SCATTERING BY A BOUNDED NON-LINEAR SINGULARITY

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ABSTRACT. An investigation is made of the effect of a non-linear addition to Schrödinger's equation for s-wave scattering of a beam of particles by a finite region of potential energy. The non-linear region is bounded and of an especially simple form so that an analytic solution is possible. The R-function for the problem is explicitly constructed and some related formulae such as the resonant energies and the scattering length are given. The analytical nature of R as a function of the momentum considered as a complex variable is discussed in relation to causality.

1. *Introduction.* This note reports on a model calculation where certain features of a non-relativistic non-linear wave equation are investigated. It is a trivial consequence of the quantum theory of coupled fields that the field equations are non-linear, the non-linearities being rather weak unless the excitation is large. As examples we can recall the Euler–Köckel Lagrangian for high intensity electromagnetic fields, the non-linear field effects emphasized by Wheeler, where the metric is field dependent, and, more recently, the existence of strong pion-pion forces in meson physics. It is clear that in any non-linear quantum-mechanical problem the response will be dependent on the intensity and therefore interesting questions of principle will arise. Discussions of non-linear field equations are often confined to attempts at obtaining a mass spectrum (1), since very high intensities will be locally reached due to the singularities in the field strengths. As a model with which to begin investigations of the effects of a non-linearity on other aspects of quantum mechanics we shall consider here an extremely simplified scattering problem. We remark that in scattering any observable effect will be very small since the intensities involved are normally minute (when measured in (electron volts)^3).

Consider a beam of particles of mass m and energy $\mathrm{E} = k_{\mathrm{E}}^2/2m$, intensity I, incident on a scattering centre which consists of a potential well of depth V and radius a' and also a region of non-linearity of radius a ($a \leqslant a'$). In any reasonable physical situation one would expect $a' \gg a$, i.e. the incident particle should feel a normal potential (or perhaps an effective potential given by some integral kernel) before feeling the effect of a non-linearity due to the coupling back of the sources with the field. This argument ignores the non-linear effects which may be present for a single particle, namely, self-mass effects on the particles of the incident beam. However, for simplicity of the mathematics and without affecting the principles involved we shall take $a = a'$ in most of the detailed calculations. In general, the coupling back will produce a non-local effect, the fields being felt over distances of the order of the Compton wavelength of the source. We shall ignore this non-locality. We remark, however, that the non-linearity itself is a velocity-dependent potential energy, which in configuration space

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will be non-local. Finally, in order to obtain analytical results, the non-linearity will be taken to be of the specific form

$$\tilde{\lambda} r^2 \phi^2(r) \quad (r < a), \tag{1}$$

where $\tilde{\lambda}$ is dimensionless and $\phi(r)$ is the spatial wave-function describing the beam of particles.

In § 2 the assumed (non-linear) wave equation is solved explicitly for the completely spherically symmetric case, and the S matrix for the scattering, a number here, is constructed. As expected, this depends now also on the intensity of the ingoing beam, the dependence being rather weak for 'reasonable' values of $\tilde{\lambda}$. As for potential scattering, it is very useful to introduce the R-function, related simply to the logarithmic derivative of the wave-function at the boundary $r = a$. This is computed in terms of elliptic functions and from it certain physical quantities, such as the position of the resonances, the scattering length and the effective range are calculated. These (exact) results can easily be compared with those of simple perturbation theory, when keeping only terms of the first non-vanishing order. The limit $\tilde{\lambda} = 0$ gives, of course, the well-known results for scattering by a potential well.

In § 3 we discuss the analytic structure of R and S when these functions are analytically continued off the real k_E-axis. It is well known that for scattering by a bounded static potential R is a meromorphic function (on the entire k_E-plane), with only real poles, a result which is normally associated with causality. Wigner (2) has defined a class of meromorphic functions, called by him R-functions, which show this behaviour. A simple expression (the derivation of which is given in an Appendix) connecting the causality condition as formulated by van Kampen (3) with the behaviour of R on the real axis is discussed and shown to be equivalent to a similar inequality derived by Wigner (4) in terms of the behaviour of the phase shift. This result is then used to discuss a non-local model for which, despite being causal in the sense just indicated, the R-function does not exhibit its usual analytic structure.

2. *The* R*-function and related formulae.* The wave equation we solve is

$$\left[-\frac{\nabla^2}{2m} + (1-\Theta(r-a))\,\tilde{\lambda} r^2 \phi^2(r) + (1-\Theta(r-a'))\,V\right]\phi(r) = E\phi(r) \quad (a' \geqslant a,\ \hbar = 1). \tag{2}$$

It is clear that the presence of the non-linear term makes the general solution of this equation extremely complicated, and on this account we restrict our discussion entirely to the case of complete spherical symmetry. This procedure is not too unphysical, however, since the $l = 0$ part of the incident wave will always penetrate into the inner region of the scattering centre, even at very small energies and thus will always be affected by the non-linearity. The higher angular momentum partial waves, on the other hand, will only be affected at higher energies, with the effect of the non-linearity tending in any case to average out over all angles.

With $u(r) = r\phi(r)$, the differential equation in the inner region ($r < a$) is then

$$\frac{d^2u}{dr^2} + (k_v^2 - \lambda u^2)\,u = 0, \tag{3}$$

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where $k_v^2 = 2m(E - V)$ is the square of the wave-number in the region $0 < r < a'$ and $\lambda = 2m\tilde{\lambda}$. The solution of equation (3) which vanishes at the origin is†

$$u = \frac{c}{\kappa} \operatorname{sn}(\kappa r), \tag{4}$$

where the modulus of the Jacobian elliptic function is given by

$$k^2 = \frac{\lambda c^2}{2\kappa^4} \tag{5}$$

with

$$\kappa = \frac{k_v}{2^{\frac{1}{2}}}\left[1 + \left(1 - \frac{2\lambda c^2}{k_v^4}\right)^{\frac{1}{2}}\right]^{\frac{1}{2}}. \tag{6}$$

The number c is the value of du/dr at $r = 0$. On account of the non-linearity it cannot now be given arbitrary values, that is to say, c will in general depend on the parameters of the problem, in particular on the intensity and on the energy of the incident beam.

The free-particle solution for the exterior region ($r > a'$) is

$$u = A\, e^{-ik_E r} + B\, e^{+ik_E r}, \tag{7}$$

where A is determined by the incident beam

$$A = e^{i\gamma}\left(\frac{mI}{4k_E^3}\right)^{\frac{1}{2}} \tag{8}$$

and B is related to A through the scattering matrix (here a number)

$$S = -\frac{B}{A}. \tag{9}$$

If we now introduce the R-function by the definition

$$R = \left.\frac{u}{r(du/dr)}\right|_{r=a} \tag{10}$$

$$= \frac{\operatorname{sn}(\kappa a)}{\kappa a \operatorname{cn}(\kappa a) \operatorname{dn}(\kappa a)} \tag{11}$$

it is straightforward to show that

$$S = e^{-2ik_E a'} \frac{(ik_v aR + 1)(k_v + k_E)\, e^{2ik_v(a'-a)} + (ik_v aR - 1)(k_E - k_v)}{(ik_v aR + 1)(k_v - k_E)\, e^{2ik_v(a'-a)} - (ik_v aR - 1)(k_E + k_v)}, \tag{12}$$

i.e. the whole effect of the non-linearity is thrown into the R-function.

Even though, as already pointed out in the introduction, on physical grounds we should expect a to be smaller than a', in order to keep the analytic properties simple we shall restrict our discussion in what follows to the case $a = a'$. Then equation (12) reduces to the form familiar in the theory of nuclear reactions,

$$S = e^{-2ik_E a} \frac{1 + ik_E aR}{1 - ik_E aR}. \tag{13}$$

† The sign of the non-linear term in equation (3) is arbitrary and chosen for convenience; if we had taken it as positive the solution which vanishes at the origin would have been

$$u = \frac{c}{\alpha} \frac{\operatorname{sn}(\alpha r)}{\operatorname{dn}(\alpha r)}; \quad \alpha^4 - \alpha^2 k_v^2 - 2\lambda c^2 = 0.$$

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We notice that in equation (11) the explicit dependence on c has divided out, the R-function being implicitly dependent on λ and c together through terms of the form λc^2. In the limit $\lambda = 0$, when we return to the usual potential well scattering, R is therefore independent of c. Moreover, in this limit $\kappa = k_v$ and $k = 0$ (i.e. the Jacobian elliptic functions go over into circular ones), and R is then given by the well-known expression

$$\mathrm{R} = \frac{1}{k_v a}\tan(k_v a). \tag{14}$$

For sufficiently small values of the dimensionless parameter $\tilde{\lambda}$ $(= \lambda/2m)$ one is tempted to use perturbation theory, by expanding our results in powers of λ. However, as the dependence on λ is always through the factor λc^2, this procedure may become questionable at certain limits on account of the dependence of c on the parameters of the problem, a dependence exhibited by the relation

$$A^*(c)\,A(c) = \frac{mI}{4k_{\mathrm{E}}^3}$$

which leads to

$$c^2\left\{\frac{k_{\mathrm{E}}^2}{\kappa^2}\mathrm{sn}^2(\kappa a) + \mathrm{cn}^2(\kappa a)\,\mathrm{dn}^2(\kappa a)\right\} = \frac{mI}{k_{\mathrm{E}}}, \tag{15}$$

where c has been taken to be real (which corresponds to fixing the phase factor in equation (8)). It is seen that c increases with the intensity of the incident beam and goes to infinity when the bombarding energy is extrapolated to zero. This energy dependence is easily understood: at very low velocities of the incident beam the wave will take a long time to traverse the region of scattering and therefore one can expect the effects of the non-linearity to become increasingly important. These effects are of course not present in the linear case, where R is not even implicitly dependent on the number c. Keeping these reservations in mind, we expand equations (5) and (6) to powers of the order $\tilde{\lambda}$. We get

$$\kappa = k_v - \frac{\lambda c^2}{4k_v^3} \tag{16}$$

and

$$k^2 = \frac{\lambda c^2}{2k_v^4}. \tag{17}$$

The partial fraction expansion of R (equation (11)) is easily obtained by using the known (5) Mittag–Leffler expansion of $(d/dv)(\log \mathrm{sn}\, v)$, and the result

$$\frac{\mathrm{sn}\, v}{\mathrm{cn}\, v\,\mathrm{dn}\, v} = \frac{1}{k'^2}\,\frac{\mathrm{cn}(v+\mathrm{K}+i\mathrm{K}')\,\mathrm{dn}(v+\mathrm{K}+i\mathrm{K}')}{\mathrm{sn}(v+\mathrm{K}+i\mathrm{K}')},$$

where k' is the complementary modulus, and K and K′ the first complete and associated complete elliptic integrals, respectively. We thus obtain

$$\mathrm{R} = \frac{1}{\kappa a k'^2}\sum_{m,n}\left\{\frac{1}{\kappa a - (2m-1)\,\mathrm{K} - (2n-1)\,i\mathrm{K}'} - \frac{1}{\kappa a - (2m-1)\,\mathrm{K} - 2ni\mathrm{K}'}\right\}. \tag{18}$$

For $\lambda = 0$ $(\mathrm{K} = \frac{1}{2}\pi,\ \mathrm{K}' = \infty)$, this reduces to

$$\mathrm{R} = \frac{1}{k_v a}\sum_n \frac{1}{(n-\frac{1}{2})\pi - k_v a}, \tag{19}$$

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which is the known expansion of equation (14), with the resonant energies

$$\mathrm{E}_{(n)} = \frac{\pi^2(n-\frac{1}{2})^2}{2ma^2} - V. \tag{20}$$

An important difference between the R's given by equations (18) and (19) is apparent at once: the former has a doubly infinite set of complex poles (one line of which is real, that corresponding to $n = 0$ in the second term of the summation), while the latter has only real poles. This latter case is the usual one and is normally associated with causality. We shall discuss this point in the following section. It is seen that in the complex κ-plane the poles of R lie on straight lines, parallel to the real axis at distances proportional to K′. When λ tends to zero all the complex poles go off to infinity like $1/\lambda$ and the only singularities left are the poles on the real axis (equation (19)).

The appearance of complex poles is of course a consequence of the doubly periodic nature of the elliptic functions. Besides equation (3) there is another non-linear radial equation which we can solve exactly. The non-linear term is taken in this case to be of the form λu^2 (instead of λu^3) and the solution is a Weierstrassian ($\wp$) elliptic function which yields an R-function of analytic structure similar to that of (18).

For the potential scattering case the zeros of the denominator of equation (19) give the resonant energies (20). In our model, on the other hand, the real zeros of the denominator of R are the roots of the equations

$$\kappa_{(n)}a = (2n-1)\,\mathrm{K}_{(n)}, \tag{21}$$

which when written in full are

$$\frac{k^2_{v(n)}}{2}\left[1+\left(1-\frac{2\lambda c^2}{k^4_{v(n)}}\right)^{\frac{1}{2}}\right]a^2 = (n-\tfrac{1}{2})^2\pi^2\left[1+\sum_{m=1}^{\infty}\left(\frac{1.3.5.....(2m-1)}{2.4.6.....2m}\right)^2 k^{2m}_{(n)}\right]^2. \tag{22}$$

Expanding in powers of λ we get

$$k^2_{v(n)} = \frac{(n-\frac{1}{2})^2\pi^2}{a^2} + \frac{3}{4}\frac{\lambda c^2 a^2}{(n-\frac{1}{2})^2\pi^2} + \ldots, \tag{23}$$

which is readily compared with (20).

It is interesting to obtain this result by perturbation theory. To the order of λ

$$\Delta k^2_{v(n)} = \frac{\lambda\int u^4_{(n)}dr}{\int u^2_{(n)}dr},$$

where

$$u_{(n)} = \frac{c}{k_{v(n)}}\sin(k_{v(n)}r).$$

Therefore,

$$\Delta k^2_{v(n)} = \frac{\lambda c^2a^2}{(n-\frac{1}{2})^2\pi^2}\frac{\int_0^{\pi}\sin^4 t\,dt}{\int_0^{\pi}\sin^2 t\,dt}$$

$$= \frac{3}{4}\frac{\lambda c^2a^2}{(n-\frac{1}{2})^2\pi^2}, \tag{24}$$

as in (23).

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Near the resonance energy $E_{(n)}$

$$R \propto \frac{\gamma_{(n)}^2}{k_{v(n)}^2 - k_E^2} \tag{25}$$

and simple algebra gives, to the order λ,

$$\gamma_{(n)}^2 = \frac{2}{a^2} + \frac{2\lambda c^2 a^2}{(n-\frac{1}{2})^2 \pi^2} + \ldots. \tag{26}$$

Finally, expressions for the scattering length, b, and the effective range, r_0, can readily be obtained. The scattering length is defined by

$$b = a - a.R \quad (k_E = 0),$$

whence

$$\mathrm{cs}\,(\kappa(0).a)\,\mathrm{dn}\,(\kappa(0).a) = \frac{1}{\kappa(0).[a-b]}, \tag{27}$$

which compares with

$$\cot(k_v(0).a) = \frac{1}{k_v(0).[a-b]} \tag{28}$$

for the linear case, where $\kappa(0)$, $k_v(0)$, are the values of these quantities at the limit $k_E = 0$. We have assumed here that the energy dependence of the parameter c (equation (15)) can be ignored in this connexion, since these effects will become important at very low momenta and the resulting deviation will thus not be seen when extrapolating to zero energy. Under the same assumption we write down the effective range formula

$$r_0 = 2\left[a - \frac{a^2}{b} + \frac{a^3}{3b^2} - \frac{a}{2mb^2}\frac{dR}{dE}\bigg|_{E=0}\right]. \tag{29}$$

3. *The causality condition and the analytic structure of the* R*-function.* As is well known (6), if the potential in Schrödinger's equation is central, static and cut-off the S-function has no poles in the first quadrant of the complex k_E-plane, when analytically continued from its value on the real axis. When the usual symmetry condition

$$S(-k_E) = S^*(k_E) \tag{30}$$

is postulated, $S(k_E)$ is found to have no poles on the whole of the upper half-plane, except on the imaginary axis. It has been shown (7) that this property corresponds directly to the R-function having real poles only. This analytic structure of R is often claimed to be simply a consequence of the causality condition.

In this section we shall construct an example to demonstrate that a non-linearity (or a non-locality) can give rise to 'spurious' poles of the R-function off the real axis —and thus of S in the upper half-plane—even though the causality condition may still be satisfied. We emphasize that this will be done in a model where the region of potential is bounded, as it is known (8) that even an exponentially falling-off local potential can give rise to similar 'redundant' poles.

The expansion of R given in § 2 (equation (18)),

$$R(z) = \frac{1}{k'^2}\frac{1}{z}\Sigma\left\{\frac{1}{z-(2m-1)K-(2n-1)iK'} - \frac{1}{z-(2m-1)K-2niK'}\right\} \tag{31}$$

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indicates the possibility of constructing such an example. The direct discussion of equation (18), however, is complicated by the fact that k', K and K′ are all dependent on k (the modulus of the elliptic functions), which in turn is a function of z.

Nevertheless, we can investigate equation (31) as a function of z for a fixed modulus. In this case the function (modulus k)

$$u = \frac{c}{q}\,\mathrm{sn}\,(qr), \tag{32}$$

where q is a wave-number, can be considered as the internal wave-function ($r < a$) in a scattering problem with a (very strange!) velocity dependent but linear bounded potential.†

The corresponding R-function is then given by equation (31) and exhibits the complex poles we have already discussed. We now show that this model is also causal.

For scattering of non-relativistic particles van Kampen (3) has given the following formulation of the causality condition: if at a time $t = -\infty$ the ingoing beam is composed of just one particle, then at any other given time t_1 the total probability of finding a particle outside a sphere of radius r_1 equal to or greater than the radius a of the scattering centre cannot be greater than one. As it is shown in the Appendix, for s-wave scattering this formulation leads to the relations

$$2a - \frac{1}{i}\mathrm{S}(k_{\mathrm{E}})\frac{d\mathrm{S}^*(k_{\mathrm{E}})}{dk_{\mathrm{E}}} \geqslant \frac{1}{k_{\mathrm{E}}}\Im\{S(k_{\mathrm{E}})\,e^{2ik_{\mathrm{E}}a}\} \tag{33}$$

and

$$\frac{d\mathrm{R}(k_{\mathrm{E}})}{dk_{\mathrm{E}}} \geqslant 0. \tag{34}$$

As a check for these expressions let us write the S-matrix as

$$\mathrm{S}(k_{\mathrm{E}}) = e^{2i\delta_0(k_{\mathrm{E}})},$$

where $\delta_0(k_{\mathrm{E}})$ is the corresponding phase-shift. From equation (33) one immediately obtains

$$\frac{d\delta_0}{dk} \geqslant -a + \frac{1}{2k_{\mathrm{E}}}\sin 2(\delta_0 + k_{\mathrm{E}}a), \tag{35}$$

an inequality previously obtained by Wigner (4). An important difference, however, should be emphasized here: in Wigner's treatment this inequality follows from the form of the partial fraction expansion of R, which in turn is considered to be a consequence of causality;‡ in our case, on the other hand, equations (33) and (34) *are* alternative expressions of the causality condition as formulated by van Kampen.

Let us come back now to the model we are considering. With $v = qa$, the R-function corresponding to solution (32) is

$$\mathrm{R}(v) = \frac{\mathrm{sn}\,(v)}{v\,\mathrm{cn}\,(v)\,\mathrm{dn}\,(v)}. \tag{36}$$

† The r-dependent part of such a potential would be the form $q^2k^2[\mathrm{sn}^2\,(qr) - \mathrm{cn}^2\,(qr)]$, k (a given constant) being the modulus of the elliptic functions.

‡ It is perhaps interesting to point out that Wigner does in fact use equation (34), as derived from the partial fraction expansion, but only as a condition which enables him to obtain inequality (35) by dropping a certain positive term in the equation giving $d\delta/dk_{\mathrm{E}}$ (see (4), p. 146).

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It is straightforward to show that (the modulus of the elliptic functions being a constant)

$$\frac{d\mathrm{R}(v)}{dv} = \frac{\mathrm{cn}^2 v + \mathrm{sn}^2 v\,\mathrm{dn}^2 v}{2\,\mathrm{cn}\,v\,\mathrm{dn}\,v}(2v - \mathrm{sn}\,(2v)), \tag{37}$$

and as

$$2v \geqslant \mathrm{sn}\,(2v) \quad (v \geqslant 0)$$

$$\frac{d\mathrm{R}(v)}{dv} \geqslant 0, \tag{38}$$

and therefore (equation (34)) the model is causal, as we wished to prove.

As already pointed out, the case of the non-linear (but formally local) wave equation we discussed in § 2 is more complicated because of the energy dependence of c, K and k. It is possible to show, however, that in a region of energy away from the limit $k_{\mathrm{E}} \to \infty$ (where $c \to \infty$), inequality (34) can still be satisfied.

We have seen, therefore, that the causality condition does not necessarily imply the usual analytic structure of the R-function when non-local (velocity-dependent) potentials are considered. The fact that velocity-dependent potentials may give rise to poles of the S-function in the upper half of the complex energy plane (and thus of R off the real axis) is transparent from the discussion given by Rosenfeld (6), which is based on considerations other than causality.†

Van Kampen (3) has considered the connexion between causality and the poles of the S- and R-functions under the assumption that the amplitude of the incident wave is the boundary value of an $L^2(0, \infty)$ function, analytic in the first quadrant. This assumption breaks down for the amplitudes describing the pure monochromatic beam we have considered, but only trivially. However, as remarked by van Kampen, one must keep in mind in these circumstances the basic fact that analytic continuation is a very unstable procedure. A slight change in the value of the functions on the real axis can have violent effects elsewhere. A change from $\sin(\kappa a)$ to $\mathrm{sn}(\kappa a)$ can be made arbitrarily small over a large region of physical values of κ, by choosing the modulus of the elliptic function sufficiently small. However, $\sin(\kappa a)$ is the boundary value of an entire function, while $\mathrm{sn}(\kappa a)$ is the boundary value of a meromorphic function, with a doubly infinite set of poles.

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APPENDIX

In the problem we have considered, outside the sphere of radius a the wave-function is given by

$$r\phi(r) = A(k_{\mathrm{E}})\,e^{-ik_{\mathrm{E}}r} + B(k_{\mathrm{E}})\,e^{+ik_{\mathrm{E}}r}$$

$$= r\phi_{\mathrm{in}}(r) + r\phi_{\mathrm{out}}(r) \quad \left\{\begin{matrix} a < r < \infty \\ 0 < k_{\mathrm{E}} < \infty \end{matrix}\right\}. \tag{A. 1}$$

† It is interesting to remark that if in the internal region the potential term was $\lambda u^* u$ instead of λu^2, the argument given by Rosenfeld should go through and there would be no singularities of S in the upper half-plane. We note that this new equation would have the same solution as equation (3) for real u. However, the new equation would not be formally analytic, and therefore the R-function off the real axis would not be that of equation (11).

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Therefore
$$r\psi_{\text{in}}(r,t) = A(k_{\text{E}})\, e^{-ik_{\text{E}}r - iEt},$$
$$r\psi_{\text{out}}(r,t) = B(k_{\text{E}})\, e^{+ik_{\text{E}}r - iEt} \quad \left(E = \frac{k_{\text{E}}^2}{2m}\right). \tag{A. 2}$$

Van Kampen's causality condition states then that
$$\int_a^\infty 4\pi r^2 \left|\psi_{\text{in}}(r,0) + \psi_{\text{out}}(r,0)\right|^2 dr \leqslant 1, \tag{A. 3}$$

where ψ_{in} is normalized by
$$\int_a^\infty 4\pi r^2 \left|\psi_{\text{in}}(r,-\infty)\right|^2 dr = 1. \tag{A. 4}$$

In equation (A. 3) we have chosen $t_1 = 0$ and have put $r_1 = a$, which clearly gives the strongest condition. We now insert (A. 4) into the right-hand side of (A. 3), use (A. 2) for ψ_{in} and ψ_{out} and evaluate the integrals in the resulting inequality as follows: for the left-hand side we have
$$r(\psi_{\text{in}}(r,0) + \psi_{\text{out}}(r,0)) = A(k_{\text{E}})\, e^{-ik_{\text{E}}r} + B(k_{\text{E}})\, e^{+ik_{\text{E}}r}$$
and we can write
$$r^2 \left|\psi_{\text{in}}(r,0) + \psi_{\text{out}}(r,0)\right|^2 = \lim_{k'_{\text{E}} = k_{\text{E}}} \left(A(k_{\text{E}})\, e^{-ik_{\text{E}}r} + B(k_{\text{E}})\, e^{+ik_{\text{E}}r}\right)$$
$$\times \left(A^*(k'_{\text{E}}) \exp\left(+ik'_{\text{E}}r\right) + B^*(k'_{\text{E}}) \exp\left(-ik'_{\text{E}}r\right)\right).$$

The integration over r is readily performed by using the well-known result
$$\int_a^\infty e^{i(p-p')r}\, dr = e^{i(p-p')a}\left\{\frac{1}{-i(p-p')} + \pi\delta(p-p')\right\}. \tag{A. 5}$$

Use of the condition $k'_{\text{E}} = k_{\text{E}}$ $(k_{\text{E}}, k'_{\text{E}} \neq 0)$ eliminates two of the resulting four δ-function terms, while the unitary of the S function†
$$|\text{S}|^2 = \frac{|B|^2}{|A|^2} = 1$$
enables us to collect the remaining two into a single term
$$\lim_{k'_{\text{E}} = k_{\text{E}}} 8\pi^2 \left|A(k_{\text{E}})\right|^2 \delta(k_{\text{E}} - k'_{\text{E}}). \tag{A. 6}$$

The principal part terms will be given below.

Let us consider now the right-hand side of the inequality. For this we write first
$$r\psi_{\text{in}}(r,-\infty) = \lim_{T \to +\infty} \{r\psi_{\text{in}}(r,-T)\}$$
$$= \lim_{T \to +\infty} \{A(k_{\text{E}}) \exp\left(-ik_{\text{E}}r + ik_{\text{E}}^2 T\right)\}.$$

Therefore
$$\int_a^\infty 4\pi r^2 \left|\psi_{\text{in}}(r,-\infty)\right|^2 dr = 4\pi \lim_{k'_{\text{E}} = k_{\text{E}}} A(k_{\text{E}})\, A^*(k'_{\text{E}})$$
$$\times \lim_{T \to \infty} \exp\left\{i(k_{\text{E}}^2 - k_{\text{E}}'^2)\, T\right\} \int_a^\infty \exp\left\{-i(k_{\text{E}} - k'_{\text{E}})\, r\right\} dr.$$

† It is clear from equation (12) that independently of the form of the R-function, S is unitary if R is real.

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Using equation (A. 5) and the result†

$$\lim_{T\to\infty}\frac{\exp\{i(k_{\mathrm{E}}^2-k_{\mathrm{E}}'^2)\,T\}}{i(k_{\mathrm{E}}-k_{\mathrm{E}}')}=\pi\delta(k_{\mathrm{E}}-k_{\mathrm{E}}')$$

we finally obtain

$$\int_a^\infty 4\pi r^2\,|\psi(r,-\infty)|^2\,dr=\lim_{k_{\mathrm{E}}'=k_{\mathrm{E}}}8\pi^2\,|A(k_{\mathrm{E}})|^2\,\delta(k_{\mathrm{E}}-k_{\mathrm{E}}'). \tag{A. 7}$$

Hence, in inequality (A. 3), (A. 4) this term cancels out with (A. 6) and the inequality thus reduces to

$$\lim_{k_{\mathrm{E}}'=k_{\mathrm{E}}}\frac{A(k_{\mathrm{E}})\,A^*(k_{\mathrm{E}}')}{i(k_{\mathrm{E}}-k_{\mathrm{E}}')}[\mathrm{S}(k_{\mathrm{E}})\,\mathrm{S}^*(k_{\mathrm{E}}')\exp\{i(k_{\mathrm{E}}-k_{\mathrm{E}}')\,a\}-\exp\{-i(k_{\mathrm{E}}-k_{\mathrm{E}}')\,a\}]$$
$$\geqslant\frac{|A(k_{\mathrm{E}})|^2}{2k_{\mathrm{E}}i}\{\mathrm{S}(k_{\mathrm{E}})\,e^{2ik_{\mathrm{E}}a}-\mathrm{S}^*(k_{\mathrm{E}})\,e^{-2ik_{\mathrm{E}}a}\},$$

where the left-hand side takes the form 0/0 in the limit $k_{\mathrm{E}}'=k_{\mathrm{E}}$. This limit is readily evaluated by applying l'Hôpital's rule and thus the causality condition is finally found to be expressed by the inequality

$$2a-\frac{1}{i}\mathrm{S}(k_{\mathrm{E}})\frac{d\mathrm{S}^*(k_{\mathrm{E}})}{dk_{\mathrm{E}}}\geqslant\frac{1}{k_{\mathrm{E}}}\Im\{\mathrm{S}(k_{\mathrm{E}})\,e^{2ik_{\mathrm{E}}a}\} \tag{A. 8}$$

as given in the text (equation (33)). Using equation (13) of § 1 it is straightforward to show that in terms of the R-function the causality condition is expressed by

$$\frac{d\mathrm{R}(k_{\mathrm{E}})}{dk_{\mathrm{E}}}\geqslant 0\quad(0<k_{\mathrm{E}}<\infty), \tag{A. 9}$$

which is equation (34) in the text.

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† This follows immediately from the identity

$$\frac{\exp\{i(k_{\mathrm{E}}^2-k_{\mathrm{E}}'^2)\,T\}}{i(k_{\mathrm{E}}-k_{\mathrm{E}}')}=\frac{1}{i(k_{\mathrm{E}}-k_{\mathrm{E}}')}+\int_0^{(k_{\mathrm{E}}+k_{\mathrm{E}}')\,T}\exp\{i(k_{\mathrm{E}}-k_{\mathrm{E}}')\,x\}\,dx$$

when letting $T\to+\infty$ (k_{E}, $k_{\mathrm{E}}'\neq 0$).

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