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Generalization of the amplitude-phase *S*-matrix formula for coupled scattering states

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Abstract

The amplitude-phase method is generalized to coupled Schrödinger scattering states with a common angular momentum quantum number. A pair of exponential-type amplitude-phase solutions $\mathbf{u}_j^{(\pm)}(r)\exp[\pm\mathrm{i}\phi_j(r)]$ for each channel is obtained, containing a common complex scalar phase function $\phi_j(r)$ and two (column) vector amplitudes $\mathbf{u}_j^{(\pm)}(r)$. The amplitude functions satisfy certain nonlinear generalized Milne equations and the scalar product of the two amplitudes determines the derivative of the common phase function. Fundamental amplitude-phase matrix solutions that are proportional to Jost-like Schrödinger matrix solutions are constructed. It is shown how a generalized amplitude-phase *S*-matrix formula can be derived from Wronskian relations involving the two amplitude-phase matrix solutions and a regular matrix solution.

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1. Introduction

The amplitude-phase method for quantum mechanical bound state and scattering problems in a single potential had its first stage of development in the 1930s [1]. Its main advantages compared to direct integration of the Schrödinger equation are its computational accuracy and its close connection to the semiclassical theories of the WKB type. Indeed, it is an exact reformulation of the original Schrödinger problem that takes advantage of an 'ansatz' of the Schrödinger solutions containing an amplitude and a related phase. The phase is determined by the history of the amplitude in the form of an integral of the inverse of the squared amplitude. The amplitude is slowly varying in regions valid for single linear combinations of (semiclassical) WKB solutions [2, 3], and the numerical computations are ideally performed on non-oscillating quantities.

It seems that little has been done to generalize the amplitude-phase method to coupled quantum states. To some extent the 'old', single-channel method has been successfully applied to the uncoupled exterior region of atomic systems [4]. In a different context of real, coupled classical parametric harmonic oscillators, a generalized amplitude-phase method was presented and it was used to identify certain Ermakov–Lewis invariants for such systems as being basically of the Wronskian type [5].

The amplitude-phase method is already considered to be an accurate numerical tool in the single-channel Regge-pole theory [3, 6–8]. This motivates a generalization of the amplitude-phase method as a tool in the coupled-states Regge-pole theory [9] as well, particularly for analysing atomic and molecular differential cross sections. It turns out that most parts in a recent formulation of the amplitude-phase method [6] can be generalized to coupled-states scattering problems. This short presentation contains only the basic steps of such a generalization which is valid also for standard partial-wave analysis. The approach to Regge-pole theory will be presented elsewhere.

Section 2 describes the basic radial Schrödinger equation where the coupled states contain a common angular momentum quantum number ℓ. In section 3, the generalized amplitude-phase Ansatz is introduced, which leads to two coupled sets of nonlinear Milne-type equations. The derivation of the S-matrix is presented in sections 4 and 5 contains concluding discussions.

2. Basic equations

The radial Schrödinger equation for each partial wave with quantum number ℓ is written in a suitable matrix form as

$$\frac{\mathrm{d}^2\mathbf{\Psi}_\ell(r)}{\mathrm{d}r^2} + \left(\mathbf{k}^2 - \mathbf{U}(r) - \frac{\ell(\ell+1)}{r^2}\mathbf{1}_n\right)\mathbf{\Psi}_\ell(r) = \mathbf{0}, \tag{1}$$

with $\mathbf{1}_n$ being a unit matrix containing n diagonal elements, $\mathbf{k}$ being the diagonal matrix of asymptotic wave numbers, i.e.

$$\mathbf{k} = \begin{pmatrix} k_1 & 0 & \cdots & 0 \\ 0 & k_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & k_n \end{pmatrix}, \tag{2}$$

and where $\mathbf{\Psi}_\ell(r)$ is given by

$$\mathbf{\Psi}_\ell(r) = \begin{pmatrix} \Psi_{11\ell}(r) & \Psi_{12\ell}(r) & \cdots & \Psi_{1n\ell}(r) \\ \Psi_{21\ell}(r) & \Psi_{22\ell}(r) & \cdots & \Psi_{2n\ell}(r) \\ \vdots & \vdots & \vdots & \vdots \\ \Psi_{n1\ell}(r) & \Psi_{n2\ell}(r) & \cdots & \Psi_{nn\ell}(r) \end{pmatrix}. \tag{3}$$

The potential matrix $\mathbf{U}(r)$ in (1) is defined such that it vanishes at $+\infty$.

A regular scattering solution satisfies

$$\mathbf{\Psi}_\ell(0) = \mathbf{0}, \tag{4a}$$

and

$$\mathbf{\Psi}_\ell(r) \sim \left(\mathbf{k}^{-1/2}\mathbf{e}_\ell^{(-)}(r) - \mathbf{k}^{-1/2}\mathbf{e}_\ell^{(+)}(r)\mathbf{S}_\ell\right)\mathbf{N}_\ell, \qquad r \to +\infty, \tag{4b}$$

where $\mathbf{S}_\ell$ is the scattering matrix, $\mathbf{N}_\ell$ is an unspecified normalization matrix and $\mathbf{e}_\ell^{(\pm)}(r)$ are the decoupled, asymptotic radial waves, i.e.

$$\mathbf{e}_\ell^{(\pm)}(r) = \begin{pmatrix} \exp(\pm\mathrm{i}(\kappa_1(r) - \ell\pi/2)) & 0 & \cdots & 0 \\ 0 & \exp(\pm\mathrm{i}(\kappa_2(r) - \ell\pi/2)) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \exp(\pm\mathrm{i}(\kappa_n(r) - \ell\pi/2)) \end{pmatrix}, \tag{5}$$

with $\kappa_j(r)$ satisfying $\mathrm{d}\kappa_j(r)/\mathrm{d}r = k_j$ such that from equations (2) and (5)

$$\frac{\mathrm{d}\mathbf{e}_\ell^{(\pm)}(r)}{\mathrm{d}r} \sim \pm\mathrm{i}\mathbf{k}\mathbf{e}_\ell^{(\pm)}(r), \qquad r \to +\infty. \tag{6}$$

Equation (6) is thus valid for Coulombic as well as non-Coulombic channels.

3. Amplitude-phase solutions

Particular amplitude-phase solutions are here defined as

$$\mathbf{f}_j^{(+)}(r) = \mathbf{u}_j^{(+)}(r)\exp(\mathrm{i}\phi_j(r_0, r)), \tag{7a}$$

$$\mathbf{f}_j^{(-)}(r) = \mathbf{u}_j^{(-)}(r)\exp(-\mathrm{i}\phi_j(r_0, r)), \tag{7b}$$

where $\mathbf{u}_j^{(\pm)}(r)$ are complex column-vector functions and $\phi_j(r_0, r)$ is a common complex phase for the jth state. To simplify the notation the ℓ-dependence of these elementary amplitude-phase quantities has been suppressed. The common phase is defined with respect to a reference point r_0 and is given by

$$\phi_j(r_0, r) = \int_{r_0}^{r} u_j^{-2}(r')\,\mathrm{d}r', \qquad u_j^2(r) = \mathbf{u}_j^{(+)}(r)\cdot\mathbf{u}_j^{(-)}(r), \tag{8}$$

where $\cdot$ denotes a complex-valued scalar product.

If the effective potential is real, the particular column-vector solutions (7*a*) and (7*b*) can be chosen as complex conjugate pairs on the real r-axis, see [5]. As soon as the effective potential becomes complex there is no such simple relationship between incoming and outgoing radial waves.

On substituting (7*a*) and (7*b*) into the radial Schrödinger equation (1), one finds the generalized Milne equations (note that the r-dependence is suppressed)

$$\mathbf{u}_j^{\prime\prime(+)} - \phi_j'^2\mathbf{u}_j^{(+)} + \left(\mathbf{k}^2 - \mathbf{U} - \frac{\ell(\ell+1)}{r^2}\mathbf{1}_n\right)\mathbf{u}_j^{(+)} + \mathrm{i}\left(\phi_j''\mathbf{u}_j^{(+)} + 2\phi_j'\mathbf{u}_j^{\prime(+)}\right) = \mathbf{0}, \tag{9a}$$

$$\mathbf{u}_j^{\prime\prime(-)} - \phi_j'^2\mathbf{u}_j^{(-)} + \left(\mathbf{k}^2 - \mathbf{U} - \frac{\ell(\ell+1)}{r^2}\mathbf{1}_n\right)\mathbf{u}_j^{(-)} - \mathrm{i}\left(\phi_j''\mathbf{u}_j^{(-)} + 2\phi_j'\mathbf{u}_j^{\prime(-)}\right) = \mathbf{0}, \tag{9b}$$

respectively. Equations (9*a*), (9*b*) are coupled through coefficients involving derivatives of the phase $\phi_j(r)$, e.g.,

$$\phi_j''(r) = -\frac{\mathbf{u}_j^{\prime(+)}(r)\cdot\mathbf{u}_j^{(-)}(r) + \mathbf{u}_j^{(+)}(r)\cdot\mathbf{u}_j^{\prime(-)}(r)}{u_j^4(r)}, \tag{10}$$

obtained from equation (8).

Note that even if the potential matrix $\mathbf{U}(r)$ is diagonal the above nonlinear differential equations for $\mathbf{u}_j^{(\pm)}(r)$ do not automatically decouple. To accomplish decoupled equations the initial conditions must be such that $\mathbf{u}_j^{(+)}(r)$ and $\mathbf{u}_j^{(-)}(r)$ have just one and the same non-zero jth element. If this is the case the bracketed terms $\left(\phi_j''(r)\mathbf{u}_j^{(\pm)}(r) + 2\phi_j'(r)\mathbf{u}_j'^{(\pm)}(r)\right)$ vanish in the jth element as well, so that both vector equations reduce to a single scalar Milne equation, given by

$$u_j''^{(\pm)}(r) + \left(k_j^2 - U_{jj}(r) - \frac{\ell(\ell+1)}{r^2}\right) u_j^{(\pm)}(r) = \left(u_j^{(\pm)}(r)\right)^{-3}. \tag{11}$$

Since an amplitude-phase method typically uses (piecewise) slowly varying Milne solutions in the single-channel case (see, e.g., [8]), it is useful to consider an adiabatic (WKB) limit of equations (9*a*) and (9*b*). A zeroth-order equation is obtained simply by neglecting terms containing derivatives of the vector-Milne solutions, see [10]. From the definition (8) it is clear that the terms in (9*a*), (9*b*) involving $\phi_j'^2$ survive and that one obtains a single eigenvalue equation

$$\left(\mathbf{k}^2 - \mathbf{U} - \frac{\ell(\ell+1)}{r^2}\mathbf{1}_n\right)\mathbf{u}_{Aj}^{(\pm)} = \phi_{Aj}'^2\mathbf{u}_{Aj}^{(\pm)}. \tag{12}$$

Each adiabatic eigenvalue $\phi_{Aj}'^2$ determines, by equation (8), the normalization of the corresponding eigenvectors $\mathbf{u}_{Aj}^{(\pm)}$. One can expect from this adiabatic consideration that there exist exact and slowly varying Milne solutions in various regions of the complex r-plane to some extent limited by the presence of classical turning points and adiabatic potential crossings. Of course, the Milne equations, and its solutions, are valid across such regions, but there is a tendency that the solutions start oscillating, see [8].

To address the full matrix problem for each partial wave, let the Milne solutions $\mathbf{u}_j^{(\pm)}(r)$, $j = 1, 2, \ldots, n$, define a matrix Milne solution, $\mathbf{u}_\ell^{(\pm)}(r)$, according to

$$\mathbf{u}_\ell^{(\pm)}(r) = \left(\mathbf{u}_1^{(\pm)}(r), \mathbf{u}_2^{(\pm)}(r), \ldots, \mathbf{u}_n^{(\pm)}(r)\right), \tag{13}$$

so that a pair of matrix amplitude-phase solutions of the radial Schrödinger equation can be written as

$$\mathbf{F}_\ell^{(\pm)}(r) = \mathbf{u}_\ell^{(\pm)}(r)\mathbf{E}_\ell^{(\pm)}(r), \tag{14}$$

where $\mathbf{E}_\ell^{(\pm)}(r)$ is a diagonal matrix of phase factors

$$\mathbf{E}_\ell^{(\pm)}(r) = \begin{pmatrix} \exp(\pm\mathrm{i}\phi_1(r_0, r)) & 0 & \cdots & 0 \\ 0 & \exp(\pm\mathrm{i}\phi_2(r_0, r)) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \exp(\pm\mathrm{i}\phi_n(r_0, r)) \end{pmatrix}. \tag{15}$$

For the purpose of analysing scattering states the Milne solutions have been selected according to the decoupled boundary conditions,

$$\mathbf{u}_\ell^{(\pm)}(+\infty) = \mathbf{k}^{-1/2} = \begin{pmatrix} k_1^{-1/2} & 0 & \cdots & 0 \\ 0 & k_2^{-1/2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & k_n^{-1/2} \end{pmatrix}, \tag{16a}$$

$$\mathbf{u}_\ell'^{(\pm)}(+\infty) = \mathbf{0}. \tag{16b}$$

This boundary condition is the unique constant matrix solution of the adiabatic equation (12) as well as the exact equations (9*a*), (9*b*) at $r = +\infty$, since the potential $\mathbf{U}(r)$ vanishes there.

As a result, from the construction (14) and the boundary conditions (16*a*), (16*b*) the amplitude-phase matrix solutions become diagonal in the limit $r \to +\infty$, where they satisfy

$$\mathbf{F}_\ell^{(\pm)}(r) \sim \mathbf{k}^{-1/2}\mathbf{E}_\ell^{(\pm)}(r), \qquad r \to +\infty. \tag{17a}$$

$$\mathbf{F}_\ell'^{(\pm)}(r) \sim \pm\mathrm{i}\mathbf{k}^{1/2}\mathbf{E}_\ell^{(\pm)}(r), \qquad r \to +\infty. \tag{17b}$$

4. *S*-matrix

The regular scattering matrix solution $\mathbf{\Psi}_\ell(r)$ and the particular amplitude-phase solutions $\mathbf{F}_\ell^{(\pm)}(r)$ satisfy the same differential equation with different boundary conditions, and thus satisfy the Wronskian relations

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\mathbf{F}_\ell^{(\pm)T}(r)\mathbf{\Psi}_\ell'(r) - \mathbf{F}_\ell'^{(\pm)T}(r)\mathbf{\Psi}_\ell(r)\right) = \mathbf{0}, \tag{18}$$

which provide two constant matrices

$$\mathbf{\Lambda}_-(\ell) = \mathbf{F}_\ell^{(+)T}(r_m)\mathbf{\Psi}_\ell'(r_m) - \mathbf{F}_\ell'^{(+)T}(r_m)\mathbf{\Psi}_\ell(r_m), \tag{19}$$

$$\mathbf{\Lambda}_+(\ell) = \mathbf{F}_\ell^{(-)T}(r_m)\mathbf{\Psi}_\ell'(r_m) - \mathbf{F}_\ell'^{(-)T}(r_m)\mathbf{\Psi}_\ell(r_m), \tag{20}$$

where the evaluation can be performed at any convenient matching point r_m. With the boundary conditions for $\mathbf{\Psi}_\ell(r)$ and $\mathbf{F}_\ell^{(\pm)}(r)$ defined at $+\infty$ by (4*b*) and (17*a*), respectively, the Wronskians can formally be determined as $r_m \to +\infty$, yielding

$$\mathbf{\Lambda}_-(\ell) = -2\mathrm{i}\lim_{r_m\to+\infty}\left\{\mathbf{E}_\ell^{(+)}(r_m)\mathbf{e}_\ell^{(-)}(r_m)\right\}\mathbf{N}_\ell, \tag{21a}$$

$$\mathbf{\Lambda}_+(\ell) = -2\mathrm{i}\lim_{r_m\to+\infty}\left\{\mathbf{E}_\ell^{(-)}(r_m)\mathbf{e}_\ell^{(+)}(r_m)\right\}\mathbf{S}_\ell\mathbf{N}_\ell. \tag{21b}$$

On eliminating $\mathbf{N}_\ell$ one obtains the *S*-matrix formula

$$\mathbf{S}_\ell = \mathbf{P}_\ell\mathbf{\Lambda}_+(\ell)\mathbf{\Lambda}_-^{-1}(\ell)\mathbf{P}_\ell, \tag{22}$$

where a diagonal r-independent phase matrix $\mathbf{P}_\ell$ is introduced as

$$\mathbf{P}_\ell = \lim_{r\to+\infty}\left\{\mathbf{E}_\ell^{(+)}(r)\mathbf{e}_\ell^{(-)}(r)\right\} = \begin{pmatrix} \exp(\mathrm{i}\alpha_{1\ell}) & 0 & \cdots & 0 \\ 0 & \exp(\mathrm{i}\alpha_{2\ell}) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \exp(\mathrm{i}\alpha_{n\ell}) \end{pmatrix}, \tag{23}$$

with

$$\alpha_{j\ell} = \lim_{r\to+\infty}[\phi_j(r_0, r) - \kappa_j(r)] + \pi\ell/2. \tag{24}$$

Equation (22) is a direct generalization of the recent single-channel *S*-matrix formula for the amplitude-phase method [6].

5. Discussion

The present amplitude-phase formula for the S-matrix is valid for complex potentials and complex angular momentum quantum numbers ($\mathrm{Re}\,\ell > -1/2$), as long as the asymptotic wave numbers are real and positive. No particular symmetries of the potential matrix have been utilized.

When using this formula numerically one has to integrate any regular Schrödinger solution from close to the origin and the Milne solutions (together with the common phase) from a very large distance to a convenient common matching point r_m, where the quantities $\mathbf{\Lambda}_{\pm}(\ell)$ (i.e., equations (19) and (20)) and $\mathbf{P}_\ell$ (i.e., equation (23)) determining the S-matrix are computed. The result is independent of the so-called reference point r_0 and it is convenient to choose this point at the matching point, i.e., $r_0 = r_m$.

The direct integration of the coupled radial Schrödinger equations may be non-trivial for heavy-particle systems. The regular solutions tend to increase exponentially in the classically forbidden regions and they typically oscillate strongly in the classically allowed regions along the r-axis. It may in such cases be advisable to use alternative methods such as the log-derivative method [11].

Since the Milne equations are nonlinear its solutions may behave very differently depending on the imposed boundary conditions. The numerical accuracy of the amplitude-phase method relies on the success of finding optimal, slowly varying Milne solutions [12]. Fortunately, for scattering problems (with open channels) where the channels decouple in the asymptotic region, it is easy to find the decoupled, constant boundary conditions (16*a*), (16*b*) for the optimal solutions. These solutions $\mathbf{u}_\ell^{(\pm)}(r)$ are expected to remain more or less monotonic from the asymptotic region and inward to the first (outer) significant transition region of the adiabatic solutions $\mathbf{u}_{Aj}^{(\pm)}$ of equation (12). Typical transition regions are located in some neighbourhood of (possibly complex) classical turning points of the adiabatic potentials and near the adiabatic potential crossing points. In the present form of the coupled-states amplitude-phase method it is advisable to perform the matching with the regular Schrödinger solution at the point r_m chosen in the outermost transition region, see [8] for improvements made in the single-channel method in this respect.

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