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Phase-function method from the Riccati form of the Schrödinger equation

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Abstract. The compatibility of the phase-function method with the Riccati form of the Schrödinger equation is investigated and the phase and amplitude equations are derived by using the method of variation of parameters.

The phase-function method (PFM) [1] is a very useful tool for nuclear scattering theory. The quantity one deals with in this method is a variable phase or phase function $\delta_l(k, \rho)$ which represents the phase shift at energy k^2 due to the potential $V(r)\theta(\rho - r)$ ($\theta(x)$ is the step function which vanishes for $x<0$ and is unity otherwise). It follows by definition that $\delta_l(k, 0)=0$ and $\delta_l(k, \infty)=\delta_l(k)$, the lth partial wave phase shift. It obeys a first-order nonlinear differential equation called the phase equation. The complete description of a wave mechanical problem needs an amplitude function $\alpha_l(k, \rho)$ in addition to the phase function. Once the phase function is known the amplitude function $\alpha_l(k, \rho)$ can be obtained by solving a first-order linear differential equation called the amplitude equation with the initial condition $\alpha_l(k, 0)=1$. Newton [2] has shown that $\alpha_l(k, \rho)$ represents the modulus of the Jost function [3] produced by a potential truncated at ρ. The phase and amplitude equations constitute the basic algorithms of the PFM. The object of the present paper is to present a derivation of these equations from the Riccati form of the Schrödinger equation using the method of variation of parameters [4].

The Riccati or nonlinear form of the Schrödinger equation forms an important basis for large-order perturbation calculations [5]. This equation has recently been used by Francisco *et al* [6] to obtain eigenvalues of the Schrödinger equation non-perturbatively. The Riccati equation satisfied by the logarithmic derivative of the wavefunction also serves as a consistency condition for the Schrödinger factorisation method [7]. This fact has been recognised by Sukumar [8] in the context of supersymmetric quantum mechanics. Thus it is of considerable interest to examine the rationale of the nonlinear form of the Schrödinger equation for development of the PFM.

Consider the lth wave radial Schrödinger equation

$$u_l''(k, r)+[k^2-l(l+1)/r^2]u_l(k, r)=V(r)u_l(k, r) \tag{1}$$

for a potential $V(r)$ at energy $E=k^2>0$ and define the logarithmic derivative of the wavefunction $u_l(k, r)$ as

$$U_l(k, r)=u_l'(k, r)/u_l(k, r). \tag{2}$$

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Here the prime denotes differentiation with respect to r and the term $l(l+1)/r^2$ stands for the centrigugal potential. Equations (1) and (2) can be combined to write

$$U_l^2(k,r)+U_l'(k,r)=V(r)+l(l+1)/r^2-k^2. \tag{3}$$

This represents the required Riccati equation. In the following we present a development of the PFM from (3).

Let us begin by treating $V(r)u_l(k,r)$ in (1) as an inhomogeneity term in the second-order linear differential equation under consideration. Then the Riccati Bessel and Neumann functions $\hat{j}_l(kr)$ and $\hat{\eta}_l(kr)$ will represent the regular and irregular solutions of the corresponding homogeneous equation. Following Lagrange's method [4] of variation of parameters we look for a solution of the inhomogeneous equation in the form

$$u_l(k,r)=A_l(k,r)\hat{j}_l(kr)-B_l(k,r)\hat{\eta}_l(kr) \tag{4}$$

where $A_l(k,r)$ and $B_l(k,r)$ are undetermined functions. Differentiation of (4) with respect to r yields

$$u_l'(k,r)=k[A_l(k,r)\hat{j}_l'(kr)-B_l(k,r)\hat{\eta}_l'(kr)]+\{A_l'(k,r)\hat{j}_l(kr)-B_l'(k,r)\hat{\eta}_l(kr)\}. \tag{5}$$

At this point we use the freedom of the method of variation of parameters to impose an extra constraint and require that the term in the curly bracket be zero such that

$$A_l'(k,r)\hat{j}_l(kr)-B_l'(k,r)\hat{\eta}_l(kr)=0. \tag{6}$$

This removes the derivatives of $A_l(k,r)$ and $B_l(k,r)$ and results in (5) taking the form

$$u_l'(k,r)=k[A_l(k,r)\hat{j}_l'(kr)-B_l(k,r)\hat{\eta}_l'(kr)]. \tag{7}$$

In the PFM one separates the radial wavefunction into an amplitude part $\alpha_l(k,r)$ and an oscillating part with the variable phase $\delta_l(k,r)$. Such a separation can be incorporated within the framework of our method provided we make the choice

$$A_l(k,r)=\alpha_l(k,r)\cos\delta_l(k,r) \tag{8a}$$

and

$$B_l(k,r)=\alpha_l(k,r)\sin\delta_l(k,r). \tag{8b}$$

From (2), (4), (7) and (8) we have

$$U_l(k,r)=\frac{k[\hat{j}_l'(kr)\cos\delta_l(k,r)-\hat{\eta}_l'(kr)\sin\delta_l(k,r)]}{[\hat{j}_l(kr)\cos\delta_l(k,r)-\hat{\eta}_l(kr)\sin\delta_l(k,r)]}. \tag{9}$$

Substituting (9) in (3) and making use of

$$\hat{Z}_l''(x)+[1-l(l+1)/x^2]\hat{Z}_l(x)=0 \tag{10}$$

we arrive at the phase equation

$$\delta_l'(k,r)=-k^{-1}V(r)[\hat{j}_l(kr)\cos\delta_l(k,r)-\hat{\eta}_l(kr)\sin\delta_l(k,r)]^2. \tag{11}$$

From (1) and (7) we have

$$A_l'(k,r)\hat{j}_l'(kr)-B_l'(k,r)\hat{\eta}_l'(kr)=k^{-1}V(r)u_l(k,r). \tag{12}$$

To get the amplitude equation we substitute (8a) and (8b) in (6) and (12). This gives

$$\alpha_l'(k,r)[\hat{j}_l(kr)\cos\delta_l(k,r)-\hat{\eta}_l(kr)\sin\delta_l(k,r)] \\ -\alpha_l(k,r)\delta_l'(k,r)[\hat{j}_l(kr)\sin\delta_l(k,r)+\hat{\eta}_l(kr)\cos\delta_l(k,r)]=0 \tag{13}$$

and

$$\alpha_l'(k,r)[\hat{j}_l'(kr)\cos\delta_l(k,r)-\hat{\eta}_l'(kr)\sin\delta_l(k,r)]$$
$$-\alpha_l(k,r)\delta_l'(k,r)[\hat{j}_l'(kr)\sin\delta_l(k,r)+\hat{\eta}_l'(kr)\cos\delta_l(k,r)]$$
$$=k^{-1}V(r)u_l(k,r). \tag{14}$$

Eliminating $\delta_l'(k,r)$ from (13) and (14) and making use of (4) and (8) we get the amplitude equation

$$\alpha_l'(k,r)=-k^{-1}V(r)\alpha_l(k,r)[\hat{j}_l(kr)\cos\delta_l(k,r)-\hat{\eta}l(kr)\sin\delta_l(k,r)]$$
$$\times[\hat{j}_l(kr)\sin\delta_l(k,r)+\hat{\eta}_l(kr)\cos\delta_l(k,r)]. \tag{15}$$

Traditionally, the PFM is developed either by using a Green function technique or by using an ansatz and a constraint [9] defined through (4), (7) and (8). The so-called Green function approach to the problem is a special instance of the more general Lagrange method used by us. Further, we have demonstrated the following.

(i) The constraint used for the PFM follows naturally from the freedom implied by the method of variation of parameters.

(ii) We have explored under which (additional) circumstances the Riccati form of the Schrödinger equation implies algorithms of the phase-function method.

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