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Geometrical characterisation of asymptotic wavefronts in N-body scattering†

Sergio Servadio
Istituto di Fisica dell'Università, Università di Pisa, Italy 56100

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Abstract. The differential geometry of admissible wavefronts for N-body scattering is investigated for each term of the multiple scattering series and within angular sectors of uniform asymptotic behaviour. The differential equations are dimension independent in form and are thus investigated in R_n. A general theorem is proved stating that, if not spherical, the wavefront must be a (ruled) $K = 0$ surface tangent to a sphere around the origin. For $n = 3$ a rather simple geometrical description is given of the most general structure.

1. Statement of the problem and discussion

The purpose of this note is to bring out the relevance of some elementary concepts of differential geometry to the description of scattering in configuration space. More specifically, I shall address myself to the question of what wavefronts characterise the asymptotic behaviour of the scattered wave and how they arise.

In the very familiar case of two-body scattering, the problem is reduced to the R_3 relative coordinate space so that the incoming plane wave sees a potential centred around the origin. If the range of the force is strictly finite the potential has compact support and the problem is equivalent to the scalar Helmholtz equation for an acoustic wave off an obstacle of finite size.

The usual ansatz is that the scattered wave behaves asymptotically as an outgoing spherical wave (which is in fact Sommerfeld's radiation condition). The sphericity of the wavefront can be traced back to the fact that the wave ultimately propagates in free space, so that a ray description of the progressing wavefront should be appropriate through the eikonal equation.

The eikonal equation (with unit energy)

$$\nabla f \cdot \nabla f = 1$$

forces the wavefronts $f^{-1}(c)$ to constitute a family of parallel surfaces (Jones 1964, Somigliana 1919). Such a family can be generated starting from any initial (smooth) surface by displacing each point along the outward normal by an equal amount. The radii of curvature of the initial surface increase linearly (with coefficient one) with such a displacement (Eisenhart 1947) so that any initial surface becomes asymptotically spherical, i.e. with asymptotically degenerate radii of curvature. (If the initial surface has zero Gaussian curvature, $K = 0$, the same holds for the whole family.)

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Although the above points to the physical origin of the spherical symmetry of the asymptotic phase, it does not fully clarify the differential characterisation of the wavefront geometry.

Take the N-body scattering problem with pairwise potentials of finite range that do not bind, and an incident plane wave χ of momentum $\boldsymbol{P}'$ in the reduced $\boldsymbol{R}_n$ (with $n = 3N - 3$) configuration space. The scattering wavefunction is the multidimensional Fourier transform

$$\Psi(\boldsymbol{x}, \boldsymbol{P}') = \int \mathrm{d}\boldsymbol{P}\, \mathrm{e}^{\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{P}}\left(\delta(\boldsymbol{P}-\boldsymbol{P}') - \frac{T(\boldsymbol{P}, \boldsymbol{P}'; P'^2 + \mathrm{i}\varepsilon)}{P^2 - P'^2 - \mathrm{i}\varepsilon}\right) = \chi + \psi(\boldsymbol{x}, \boldsymbol{P}')$$

in terms of the kernel $T(\boldsymbol{P}, \boldsymbol{P}'; z)$ of the full T-matrix

$$T(z) = V - V(H-z)^{-1}V.$$

The Hamiltonian

$$H = K + \sum_{i<j} V_{ij} = K + V$$

is the sum of the total kinetic energy K and the pair potentials V_{ij} (Yakubovskii 1967).

To simplify the notation let us restrict to a three-body system ($i = 1, 2, 3$). Let Greek letters label the pairs, e.g. $\alpha = 1$ is the pair of particles 2 and 3. Resolve $T(z)$ into Faddeev's components

$$T(z) = \sum_{\alpha} M_{\alpha}(z)$$

where

$$M_{\alpha}(z) = T_{\alpha}(z) - T_{\alpha}(z)(K - z - \mathrm{i}\varepsilon)^{-1} \sum_{\beta \neq \alpha} M_{\beta}.$$

Here T_{α} is the T-matrix with only pair α interacting and it carries a $\delta(\ldots)$ for the third particle going through.

Upon iteration, one generates the multiple scattering series for $T(z)$, and so for $\psi(\boldsymbol{x}, \boldsymbol{P}')$. The starting terms for $T(z)$ are

$$T(z) = \sum_{\alpha}\left(T_{\alpha}(z) + T_{\alpha}(z)\frac{1}{K - z - \mathrm{i}\varepsilon}\sum_{\beta \neq \alpha} T_{\beta}(z) + \ldots\right)$$

where $1/(K - z - \mathrm{i}\varepsilon)$ is the propagator for the intermediate state in between scatterings.

Each term in the multiple scattering series for $\psi(\boldsymbol{x}, \boldsymbol{P}')$ is characterised by the overall energy pole, the propagators and the appropriate $\delta(\ldots)$ functions at each vertex. When due account is taken of the $\delta(\ldots)$'s, the term reduces to a multidimensional Fourier transform of a kernel having the energy pole and additional intermediate state singularities whose location is determined by the kinematics (Merkur'ev 1971). For its asymptotic behaviour as $\rho = |\boldsymbol{x}| \to \infty$ the residue at the energy pole has to be picked with a one-dimensional integration. An outer integration gets in general a leading O(1) term from a propagator singularity and an $\mathrm{O}(\rho^{-1/2})$ term by application of the stationary phase method. The two contributions are distinct and additive only within angular sectors in $\boldsymbol{x}$-space of uniform asymptotic behaviour. Failure occurs over the matching regions analogous to the boundary of the geometrical shadow in optics (where the pole and the stationary phase point coalesce).

Away from the matching each contribution has a well defined asymptotic behaviour

$$\psi \sim (e^{if(x)}/\rho^{\alpha})(\text{amplitude})$$

with $0 < \alpha \leq \frac{1}{2}(n-1)$.

The phase function $f(x)$ is guaranteed to satisfy the eikonal equation and, by the very Fourier transform construction, to be homogeneous of degree one with the origin as the point of homogeneity. It then appears that the allowed geometries of the asymptotic wavefronts are strongly limited by the differential system

$$\nabla f \cdot \nabla f = 1 \tag{1.1}$$

$$(x \cdot \nabla) f = f. \tag{1.2}$$

That interesting geometries must actually occur is suggested by the following heuristic considerations.

The potential in R_n is $\Sigma_{i<j} V_{ij}$ and each term has a translational symmetry in those coordinates on which it does not depend, along which it is 'flat'. The geometry of a multiply scattered term (note the very close relation with Keller's geometrical theory of diffraction) must be a result of the successive modification of the geometry of the progressing wavefront (Fock 1950). Thus, different scattered terms will have a different number of non-vanishing curvatures, different symmetries and a different associated expansion coefficient α.

It is well known in geometry that the fall-off coefficient α is associated with how the area of the wavefront $f^{-1}(c)$ increases in passing to a neighbouring (parallel) surface (Thorpe 1979); (2α) equals the rank of the second fundamental form of the wavefront set, i.e. the number of its non-vanishing curvatures. This is related to the fact that, proceeding in free space, such a ψ obeys

$$(\nabla^2 + 1)\psi = 0$$

so that the current

$$j = \text{Re}(i\psi^* \nabla \psi)$$

is conserved.

Pushing the analysis a bit farther, one can see that a better understanding of ψ comes from calculating the finite radii of principal curvature R_i with $i = 1, 2, \ldots, 2\alpha$ of $f^{-1}(c)$; ψ can then be cast into the form

$$\psi \sim (e^{if(x)}/\Pi_{i=1}^{2\alpha} R_i^{1/2}) g(\nabla f)$$

with an amplitude g that depends only on the wavefront normal (unit) vector ∇f. The amplitude is then constant along the (straight) integral lines of ∇f, i.e. along the rays. In addition, if the directional derivative

$$(\hat{\lambda} \cdot \nabla) \nabla f$$

is zero along some tangent field $\hat{\lambda}$ (direction of vanishing curvature), then also

$$(\hat{\lambda} \cdot \nabla) g = 0$$

and g is constant along the integral lines of $\hat{\lambda}$.

This picture affords, in a sense, a separation of geometrical and dynamical features of the wavefunction.

Although the statements we shall make are of a local character, the geometry of the surfaces allows these structures to be continued and interpreted in a larger domain.

We shall prove that in any dimensionality a candidate wavefront is either a sphere or a surface of zero Gauss curvature ($G=0$) enveloped around a sphere. Surfaces with $G=0$ in R_n are 'developable'; they have $\infty^{2\alpha}$-many tangent planes with

$$\alpha < \tfrac{1}{2}(n-1)$$

or, equivalently, $\infty^{2\alpha}$-many independent normal vectors. They are always ruled surfaces.

The only ruled surfaces in R_2 being the lines, R_2 admits only lines and circles.

In R_3 there is a richer structure. The most general case is locally like a cone enveloping the sphere but with the apex drifting along the generator. It can be generated as follows. Let a ruling slide over the unit sphere holding one of its points fixed (which point is held fixed is a function of time). The surface thus generated is taken as the level set of a function f at the value one. Propagate the function by the eikonal or the homogeneity condition. (The result is independent of that choice.)

An analogous complete description in higher dimensionalities must take into account more possibilities, essentially because the surface has more curvatures which need not vary in the same linear manner along the ruling. Moreover it might happen that there is more than one ruling through each point.

In the particularly interesting case of the three-body problem one can check that the troublesome single- and double-scattering terms are characterised by eikonal surfaces fitting exactly into our scheme. The geometry of their wavefronts plays an important role both in the calculation of interference fluxes and in the study of recurrence relations à la Sommerfeld–Luneburg (Keller *et al* 1956) between successive coefficient amplitudes of the asymptotic expansion. In particular, interference fluxes in which an inner integration can be done by quadratures independently of the dynamics, i.e. of the t-matrices (Servadio 1981), find their most natural explanation in terms of rays emerging parallel from the scattering region. The summation is over rays that have had the same dynamical history, differing only for intercollision times. The two interfering wavefronts are recognised as being ruled surfaces tangent to each other along a ruling carrying the parallel emerging rays.

In view of these applications it appears worthwhile to explain in detail how the differential system (1.1) and (1.2) constrains the geometry of the wavefront. Since in actual calculations it is necessary to parametrise a wavefront in order to calculate its curvatures and integrals over its set, after proving the main theorem in R_n we shall restrict to R_3 and, as an exercise, analyse its structures in detail.

2. Mathematical section

2.1. The R_n case

We shall prove the following theorem.

Theorem. If not a spherical cap, the surface $f^{-1}(c)$ is a $K=0$ surface.

Proof. By taking ∇ of (1.1) and using the symmetry

$$\partial^2 f/\partial x_i\, \partial x_j = \partial^2 f/\partial x_j\, \partial x_i$$

(which in a sense is the Frobenius integrability condition for reconstructing $f^{-1}(c)$ from its gradient vector field) one sees that

$$(\hat{N}\cdot\nabla)\hat{N}=0$$

where

$$\hat{N}=\nabla f.$$

Similarly, (1.2) readily gives

$$(\boldsymbol{x}\cdot\nabla)\hat{N}=0.$$

Combining the two, for any α and β

$$[(\alpha\boldsymbol{x}+\beta\hat{N})\cdot\nabla]\hat{N}=0;$$

so, if $\alpha=1/f$ and $\beta=-1$,

$$[(\boldsymbol{x}/f-\hat{N})\cdot\nabla]\hat{N}=0.$$

Provided $\boldsymbol{x}\wedge\hat{N}\neq 0$, this is a curvature equation since the vector $(\boldsymbol{x}/f-\hat{N})$ lies on the tangent plane at $\boldsymbol{x}$. The theorem is thus proved.

It is well known that $K=0$ surfaces are also ruled (an elementary proof can be given by mimicking the proof in R_3 by do Carmo (1976); alternatively, one can prove it directly from our hypothesis), the rulings being the (straight) integral lines of the directions of vanishing curvature. Then, if we call

$$\hat{\lambda}=\boldsymbol{x}/f-\hat{N}$$

the ruling vector field, for any λ we have

$$f(\boldsymbol{x})=f(\boldsymbol{x}+\lambda\hat{\lambda}).$$

The $(n-1)$-surface $f^{-1}(c)$ has ∞^{n-2}-many such rulings (generators) if non-overlapping rulings are considered distinct. Each ruling has a point of closest approach to the origin where $\hat{N}$ is radial, the point being a distance $|\boldsymbol{x}|=c$ from the origin. If (2α) is the rank of the second fundamental form of the surface there is a (2α)-manifold of points of closest approach to the origin which is the 'tangency manifold' between the surface $f^{-1}(c)$ and the sphere of radius c. There are $\infty^{2\alpha}$-many different normal vectors $\hat{N}$ to our wavefront surface, so that the number (2α) of non-vanishing curvatures is connected with how many independent directions are present in the ray system associated with our eikonal surface.

The importance of the 'tangency manifold' in actual calculations can be fully appreciated in the study of double-scattering waves in the three-body problem. One sees that it is exactly the matching region between two contributions, one of which is a ruled cone-like eikonal and the other a spherical eikonal (Servadio 1981).

2.2. The R_3 case

To see more easily some features of the wavefronts, let us restrict to R_3 and analyse its $K=0$ surfaces. The 'tangency manifold' is in general a line called the directrix and the rulings are the generators. Let the rulings be parametrised by the arc length λ with $\lambda=0$ on the directrix. Since the rulings are lines of principal curvature, so must be their orthogonal trajectories $\lambda=$ constant. Let these be the integral lines of a $\hat{\mu}$ vector field parametrised by the arc length μ. Call $R(\lambda, \mu)$ the associated radius of curvature:

$$(\hat{\mu} \cdot \nabla)\hat{N} = (R(\lambda, \mu))^{-1}\hat{\mu}. \tag{2.1}$$

It is well known that

$$\partial^2 R(\lambda, \mu)/\partial\lambda^2 = 0$$

so that we can parametrise

$$R(\lambda, \mu) = A(\mu)[k(\mu) + \lambda].$$

Any $\boldsymbol{x}$ on $f^{-1}(c)$ can be written as

$$\boldsymbol{x}(\mu, \lambda) = \boldsymbol{a}(\mu) + \lambda\,\hat{\lambda}(\mu)$$

where $\boldsymbol{a}(\mu)$ takes to the directrix and $\lambda\,\hat{\lambda}(\mu)$ along the generator. Then, the curvature equation (2) requires the proportionality

$$\partial\boldsymbol{a}/\partial\mu = k(\mu)\partial\hat{\lambda}/\partial\mu$$

and the coordinate velocity field along $\hat{\mu}$

$$\partial\boldsymbol{x}/\partial\mu = \partial\boldsymbol{a}/\partial\mu + \lambda\ \partial\boldsymbol{b}/\partial\mu = (k(\mu) + \lambda)\partial\hat{\lambda}/\partial\mu$$

vanishes at $\lambda = k(\mu)$.

The motion of the generator can be thought of as having the point of curvilinear coordinates $(\lambda = -k(\mu), \mu)$ fixed. The surface is generated by sliding the ruling over the spherical surface and instantaneously having $\boldsymbol{x}_A(\mu) = \boldsymbol{a}(\mu) - k(\mu)\hat{\lambda}(\mu)$ fixed, i.e. rotating around an axis through the $\boldsymbol{x}_A$ point. The instantaneous centre of rotation moves with velocity

$$\mathrm{d}\boldsymbol{x}_A/\mathrm{d}\mu = -(\mathrm{d}k/\mathrm{d}\mu)\hat{\lambda}(\mu)$$

and so it drifts along the generator. The vector $\hat{N}$ is parallel to the axis of rotation and is found to be

$$\hat{N}(\mu) = \boldsymbol{a}(\mu)/c.$$

(Obviously it points, if drawn out of the origin, towards the appropriate point of the directrix.) Thus, the directrix is the image of the Gauss map.

If $k(\mu) = \text{constant}$, then $f^{-1}(c)$ is a cone of rotational symmetry.

If $k(\mu) = \infty$, the cone degenerates into a cylinder.

If $k(\mu) = 0$, the cone flattens out into a plane.

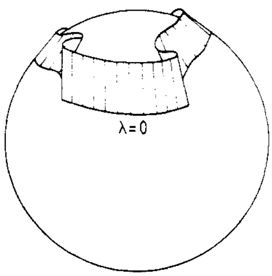

Figure 1. The R_3 case showing the $\lambda = 0$ directrix.

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