Remarks on the Determination of a Central Field of Force from the Elastic Scattering Phase Shifts

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It is shown by an explicit example that a central field of force is not uniquely determined by the phase shifts for an S-wave. Hylleraas' recent paper is discussed, and an error in his argument is pointed out.

INTRODUCTION

It is interesting to know to what extent a central field of force is determined by the phase shifts which are used in computing the elastic scattering cross sections according to quantum mechanics. Recently two methods[1,2] have been suggested which would even allow determination of the field of force from the phase shifts for one single value of the angular momentum (for example, $l=0$). Clearly, these methods can be generally valid only if no two different potentials give rise to the same phase shifts.

In this note we shall exhibit, however, two potentials, V_1 and V_2 ($V_1 \neq V_2$), which yield the same phase shifts for S-waves (cf. (13a) and (13b)).

Let $\psi(r)$ be the wave function (for angular momentum 0) of a particle moving in a central field $V(r)$, and set $\phi = r\cdot\psi$. In the non-relativistic case, ϕ satisfies the differential equation

$$d^2\phi/dr^2 + k^2\phi = V(r)\cdot\phi, \qquad (1)$$

k being the wave number. (The units are so chosen that the energy of the particle equals k^2. If ordinary units are used both E and V must be multiplied by $h^2/2m$, where m is the mass of the particle.) We assume that the integral $\int_0^\infty |V(r)|dr$ converges, so that the usual scattering theory may be applied.

Following R. Jost's paper on the S-matrix,[3] we introduce two independent solutions of (1), *viz.*, $f(k, r)$ and $f(-k, r)$, which for large r are asymptotically equal to e^{-ikr} and to e^{ikr}, respectively, and we set

$$f(k) = f(k, 0); \quad f(-k) = f(-k, 0). \qquad (2)$$

For real values of k the functions $f(k, r)$ and $f(-k, r)$ are complex conjugate, and $f(k) \neq 0$. Since $\phi = r\cdot\psi$, an admissible solution of (1) must vanish for $r=0$. Hence,

$$\phi(r) = (1/2i|f(k)|) \times \{f(k)f(-k, r) - f(-k)f(k, r)\}. \qquad (3)$$

Asymptotically, $\phi(r) \sim \sin(kr+\eta)$, where the phase shift η is determined by

$$e^{i\eta} = f(k)/|f(k)| \quad \text{or} \quad S(k) = e^{2i\eta} = f(k)/f(-k). \qquad (4)$$

(The $S(k)$ are the proper values of the S-matrix associated with Eq. (1).) As has been shown by Jost,[3] the function $f(k, r)$ may also be used (and is analytic in k) for complex k with negative imaginary parts, in particular for $k = -i\kappa$, where $\kappa > 0$. A bound stationary state is obtained if the exponentially decreasing solution $f(-i\kappa, r)$ vanishes at $r=0$, i.e., if $f(-i\kappa) = 0$. Its energy is then given by

$$E = k^2 = -\kappa^2 \qquad [f(-i\kappa) = 0, \quad \kappa > 0]. \qquad (5)$$

It follows from (4) and (5) that two potentials with the same function $f(k)$ yield the same phase shifts and the same stationary energy values.

CONSTRUCTION OF THE EXAMPLE

The potentials considered are Eckart potentials[4] of the form

$$V(r) = K[\sigma, \beta, \lambda] \equiv -\sigma\lambda^2\beta e^{-\lambda r}/(1+\beta e^{-\lambda r})^2, \qquad (6)$$

where $\lambda > 0$, and $\beta > -1$. We shall restrict ourselves to the values $\sigma = 2$ and $\sigma = 6$. (With respect to this choice cf. the Appendix.)

[1] Carl-Erik Fröberg, Phys. Rev. **72**, 519 (1947).
[2] E. A. Hylleraas, Phys. Rev. **74**, 48 (1948).
[3] R. Jost, Helv. Phys. Acta **22**, 256 (1947).
[4] C. Eckart, Phys. Rev. **35**, 1303 (1930).

(a) $\sigma=2$

(This potential is also discussed by Jost (reference 3, p. 260).) Here

$$f(k,r)=e^{-ikr}(2k+i\mu(r))/(2k-i\lambda), \tag{7}$$

with

$$\mu(r)=\lambda(\beta e^{-\lambda r}-1)/(\beta e^{-\lambda r}+1). \tag{7a}$$

Clearly,

$$\mu(0)=\nu\equiv\lambda(\beta-1)/(\beta+1);\quad \mu(\infty)=-\lambda. \tag{8}$$

It is easily verified that (7) is a solution of the Schrödinger equation (1), since $d\mu/dr=\frac{1}{2}(\mu^2-\lambda^2)=-2\lambda^2\beta e^{-\lambda r}/(1+\beta e^{-\lambda r})^2$, and $d^2\mu/dr^2=\mu\cdot(d\mu/dr)$. Moreover, for large r, $f(k,r)\sim e^{-ikr}$, since $\mu(\infty)=-\lambda$. From (7) we obtain (cf. (8))

$$f(k)\equiv f(k,0)=(2k+i\nu)/(2k-i\lambda). \tag{9}$$

The function $f(-i\kappa)$ vanishes for $\kappa=\frac{1}{2}\nu$, so that there exists a bound stationary state, with energy $E=-\frac{1}{4}\nu^2$, if $\nu>0$, i.e., if $\beta>1$.

(b) $\sigma=6$

As may again be directly verified, here

$$f(k,r)=e^{-ikr}\frac{4k^2+6ik\mu(r)+\lambda^2-3\mu(r)^2}{(2k-i\lambda)(2k-2i\lambda)}, \tag{10}$$

$$f(k)=\frac{4k^2+6ik\nu+\lambda^2-3\nu^2}{(2k-i\lambda)(2k-2i\lambda)}, \tag{11}$$

where $\mu(r)$ and ν are defined by (7a) and (8), respectively. The bound stationary states are obtained from the equation $f(-i\kappa)=0$, $(\kappa>0)$. There exists one stationary state if $2-\sqrt{3}<\beta\leqq 2+\sqrt{3}$, and there exist two if $\beta>2+\sqrt{3}$. ($2\pm\sqrt{3}$ are the two roots of the equation $\lambda^2-3\nu^2=0$.)

Consider now $V_1(r)=K[6,1,\lambda]$ (λ arbitrary). Then $\nu=0$ (cf. (8)), and, by (11),

$$f_1(k)=(2k+i\lambda)/(2k-2i\lambda). \tag{12}$$

Set, further, $V_2(r)=K[2,\beta',\lambda']$ (β' and λ' to be determined). By (9), $f_2(k)=(2k+i\nu')/(2k-i\lambda')$. Hence $f_1(k)=f_2(k)$ if $2\lambda=\lambda'$, and $\lambda=\nu'=\lambda'(\beta'-1)/(\beta'+1)$, i.e., $\beta'=3$. Consequently, the two potentials

$$V_1(r)=-6\lambda^2e^{-\lambda r}/(1+e^{-\lambda r})^2, \tag{13a}$$

and

$$V_2(r)=-24\lambda^2e^{-2\lambda r}/(1+3e^{-\lambda r})^2, \tag{13b}$$

lead to the same function $f(k)$, and therefore to the same phase shift η (cf. (4)).

$V_1(r)$ and $V_2(r)$ have the common value $-3\lambda^2/2$ at $r=0$, their integrals (extended over all r) are both equal to -3λ, and they give rise to stationary states with the same energy, *viz.*, $E=-\frac{1}{4}\lambda^2$.

If V_1 and V_2 are expressed as

$$V_1(r)=-3\lambda^2/2\cosh^2(\tfrac{1}{2}\lambda r),$$
$$V_2(r)=-2\lambda^2/\cosh^2(\lambda(r-a));\quad a=(\ln 3)/2\lambda,$$

it is seen that $V_1(r)$ has its minimum at $r=0$, and defines an attractive force for all r, while $V_2(r)$ reaches its minimum at $r=a$, defining a repulsive force for $r<a$, and an attractive force for $r>a$. Moreover, the two potentials differ in their asymptotic behavior. The expression

$$D=\left\{\int_0^\infty (V_1(r)-V_2(r))^2dr\Big/\int_0^\infty (V_1(r)+V_2(r))^2dr\right\}^{\frac{1}{2}},$$

may serve as a measure for the deviation of $V_1(r)$ from $V_2(r)$. One finds $D=0.162$.

Evidently our result only proves that the phase shifts for the angular momentum zero do not determine the potential $V(r)$, but we cannot yet assert that the knowledge of all phase shifts (for arbitrary values of the angular momentum) is insufficient for the unique determination of $V(r)$. C. Møller[5] has proved that one can construct infinitely many different Hamiltonians which yield the same phase shifts, i.e., the same S-matrix. It is not obvious, however, that one can find among them a Hamiltonian which corresponds to an ordinary central field of force.

REMARKS ON HYLLERAAS' PAPER

We again restrict ourselves to the case $l=0$. For a given $V(r)$, Hylleraas[2] introduces two solutions of the Schrödinger equation,[6] *viz.*, $v_1(r)$, which is given by Eq. (3) above, and $v_2(r)$, which may be expressed as

$$v_2(r)=(1/2|f(k)|)\times\{f(k)f(-k,r)+f(-k)f(k,r)\}, \tag{14}$$

[5] C. Møller, Kgl. Danske Vid. Sels. Math.—Fys. Medd 24, No. 19 (1946). Cf. p. 33.

[6] For the details the reader is referred to Hylleraas' paper. (H 13), for example, is a reference to Eq. (13) of his paper.

and which asymptotically equals $\cos(kr+\eta)$. Let $V(r)$ and $U(r)$ be two potentials, η and ξ the corresponding phase shifts, and v_1, v_2 and u_1, u_2 the associated wave functions. Set $Y_k(r)=u_1v_1$, and $Z_k(r)=u_1v_2+u_2v_1$. Hylleraas asserts the general validity of the equation

$$V(r)-U(r) = (4/\pi)(d/dr)\int_0^\infty \sin(\eta-\xi)Z_k(r)dk. \quad (15)$$

[The foregoing equation differs from Hylleraas' (cf. (H 13)) in two minor points. (a) In order to avoid the appearance of divergent integrals we have interchanged differentiation with respect to r and integration with respect to k. (b) The signs of V and U are inverted, because Hylleraas' V corresponds to our $-V$ in the Schrödinger equation (cf. his Eq. (3)).] One would infer from (15) that $\eta=\xi$ implies $V(r)=U(r)$, whereas we have seen above that $V(r)$ is not uniquely determined by η.

Hylleraas bases his proof on the assumption that his equations (H 14) and (H 15) are equivalent, and that it is therefore sufficient to establish (H 14). In reality, these two equations are independent, since (H 14) corresponds to an orthogonality relation, and (H 15) to a completeness relation. The latter appears particularly doubtful if either one of the potentials V, U gives rise to a bound state, because then the solutions of the Schrödinger equation which belong to the continuous spectrum do not form a complete system of functions.

The writer has checked Eq. (H 15) for $V=K[2, \beta, \lambda]$, $U=K[2, \beta', \lambda']$. Then the functions Y_k and Z_k may be computed from (7), (3), and (14), and the integral in (H 15) evaluated explicitly. The following result was obtained: (H 15) holds if and only if the Schrödinger equations for both V and U have no discrete spectra, i.e., if $\beta\leqq 1$ and $\beta'\leqq 1$. This seems to indicate that Hylleraas' formula (cf. Eq. (15) above) may be generally valid if neither V nor U give rise to bound states. (Note that this holds for the example which Hylleraas discusses at the end of his paper.) The writer has not attempted a proof of this conjecture.

APPENDIX

For arbitrary values of σ, the function $f(k, r)$ associated with the potential $V(r)=K[\sigma, \beta, \lambda]$ (cf. (6)) is found to be

$$f(k, r)=e^{-ikr}(1+\beta e^{-\lambda r})^\tau F(\tau+(2ik/\lambda), \tau, 1+(2ik/\lambda), -\beta e^{-\lambda r}), \quad (16)$$

where $\tau=\frac{1}{2}(1-(1+4\sigma)^{\frac{1}{2}})$, and F is the hypergeometric function. If $\sigma=n(n+1)$ $[n=1, 2, \cdots]$, then $\tau=-n$, and F is a polynomial of n-th degree. One obtains the expressions (7) and (10) by setting $n=1$ and 2, respectively, and inserting $(\lambda+\mu(r))/(\lambda-\mu(r))$ for $\beta e^{-\lambda r}$.

Note added in proof: In the meantime the writer has worked out a number of additional examples. In particular, it is possible to construct potentials which (for S-waves) give equal phase shifts, but bound states of different energy values. This fact is of interest with respect to the theory of the S-matrix. It is also possible to find a non-vanishing potential which does not give any S-scattering. A detailed account will be published later.

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Condensation of Pure He^3 and Its Vapor Pressures between 1.2° and Its Critical Point

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On October 13, 1948 the authors succeeded in condensing[1] pure He^3 prepared by E. S. Robinson and R. M. Potter of the laboratory. The isotope was "grown" from pure tritium solutions by β-decay of the tritium. The latter

[1] Although the evidence is not conclusive, indications are that we have observed a transition to a liquid rather than a solid state. This is suggested by the similarity of Fig. 1 to what one would expect for a gas-liquid transition and by the approximate agreement between observed densities and those calculated from the critical constants by use of van der Waal's and Dieterici's equations of state.