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Physics Letters A 339 (2005) 83–88

PHYSICS LETTERS A

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A dressing of zero-range potentials and electron–molecule scattering problem at low energies

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Received 25 October 2004; received in revised form 10 January 2005; accepted 11 January 2005

Communicated by B. Fricke

Abstract

A dressing technique is used to improve zero range potential (ZRP) model. We consider a Darboux transformation starting with a ZRP, the result of the "dressing" gives a potential with non-zero range that depends on a seed solution parameters. Concepts of the partial waves and partial phases for non-spherical potential are used in order to perform Darboux transformation. The problem of scattering on the regular X_n and YX_n structures is studied. The results of the low-energy electron–molecule scattering on the dressed ZRPs are illustrated by model calculation for the configuration and parameters of the silane (SiH_4) molecule.

Keywords: Low-energy scattering; Multiple scattering; Ramsauer–Townsend minimum; Silane; Zero range potential

1. Introduction

The ideas of zero range potential (ZRP) approach were recently developed [1–3] to widen limits of the traditional treatment by Demkov and Ostrovsky [4] and Albeverio et al. [5]. The advantage of the theory is the possibility of obtaining an exact solution of scattering problem. The ZRP is conventionally represented as the boundary condition on the wave function at some point. Alternatively, the ZRP can be represented as pseudopotential (Breit [3,8]).

On the other hand, the factorization of a Schrödinger operator allows to construct in natural way exactly solvable potentials [9]. The method has the direct link to Darboux transformations (DT) theory [10]. General starting point of the theory goes up to the Matveev theorem (see, e.g., [11]). The transformation can be also defined on the base of covariance property of the Schrödinger equation with respect to a transformation of wave function and potential energy.

Darboux formulas in multi-dimensional space could be applied in the sense of Andrianov, Borisov

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doi:10.1016/j.physleta.2005.01.096

and Ioffe ideas [14] combined with ones for the radial Schrödinger equation [10,15]. In the circumstances, DT technique can be used so as to correct ZRP model.

We attempt to modify the ZRP by means of a special choice of DT in order to widen possibilities of the ZRP model (Section 2). In Section 3 we consider partial waves decomposition for a wave function for a non-spherical potential so as to dress a multi-centered potential, which includes n ZRPs [6]. The problem we consider is generic: it includes a three-dimensional potential. In order to construct DT we use results of division theory of differential operators [12]. As an important example, we consider electron scattering by the X_n and YX_n structures within the framework of the ZRP model (Section 4). In Section 5 we present our calculations of integral cross section for the electron–silane scattering on the base of the modified (dressed) ZRPs.

2. Zero range potentials and dressing

Our first observation shows that generalized ZRPs (see [1]) appear as a result of Darboux transformations. In order to demonstrate it we consider a radial Schrödinger equation for partial wave ψ_l with orbital momentum l. The atomic units are used throughout the present Letter $\hbar = m_e = 1$

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} + u_l - E\right)\psi_l(r) = 0, \tag{2.1}$$

where u_l are potentials for the partial waves with the following asymptotics at infinity

$$\psi_l(r) \sim \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr}. \tag{2.2}$$

Eq. (2.1) describes scattering of a particle with energy E and momentum $k = \sqrt{2E}$. In the absence of the potential, partial shifts $\delta_l = 0$ and partial waves can be expressed via Bessel functions with half-integer indices [7]. Let us demonstrate that generalized ZRP can be introduced by DT. For our purpose it is convenient to use a chain of DTs (Crum formulas [13] with the wave and prop functions multiplied by r), which for our equation look like

$$\psi_l^{(1)} = \text{const} \cdot \frac{W(r\psi_l, r\phi_1, \ldots, r\phi_{2l+1})}{rW(r\phi_1, \ldots, r\phi_{2l+1})}, \tag{2.3}$$

$$u_l^{(1)} = u_l - \bigl(\ln W(r\phi_1, \ldots, r\phi_{2l+1})\bigr)'', \tag{2.4}$$

where W is Wronskian, and

$$\phi_m = \sqrt{\frac{\pi}{2\kappa_m r}} H^{(1)}_{l+1/2}(\kappa_m r), \quad m = \overline{1, 2l+1} \tag{2.5}$$

and κ_m satisfy algebraical equation $\kappa_m^{2l+1} = \mathrm{i}\alpha_l$ with real α_l. Here we assume $u_l = 0$. The transformation (2.3) combines the solution ψ_l and functions ϕ_m. The Crum formulas result from the replacement of a chain of $2l + 1$ first order transformations by a single $(2l + 1)$th order transformation, which happens to be more efficient in practical calculations. Direct substitution of (2.5) to Wronskian shows that

$$W(r\phi_1, \ldots, r\phi_{2l+1}) = \text{const}. \tag{2.6}$$

It means that dressed potential $u_l^{(1)}(r > 0) = 0$. The transformation (2.4) allows to calculate potential in range $r > 0$. We state that DTs also yield a generalized ZRP at $r = 0$. In order to prove this we perform transformation (2.3) and show that $\psi_l^{(1)}$ is a solution for a generalized ZRP. Since potential is equal zero in the region $r > 0$, it is enough to determine asymptotic behavior of the wave function. Substituting $\psi_l = \sqrt{\frac{\pi}{2kr}} J_{l+1/2}(kr)$ to the Crum formulas, and using well-known properties of Bessel functions, we obtain

$$\psi_l^{(1)} \sim \text{const} \cdot \left\{(-\mathrm{i})^l \frac{\mathrm{e}^{\mathrm{i}kr}}{kr} \frac{\Delta(\mathrm{i}k, \kappa_1, \ldots, \kappa_{2l+1})}{\Delta(\kappa_1, \ldots, \kappa_{2l+1})} - \mathrm{i}^l \frac{\mathrm{e}^{-\mathrm{i}kr}}{kr} \frac{\Delta(-\mathrm{i}k, \kappa_1, \ldots, \kappa_{2l+1})}{\Delta(\kappa_1, \ldots, \kappa_{2l+1})}\right\}, \tag{2.7}$$

where Δ is Wandermond determinant. Considering one as the product

$$\Delta(\mathrm{i}k, \kappa_1, \ldots, \kappa_{2l+1}) = \text{const} \cdot \prod_{m=1}^{2l+1} (\kappa_m - \mathrm{i}k) \tag{2.8}$$

we obtain an asymptotics, which coincides with the asymptotics of the solution

$$\psi_l^{(1)} = \text{const} \cdot \bigl(H^{(1)}_{l+1/2}(kr)\mathrm{e}^{2\mathrm{i}\delta_l} - H^{(2)}_{l+1/2}(kr)\bigr),$$
$$\exp(2\mathrm{i}\delta_l) = \prod_{m=1}^{2l+1} \frac{\kappa_m - \mathrm{i}k}{\kappa_m + \mathrm{i}k}. \tag{2.9}$$

It easy to show that the wave function (2.9) describes a scattering by generalized ZRP with orbital momentum l. One is conventionally represented as the boundary condition at $r = 0$ on the wavefunction. It can be