8) one sees that $\psi(x,k) = \langle x|\Omega_-|k\rangle$.) Hence the T-matrix can be expressed in terms of generalized eigenfunctions and one finds (cf. [23]) that

$$T(k,k') = (2\pi)^{-3}\int \mathrm{e}^{-\mathrm{i}k\cdot x}V(x)\psi(x,k')\,\mathrm{d}^3x\,. \tag{23}$$

Thus the iterative solution of (22) yields a perturbative expansion for T, called the Born series.

Moreover, comparing (21) and (22), expanding the right hand side of (22) in powers of $|x|^{-1}$, we see from the leading term that

$$f^{k_0}(\omega) = -(2\pi)^{-1}\int \mathrm{e}^{-\mathrm{i}|k_0|\omega\cdot y}V(y)\psi(y,k_0)\,\mathrm{d}^3y\,.$$

Thus $f^{k_0}(\omega) = -4\pi^2 T(\omega|k_0|, k_0)$.

In naive scattering theory, $f^{k_0}(\omega)$ is called the scattering amplitude: One simply uses the stationary solutions of Schrödinger's equation with the asymptotic behavior (21) to obtain the cross section from the quantum probability flux through Σ generated by the scattered wave, suggesting the identification of the differential cross section with

$$\sigma^{k_0}_{\text{naive}}(\Sigma) := \int_{\Sigma} |f^{k_0}(\omega)|^2 \, \mathrm{d}\Omega \,, \tag{24}$$

in agreement with the result (14) sketched in the previous section. However, such a heuristic derivation of the formula (24) for the differential cross section, based solely on the stationary picture, is unconvincing—even for physicists.

One can try to extract the time dependent picture from the stationary one by constructing wave packets from the generalized eigenfunctions $\psi(x,k)$; see [23]. Stationary phase ideas then suggest the development over time of a transmitted and a scattered wave, corresponding to the two terms in (21). However, unless the impact parameter is randomized, their relative sizes—and hence the total cross section—will depend upon delicate cancellations contingent upon detailed geometrical considerations, as indicated already at the end of Section 4.

6 Scattering into cones: the cone cross section

The analysis in Section 4 is based on the formula (11) for the scattering cross section, which is obtained by applying Born's statistical law to momentum measurements in the distant future. But what does the setup for scattering experiments, involving detectors covering certain solid angles, have to do with the measurement of momentum? After all, not every measurement is a momentum measurement. And in scattering experiments each particle is ultimately detected at fairly definite (though random) location—that of the detector that fires—after which the state of the particle can hardly be regarded as a global plane wave, which is what momentum measurements might reasonably be expected to produce. If it is, in fact, appropriate to regard the final detection in a scattering experiment as a measurement of momentum, it cannot be a priori that this is so. Rather this must be justified by a quantum mechanical analysis that takes the relevant experimental details into account.

These experimental details, involving detectors that locate particles at a distant time in a given solid angle, suggest that the *cone cross section*

$$\sigma^{\psi}_{\text{cone}}(\Sigma) := \lim_{t\to\infty} \int_{C_\Sigma} |\psi_t(x)|^2 \, \mathrm{d}^3 x \,, \tag{25}$$

the asymptotic probability of finding the particle in the cone C_Σ,[9] is the more fundamental definition of scattering cross section, more directly connected with what is measured in a scattering experiment, and from which other formulas for the cross section, such as (11), must be derived. This was accomplished by Dollard [12] (see also [23, p. 356] and [16]), whose scattering-into-cones theorem

$$\lim_{t\to\infty}\int_{C_\Sigma} |\psi_t(x)|^2\, \mathrm{d}^3x = \int_{C_\Sigma} |\widehat{\Omega_+^{-1}\psi}(k)|^2\, \mathrm{d}^3k \tag{26}$$

says that $\sigma^\psi_{\text{cone}} = \sigma^\psi$—that the cone cross section is given by the simpler, more standard, though less fundamental object (11).

7 The flux cross section and the flux across surfaces theorem

It is widely believed that the cone cross section (25) more or less directly conveys the statistics—the relative frequency of detector firings—for the results of a scattering experiment. But in a scattering experiment does one actually determine whether the particle is in the cone C_Σ at some large fixed time? Rather, is it not the case that one of a collection of distant detectors, surrounding the scattering center at a fairly definite distance, fires at some random time, a time that is not chosen by the experimenter? And isn't that random time simply the time at which, roughly speaking, the particle crosses the surface of the detector or detectors subtended by the cone?

What a scattering experiment is fundamentally concerned with is not scattering into cones but flux across surfaces. Thus the quantum flux $j^{\psi_t} = \mathrm{Im}\psi_t^*\nabla\psi_t$, the probability current for the probability density $\rho_t(x) = |\psi_t(x)|^2$ in the quantum continuity equation

$$\frac{\partial\rho_t}{\partial t} + \mathrm{div} j^{\psi_t} = 0\,, \tag{27}$$

should play a fundamental role in scattering theory. It is hard to resist the suggestion that the quantum flux integrated over a surface gives the probability that the particle crosses that surface, i.e., that

$$j^{\psi_t}\cdot \mathrm{d}A\mathrm{d}t \tag{28}$$

is the probability that a particle crosses the surface element $\mathrm{d}A$ in the time $\mathrm{d}t$. This suggestion must be taken "cum grano salis" since $j^{\psi_t}\cdot \mathrm{d}A\mathrm{d}t$ may

[9] Note that C_Σ in (25) is the cone in position space spanned by Σ.

somewhere be negative, in which case it can't be a probability. However, in the scattering regime, the regime we are interested in, this quantity is presumably positive far away from the scattering center when $\mathrm{d}A$ is oriented outwards.

Hence, if the detectors are sufficiently distant from the scattering center the flux will typically be outgoing and (28) will be positive, [10] so that it appears natural to identify the probability that the particle crosses some distant surface during some time interval, with the integral of (28) over that time interval and that surface. With this identification, the integrated flux provides us with a physically fundamental definition of the cross section:

$$\sigma_{\text{flux}}^{\psi}(\Sigma) := \lim_{R\to\infty} \int_0^{\infty} \mathrm{d}t \int_{R\Sigma} j^{\psi_t} \cdot \mathrm{d}A\,, \tag{29}$$

where $R\Sigma$ is the intersection of the cone C_Σ with the sphere of radius R. And a derivation of the formula (11) from microscopic first principles then amounts to a proof of the *flux-across-surfaces theorem*:

$$\lim_{R\to\infty} \int_0^{\infty} \mathrm{d}t \int_{R\Sigma} j^{\psi_t} \cdot \mathrm{d}A = \int_{C_\Sigma} |\widehat{\Omega_+^{-1}\psi}(k)|^2 \, \mathrm{d}^3 k\,. \tag{30}$$

The fundamental importance of the flux-across-surfaces theorem was first recognized by Combes, Newton and Shtokhamer [8]. The first proof of the free flux-across-surfaces theorem, i.e., for $V = 0$, was given in [10]; a simplified version of the proof can be found in [14,27]. For proofs of the flux-across-surfaces theorem for various classes of short and long range potentials and under a variety of conditions on the wave function, see [3,2,26]. (For more details on the proofs, we refer the reader to the last section of this paper.)

Note that the flux-across-surfaces theorem (30) also shows that the scattering cross section (29), defined via the quantum flux, indeed yields a probability measure on the unit sphere. In fact, in the course of establishing (30) one also obtains that

$$\lim_{R\to\infty} \int_0^{\infty} \mathrm{d}t \int_{R\Sigma} j^{\psi_t} \cdot \mathrm{d}A = \lim_{R\to\infty} \int_0^{\infty} \mathrm{d}t \int_{R\Sigma} \left| j^{\psi_t} \cdot \mathrm{d}A \right| . \tag{31}$$

This shows that the flux is asymptotically outgoing and that the identification of (28) with the crossing probability is consistent in the scattering regime.

[10] In [11] the current positivity condition, which states that the flux through a (given) surface is outgoing at all times, was introduced. In [14] it is shown that this condition is naturally associated with the dilation operator, whose spectral decomposition is used in proving asymptotic completeness.

8 Random trajectories and the Bohmian cross section

There remains, however, a very serious difficulty with regarding the flux cross section (29) as the basic quantity for the derivation of scattering theory from microscopic first principles, one that perhaps can best be appreciated by asking: Precisely which microscopic principles have been used for the derivation?

Schrödinger's equation alone is certainly insufficient, since the derivation involves quantum probability formulas and these transcend the Schrödinger dynamics. A better answer would be standard textbook quantum theory, involving, as well as Schrödinger's equation, the quantum measurement postulates for the statistics of the results of measurements of quantum observables. However, this theory, with the macroscopic notion of measurement playing a *fundamental* role, is not a fully microscopic theory and thus can't genuinely be regarded as defining the microscopic first principles that we seek.

Moreover, even if we ignore this difficulty—as most physicists no doubt would be inclined to do—there remains the severe difficulty that there is no quantum observable, as understood in textbook quantum theory, to which the quantum flux corresponds via the quantum measurement formalism. The quantum flux is usually not regarded as having any operational significance. It is not related to any standard quantum mechanical measurement in the way, for example, that the density ρ, as the spectral measure of the position operator, gives the statistics for a position measurement.

We have proposed that the (time-integrated) flux be identified with a crossing probability, the probability that the particle crosses a given piece of surface—which, as we have emphasized, to the extent that we are allowed to use such concepts at all in orthodox quantum theory, it does at a random time. Thus the relevant observable should be the position of the particle at a random time, the time at which it crosses the surface. This time should, in orthodox quantum theory, be associated with a time-operator. But the notion of time-operator is exceedingly problematical, and the notion of the position at this random time is utterly hopeless from an orthodox perspective.

There is, however, a suitable candidate for a theory embodying the appropriate first principles, namely, Bohmian mechanics [6,13,4], which provides a rigorous foundation for the "suggestions" and "natural identifications" of Section 7. In Bohmian mechanics a particle moves along a trajectory $X(t)$ determined by (using now general units)

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = v^{\psi_t}(X(t)) = \frac{\hbar}{m}\mathrm{Im}\frac{\nabla\psi_t}{\psi_t}(X(t))\,, \tag{32}$$

where ψ_t is the particle's wave function, evolving according to Schrödinger's equation. Moreover, if an ensemble of particles with wave function ψ is prepared, the positions X of the particles are distributed according to the quantum equilibrium distribution $\mathbb{P}^\psi$ with density $\rho = |\psi|^2$.

In particular, since $|\psi_t|^2 v^{\psi_t} = j^{\psi_t}$, the continuity equation for the probability shows that the probability flux $(|\psi_t|^2, |\psi_t|^2 v^{\psi_t})$ is conserved, i.e., the flow (32) carries an initial $|\psi|^2$ probability density for the particle to the density $|\psi_t|^2$ at time t. Thus, given an initial wave function ψ, the solutions $X^\psi(t) \equiv X^\psi(t, X_0)$ of equation (32) are random trajectories, with $X^\psi(t)$ having distribution $|\psi_t(x)|^2$, and where the randomness comes from that of the $\mathbb{P}^\psi$-distributed initial position X_0.

Let now Σ be any smooth piece of oriented surface in $\mathbb{R}^3$ and consider the number $N^\psi(\Sigma, I)$ of crossings by the trajectory $X^\psi(t)$ of Σ in the time interval I. Consider also $N_+^\psi(\Sigma, I)$, the number of crossings in the direction of the orientation, and $N_-^\psi(\Sigma, I)$, the number of crossings in the opposite direction, of Σ in the time interval I. Then $N^\psi(\Sigma, I) = N_+^\psi(\Sigma, I) + N_-^\psi(\Sigma, I)$ and we define the number of signed crossings by $N_{\mathrm{s}}^\psi(\Sigma, I) := N_+^\psi(\Sigma, I) - N_-^\psi(\Sigma, I)$.

We now compute the expectation values with respect to the probability $\mathbb{P}^\psi$ of these random variables in the usual manner. For a crossing of an infinitesimal surface element of (vector) size $\mathrm{d}A$ to occur in the time interval $(t, t + \mathrm{d}t)$, the particle must be in a cylinder of size $|v^{\psi_t}\mathrm{d}t \cdot \mathrm{d}A|$ at time t. Thus $\mathbb{E}^\psi(N^\psi(\mathrm{d}A, \mathrm{d}t)) = |\psi_t|^2 |v^{\psi_t}\mathrm{d}t \cdot \mathrm{d}A| = |j^{\psi_t} \cdot \mathrm{d}A|\,\mathrm{d}t$, and similarly $\mathbb{E}^\psi(N_{\mathrm{s}}^\psi(\mathrm{d}A, \mathrm{d}t)) = j^{\psi_t} \cdot \mathrm{d}A\,\mathrm{d}t$. Hence

$$\mathbb{E}^\psi(N^\psi(\Sigma, I)) = \int\limits_I \int\limits_\Sigma |j^{\psi_t} \cdot \mathrm{d}A|\,\mathrm{d}t \tag{33}$$

and

$$\mathbb{E}^\psi(N_{\mathrm{s}}^\psi(\Sigma, I)) = \int\limits_I \int\limits_\Sigma j^{\psi_t} \cdot \mathrm{d}A\,\mathrm{d}t\,. \tag{34}$$

Consider now a particle with wave function ψ localized, say, at time $t = 0$ in some region $B \subset \mathbb{R}^3$ with smooth boundary ∂B. The random variables t_B^ψ, the first exit time from B, $t_B^\psi := \inf\{t \geq 0 \,|\, X^\psi(t) \notin B\}$, and X_B^ψ, the position of first exit, $X_B^\psi := X^\psi(t_B)$, are the basic quantities describing the exit of the particle from B. If $j^{\psi_t} \cdot \mathrm{d}A$ is, for all $t > 0$, positive everywhere on ∂B, the particle can cross ∂B at most once and only outwards. We then have that for $\Sigma \subset \partial B$

$$\mathbb{P}^\psi(X_B^\psi \in \Sigma) = \mathbb{E}^\psi(N_{\mathrm{s}}^\psi(\Sigma))\,, \tag{35}$$

where we have written $N_\mathrm{s}^\psi(\Sigma)$ for $N_\mathrm{s}^\psi(\Sigma,(0,\infty))$, with a similar notation for N^ψ and $N_\pm^\psi$. More generally, since $|I_{\{X_B^\psi\in\Sigma\}} - N_\mathrm{s}^\psi(\Sigma)| \le N_-^\psi(\partial B) = \frac{1}{2}(N^\psi(\partial B) - N_\mathrm{s}^\psi(\partial B))$, where $I_{\{\cdot\}}$ is the indicator function of $\{\cdot\}$, we have that

$$|\mathbb{P}^\psi(X_B^\psi \in \Sigma) - \mathbb{E}^\psi(N_\mathrm{s}^\psi(\Sigma))| \le \frac{1}{2}\left(\mathbb{E}^\psi(N^\psi(\partial B)) - \mathbb{E}^\psi(N_\mathrm{s}^\psi(\partial B))\right). \quad (36)$$

We now define the Bohmian cross section as the probability that the particle crosses the surface covered by the relevant detector or detectors at some future time. More precisely, we define the Bohmian cross section as the $R\to\infty$ limit of the probability that the particle will leave the ball $B = B_R$, of radius R centered at the origin, through $R\Sigma$, $\Sigma \subset S^2$,

$$\sigma_\mathrm{Bohm}^\psi(\Sigma) := \lim_{R\to\infty} \mathbb{P}^\psi(X_{B_R}^\psi \in R\Sigma). \quad (37)$$

This is physically the most fundamental definition of the cross section, corresponding more or less directly to what is measured in a scattering experiment. This definition involves a quantity, the first exit position $X_{B_R}^\psi$, which, while perfectly straightforward for Bohmian mechanics, cannot be expressed in orthodox quantum theory.

It follows from (31) and (33–36) that $\sigma_\mathrm{Bohm}^\psi = \sigma_\mathrm{flux}^\psi$.

9 Overview

Using (37) instead of (11) in the analysis leading to (16), we arrive at

$$\sigma_\mathrm{diff}^{k_0}(\Sigma) := \lim_{|\hat\phi(k)|^2\Rightarrow\delta(k-k_0)} \lim_{L\to\infty} \int_{y\in\Gamma_L} \lim_{R\to\infty} \mathbb{P}^{\phi_y}(X_{B_R}^{\phi_y} \in R\Sigma)\, \mathrm{d}^2 y, \quad (38)$$

for $k_0 \notin C_\Sigma$, as the fundamental definition of the differential scattering cross, describing the scattering rate for a beam of particles of momentum k_0. Our derivation of scattering theory from microscopic first principles thus becomes the demonstration from Bohmian mechanics of the emergence of (14) from (38). It is worth noting that (38) is somewhat complicated, involving three explicit limits, each crucial and with the order of the limits important. For example, because the limit $R\to\infty$ is taken first, the wave functions ϕ_y are asymptotically in the support of B_R.

The derivation begins with the analysis of Section 8 and proceeds via the flux-across-surfaces theorem, (30) and (31), to (16). Then, using the computation of Amrein, Jauch, and Sinha described in Section 4, we arrive at (14), which in turn can be computed using the stationary methods described in Section 5. One of the frequent objections against Bohmian mechanics is that it lacks the resources to cope, e.g., with momentum, based as it is solely upon position. It is thus worth emphasizing that our analysis shows how the usual textbook scattering formulas involving momentum matrix elements naturally emerge from Bohmian mechanics.

We wish to comment now on a crucial step in the derivation: the flux-across-surfaces theorem. Note that there is a peculiarity in the statement of that theorem: The right hand side of (30) is well defined for all wave functions in the range of Ω_+, but one cannot expect the theorem to hold for all such wave functions because the left hand side, involving the flux, is defined only if the wave function obeys certain smoothness conditions.

The usual mathematical physics of scattering theory, with its focus on asymptotic completeness, neither relies upon nor needs such smoothness properties, nor does Dollard's theorem (26), but to treat the flux, extra conditions and new techniques are required. One might expect that (30) holds whenever the wave functions are sufficiently smooth and are moving freely asymptotically in time, i.e., are in the range of Ω_+. But this has not yet been shown! One typical problem, for example, is that the standard techniques in time-dependent scattering theory yield the required "propagation estimates" only for wave functions with energy cutoffs for small and large energies (cf. [3,2]). When proving asymptotic completeness, these are harmless because they can be easily removed at the appropriate time by simple density-in-L^2 arguments. However, this does not work in (30) because of the unboundedness of the form $\int_0^\infty \mathrm{d}t \int_{R\Sigma} j^{\psi_t} \cdot \mathrm{d}A$. On the other hand, the few known propagation estimates for wave functions without energy cutoffs (cf. [20,28]) are not strong enough for proving the flux-across-surfaces theorem.

One way to come to grips with this is to turn to generalized eigenfunction expansions (see [18,26,21]). However, while no energy cutoffs are then needed, the class of allowed potentials in [26] is less general than in the standard approaches [3,2]. Nevertheless, the eigenfunction expansions have proven to be a general and rather promising tool. Further mathematical work on generalized eigenfunctions would surely be of interest for the foundations of scattering theory. We recall in this respect also the use of (22) for actual computation.

It would be very interesting to know whether the energy cutoffs on the wave functions can be circumvented without sacrificing the less restrictive conditions on the potential appearing in the standard approaches to the proof of (30). As mentioned before, the most general and most satisfying result would be that any sufficiently smooth wave function whose motion is asymptotically free, i.e., that is in the range of Ω_+, satisfies (30). This would justify the name scattering states for the set $\mathrm{Ran}(\Omega_+)$. On the other hand it would be interesting to understand whether (37) is a well defined probability measure also for states in the singular continuous spectral subspace, even though the formula (30) could then no longer hold.

For the case of many-particle scattering, asymptotic completeness has been established by Soffer and Sigal (see [9,24] and the references therein). Moreover, Bohmian mechanics for many-particle systems is perfectly well defined [4]. However, we are not aware of any work on a many-particle analogue of the flux-across-surfaces theorem, which would be necessary for a more complete understanding of many-particle scattering phenomena in terms of microscopic first principles.

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