Scattering *S*-matrix derived from invariants of the Ermakov–Lewis type

2004 J. Phys. A: Math. Gen. 37 L589

(http://iopscience.iop.org/0305-4470/37/44/L07)

J. Phys. A: Math. Gen. **37** (2004) L589–L591 PII: S0305-4470(04)84848-0

LETTER TO THE EDITOR

Scattering *S*-matrix derived from invariants of the Ermakov–Lewis type

Karl-Erik Thylwe

Department of Mechanics, KTH, Royal Institute of Technology, SE-100 44 Stockholm, Sweden

E-mail: ket@mech.kth.se

Received 11 August 2004, in final form 10 September 2004
Published 20 October 2004
Online at stacks.iop.org/JPhysA/37/L589
doi:10.1088/0305-4470/37/44/L07

Abstract
An amplitude-phase formula for the *S*-matrix due to a central potential is derived. The derivation makes use of invariants of the Ermakov–Lewis type.

PACS numbers: 02.30.Hq, 02.30.Ik, 03.65.Ca, 03.65.Sq

Important equations of the amplitude-phase method [1] can be interpreted as a so-called Ermakov system [2–4]. Ermakov systems of various complexities have been studied because of their invariants [2, 5–10]. In the amplitude-phase analysis, such invariants are expressed in terms of two functions that are solutions to either the Schrödinger equation or the nonlinear Milne equation [10]. Invariants of the Ermakov–Lewis type therefore appear in the matching of different particular amplitude-phase solutions of the Schrödinger equation. Physical quantities derived by the amplitude-phase method may also be expressed in terms of these invariants.

In this letter, it is shown how a useful amplitude-phase formula for the *S*-matrix can be derived from invariants of an Ermakov system defined by the radial Schrödinger equation and the Milne equation. For this particular Ermakov system, it has been shown that several invariants containing first-order, second-order and fourth-order derivatives derive from Wronskian relations of the Schrödinger equation [10] (see also [11]).

Consider the radial Schrödinger equation for a quantal particle of mass m and energy E in a scattering potential $V(r)$, i.e.

$$\frac{\mathrm{d}^2\Psi_\ell(r)}{\mathrm{d}r^2} + \left[\frac{2m}{\hbar^2}(E - V(r)) - \frac{\ell(\ell+1)}{r^2}\right]\Psi_\ell(r) = 0, \tag{1}$$

where ℓ is the partial-wave quantum number and $V(+\infty) = 0$. The scattering solution is regular at the origin, i.e.

$$\Psi_\ell(0) = 0, \tag{2}$$

and as $r \to +\infty$ it satisfies

$$\Psi_\ell(r) \sim N_\ell(\mathrm{e}^{-\mathrm{i}[\kappa(r)-\pi\ell/2]} - S_\ell\,\mathrm{e}^{\mathrm{i}[\kappa(r)-\pi\ell/2]}), \qquad r \to +\infty, \tag{3}$$

where N_ℓ is a normalization factor and $\kappa(r)$ satisfies the relation

$$\frac{\mathrm{d}\kappa(r)}{\mathrm{d}r} \to k, \qquad r \to +\infty, \tag{4}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{5}$$

A pair of amplitude-phase solutions of the Schrödinger equation is given by

$$F^{\pm}(r_0, r) = u_\ell(r)\,\mathrm{e}^{\pm \mathrm{i}\phi(r_0,r)}, \tag{6a}$$

$$\phi(r_0, r) = \int_{r_0}^{r} \frac{\mathrm{d}r'}{u_\ell^2(r')}, \tag{6b}$$

where r_0 is an unspecified reference point and u_ℓ satisfies the nonlinear Milne equation

$$\frac{\mathrm{d}^2 u_\ell}{\mathrm{d}r^2} + \left[\frac{2m}{\hbar^2}(E - V(r)) - \frac{\ell(\ell+1)}{r^2}\right] u_\ell = u_\ell^{-3}. \tag{7}$$

The Milne equation results from inserting the ansatz (6*a*) into the radial Schrödinger equation (1) and applying the relation (6*b*). The Wronskian determinant of the two solutions (6*a*) is constant.

The relevant scattering solution of (7) is constant in the limit as $r \to +\infty$. It is specified by the boundary condition:

$$u_\ell(+\infty) = k^{-1/2}. \tag{8}$$

With the aid of (1), (6*a*), (6*b*) and (7), one derives the Ermakov–Lewis invariants that contain first-order derivatives with respect to r; see [10]:

$$\Lambda_-(\ell) = \left[\Psi_\ell'(r)u_\ell(r) - \Psi_\ell(r)u_\ell'(r) - \mathrm{i}\frac{\Psi_\ell(r)}{u_\ell(r)}\right]\mathrm{e}^{\mathrm{i}\phi(r_0,r)}, \tag{9a}$$

$$\Lambda_+(\ell) = \left[\Psi_\ell'(r)u_\ell(r) - \Psi_\ell(r)u_\ell'(r) + \mathrm{i}\frac{\Psi_\ell(r)}{u_\ell(r)}\right]\mathrm{e}^{-\mathrm{i}\phi(r_0,r)}. \tag{9b}$$

It is straightforward to verify that $\mathrm{d}\Lambda_\pm(\ell)/\mathrm{d}r = 0$. In particular, the regular solution and the scattering Milne solution satisfy (9*a*) and (9*b*). The determination of the invariants, $\Lambda_\pm(\ell)$, requires an integration of Milne's solution from $+\infty$ to any matching point in common with the regular, radial Schrödinger solution that is integrated from the origin.

It is possible to determine the values of these invariants from the boundary conditions at $+\infty$, i.e. from equations (3) and (8), which gives

$$\Lambda_-(\ell) = -2\mathrm{i}k^{1/2}N_\ell\,\mathrm{e}^{\mathrm{i}\Delta(\ell)}, \tag{10a}$$

$$\Lambda_+(\ell) = -2\mathrm{i}k^{1/2}N_\ell S_\ell\,\mathrm{e}^{-\mathrm{i}\Delta(\ell)}, \tag{10b}$$

where

$$\Delta(\ell) = \lim_{r\to+\infty}\left[\phi(r_0, r) - \kappa(r) + \pi\ell/2\right]. \tag{11}$$

From (10*a*) and (10*b*) one obtains

$$S_\ell = \frac{\Lambda_+(\ell)}{\Lambda_-(\ell)}\,\mathrm{e}^{2\mathrm{i}\Delta(\ell)}. \tag{12}$$

In applications of (12), it is convenient to let the phase reference point r_0 be identical to the (unspecified) point r at which the invariants $\Lambda_\pm(\ell)$ in (9*a*) and (9*b*) are calculated. Then the phase $\phi(r_0, r)$ in (11) can be obtained numerically together with the integration of the Milne equation (7) from the asymptotic boundary condition (8) to the matching point $(= r_0)$.

Formula (12) is valid for complex potentials and complex angular momenta that do not alter the given boundary conditions (3) and (8).

In this letter, it is demonstrated how the amplitude-phase method can benefit from invariants of Ermakov systems. The invariants $\Lambda_{\pm}(\ell)$ become important ingredients in the derivation of the *S*-matrix formula. The invariants are also important ingredients in the final *S*-matrix formula. Since these types of invariants are possible to generalize to coupled Schrödinger and the related coupled Milne equations, the present formulation is a first step to generalize the amplitude-phase method to coupled scattering states [12].

In numerical applications, one has the freedom to choose the matching point conveniently on the real axis or in the complex *r*-plane. For effective potentials with barriers it may be numerically advantageous to use additional Milne solutions in regions where the present 'scattering Milne solution' becomes large and oscillatory. In such cases, the *S*-matrix formula has to be re-expressed to include the additional Milne solutions.

Acknowledgment

The author is indebted to Professor P O Fröman who has read the manuscript and suggested valuable improvements in the presentation.

References

[1] Milne W E 1930 *Phys. Rev.* **35** 863
Wilson H A 1930 *Phys. Rev.* **35** 948
Young H A 1931 *Phys. Rev.* **38** 1612
Young H A 1932 *Phys. Rev.* **39** 455
Wheeler J A 1937 *Phys. Rev.* **52** 1123
Newman W I and Thorson W R 1972 *Can. J. Phys.* **50** 2997
Newman W I and Thorson W R 1972 *Phys. Rev. Lett.* **29** 1350
[2] Ermakov V P 1880 *Univ. Izv. Kiev Serie III* **9** 1
[3] Korsch H J and Laurent H 1981 *J. Phys. B: At. Mol. Phys.* **14** 4213
[4] Matzkin A 2001 *J. Phys. A: Math. Gen.* **34** 7833
[5] Lewis H R 1967 *Phys. Rev. Lett.* **18** 510
Lewis H R 1967 *Phys. Rev. Lett.* **18** 636 (erratum)
Lewis H R 1968 *J. Math. Phys.* **9** 1976
Lewis H R and Riesenfeldt W B 1969 *J. Math. Phys.* **10** 1458
Lewis H R and Leach P G L 1982 *J. Math. Phys.* **23** 2371
[6] Lutzky M 1978 *Phys. Lett.* A **68** 3
[7] Ray J R and Reid J L 1979 *Phys. Lett. A* **71** 317
Ray J R and Reid J L 1979 *J. Math. Phys.* **20** 2054
[8] Athorne C 1992 *J. Differ. Equ.* **100** 82
Govindert K S, Athorn C and Leach P G L 1993 *J. Phys. A: Math. Gen.* **26** 4035
[9] Haas F 2002 *J. Phys. A: Math. Gen.* **35** 2925
[10] Thylwe K-E 2002 *J. Phys. A: Math. Gen.* **35** 4359
[11] Fernandez G and Moya-Cessa H 2003 *Phys. Rev.* A **67** 063803
[12] Thylwe K-E and Korsch H J 1998 *J. Phys. A: Math. Gen.* **31** L279