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DRESSING OF ZERO-RANGE POTENTIALS INTO REALISTIC MOLECULAR POTENTIALS OF FINITE RANGE

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Abstract: The zero-range potentials of the radial Schrodinger equation and their dressing are investigated. A sequence of Darboux transformations involving a set of parameters yields solvable potentials of a finite-range with physically meaningful properties. In particular, the newly obtained potential is matched to that resulting from the *ab initio* computation methods in terms of discrete and continuous spectrum parameters. The approach, being a companion to conventional quantum simulation methods, combines symbolical and numerical calculations and is expected to work best for molecules with high spherical symmetry, typically fullerenes.

Keywords: effective potentials, zero-range potentials, Darboux transformation, dressing method, fullerenes

1. Introduction

In many situations heavy molecular calculations can be simplified by using effective potentials making any relevant evaluations easier. One of the simplest physically meaningful potential to treat is a point-potential and the corresponding approach that allows to grasp the geometrical structure of an object neglecting real interaction details at low energies is the so-called zero-range potential (ZRP) method. The method has been well developed up to now [1–6] and extended further into the generalized zero-range potential (gZRP) method that takes into account the effects of higher spherical waves in the scattering problem by matching the data with those obtained from an experiment or other calculations [7–12].

Within the framework of the present work, we focus on the ZRP approach and extend it by means of a dressing procedure in the form of the Darboux transformation (DT) [11, 10]. Multiple application of DT with certain parameters yields a potential of a finite range that captures the discrete and continuum spectra properties and, thus, is believed to appropriately describe a molecule.

2. Darboux transformation and dressing of ZRP

Let us consider the one-dimensional Sturm-Liouville equation:

$$L\psi = \lambda\psi \tag{1}$$

where

$$L = -\frac{d^2}{dx^2} + u(x) \tag{2}$$

Now we apply such algebraic-differential transformation (referred to as the Darboux transformation [13]):

$$D = \frac{d}{dx} - \sigma(x) \tag{3}$$

that the transformed equation preserves the same form:

$$L^{[1]}\psi^{[1]} = \lambda\psi^{[1]} \tag{4}$$

where $\psi^{[1]} = D\psi$, $L^{[1]} = -\frac{d^2}{dx^2} + u^{[1]}(x)$ and the transformed potential is:

$$u^{[1]}(x) = u(x) - 2\sigma'(x) \tag{5}$$

It is straightforward to check that:

$$\sigma(x) = \frac{\Phi_1'}{\Phi_1} \tag{6}$$

with Φ_1 being a particular solution to the original equation, *i.e.* it satisfies:

$$-\Phi_1'' + u(x)\Phi_1 = \lambda_1\Phi_1$$

for some λ_1.

It can be shown that in case of a multiple application of the Darboux transformation, the expression (6) is generalized into:

$$\sigma(x) = \frac{d}{dx}[\log W(\Phi_1, \ldots, \Phi_N)]$$

resulting in the following transformation of the potential:

$$u^{[N]}(x) = u(x) - 2\frac{d^2}{dx^2}[\log W(\Phi_1, \ldots, \Phi_N)] \tag{7}$$

The corresponding transformation of the solution is given by the Crum's formula [14, 15]:

$$\psi^{[N]} = D^{[N]}\psi = \frac{W(\Phi_1, \ldots, \Phi_N, \psi)}{W(\Phi_1, \ldots, \Phi_N)} \tag{8}$$

where W denotes the determinants of the Wronskian matrices.

In spherical geometry the Schrodinger equation

$$-\left(\psi''+\frac{2}{r}\psi'\right)=k^2\psi, \tag{9}$$

with notation $\psi=\psi(r)$ can be brought to the form (1) eligible for direct application of the obtained transformation formulas. Namely, performing substitution $\psi=\chi/r$, a one-dimensional wave equation with respect to χ is readily obtained while the potential term remains zero.

Therefore, the formulas (7) and (11) in spherical coordinates should be replaced with:

$$u^{[N]}(r)=-2\frac{d^2}{dr^2}\left[\log W(r\Phi_1,\ldots,r\Phi_N)\right] \tag{10}$$

and

$$\psi^{[N]}=D^{[N]}\psi=\frac{W(r\Phi_1,\ldots,r\Phi_N,r\psi)}{rW(r\Phi_1,\ldots,r\Phi_N)} \tag{11}$$

Following an idea of a previous work [10, 11], we state that the application of DT to the spherical Bessel function as seed solution:

$$\psi_0(r)=j_0(kr)=\sin(kr)/(kr) \tag{12}$$

with the Hankel function as the prop function:

$$\Phi_0(r)=h_0^{(1)}(-i\kappa_0 r)=\exp(\kappa_0 r)/(\kappa_0 r) \tag{13}$$

results in ZRP behavior of the transformed solution $\psi_0^{[1]}(r)$:

$$\psi^{[0]}(r)\equiv\psi_0^{[1]}(r)=C\left[s_0 h_0^{(1)}(kr)-h_0^{(2)}(kr)\right] \tag{14}$$

$$u_0^{[1]}(r)=0 \tag{15}$$

The obtained ZRP with characteristic κ_0 being pole $k=i\kappa_0$ of scattering matrix $s_0=-\frac{(k+i\kappa_0)}{(k-i\kappa_0)}$ can be represented as the boundary condition:

$$\left.\frac{d\log(r\psi)}{dr}\right|_{r=0}=-\kappa_0=-1/a_0 \tag{16}$$

with a_0 termed as the scattering length.

Next, the application of DT to (14) choosing the prop function as:

$$\Phi_1(r)=A_1 h_0^{(1)}(-i\kappa_1 r)+B_1 h_0^{(2)}(-i\kappa_1 r) \tag{17}$$

yields the finite range potential:

$$u^{[1]}(r)\equiv u_0^{[2]}(r)=-2\frac{d^2}{dr^2}\log\left[r\Phi_1(r)\right] \tag{18}$$

As follows from the Crum's formula (11), the behavior of the transformed solution $\psi_0^{[2]}$ is similar to (14) but only asymptotically:

$$\psi^{[1]}(r)\underset{r\to\infty}{\approx}C\left[s_0^{[1]}h_0^{(1)}(kr)-h_0^{(2)}(kr)\right] \tag{19}$$

while the scattering matrix $s_0^{[1]}=\frac{(k+i\kappa_0)(k+i\kappa_1)}{(k-i\kappa_0)(k-i\kappa_1)}$ contains one more pole $k=i\kappa_1$.

We note that the normalization constant value here is not the same as in (14), since we use C to denote the generic constant the value of which is not of particular importance.

Instead of single DT, one may perform a chain of N consecutive DTs applied to the ZRP solution (14) with prop functions:

$$\Phi_m(r) = A_m h_0^{(1)}(-i\kappa_m r) + B_m h_0^{(2)}(-i\kappa_m r), \qquad m = 1, \ldots, N \tag{20}$$

The solution transforms according to (11) and the asymptotical expansion still has the same form as (19):

$$\psi^{[N]}(r) \underset{r\to\infty}{\approx} C\left[s_0^{[N]} h_0^{(1)}(kr) - h_0^{(2)}(kr)\right] \tag{21}$$

with $s_0^{[N]} = (-1)^{N+1}\frac{(k+i\kappa_0)(k+i\kappa_1)\cdot\ldots\cdot(k+i\kappa_N)}{(k-i\kappa_0)(k-i\kappa_1)\ \ldots\ (k-i\kappa_N)}$.

Thus, using DT we may add scattering matrix poles $k = i\kappa_m$ lying on positive imaginary k-semiaxis (*i.e.* $\kappa_m > 0$) corresponding to the bounded states of the molecule that is considered as known (or may be found by solving the discrete spectrum problem using the ZRP formulation).

This tranformation yields finite range N-dressed potential according to the general expression (10).

We note that although the scattering matrix $s_0^{[N]}$ in (21) is independent of the choice of constants $A_m, B_m, m = 1, \ldots, N$, these constants (namely, the ratios A_m/B_m) affect the singular behavior of the transformed solution at the origin. This modifies the conventional ZRP boundary condition (16)

$$\left.\frac{d\log(r\psi)}{dr}\right|_{r=0} = \left(\frac{d}{dr}\frac{W(r\Phi_1, \ldots, r\Phi_N, r\psi)}{W(r\Phi_1, \ldots, r\Phi_N)}\right)\Bigg/\left.\frac{W(r\Phi_1, \ldots, r\Phi_N, r\psi)}{W(r\Phi_1, \ldots, r\Phi_N)}\right|_{r=0} = \text{const} \tag{22}$$

In the particular case $N = 1$, $A_1 = B_1$, this modification reads [11]:

$$\left.\frac{d\log(r\psi)}{dr}\right|_{r=0} = \frac{k^2 + \kappa_1^2}{\kappa_0} \tag{23}$$

3. Application

In order to obtain an analytical potential well describing a molecular structure, we apply the dressing method as described in the previous section choosing parameters of the prop functions (20) in a way that the obtained potential (10) must be physically meaningful.

As has been mentioned before, spectral parameters $\kappa_m, m = 0, \ldots, N$ might be chosen according to the discrete spectrum of the molecule.

The choice of constants $A_m, B_m, m = 1, \ldots, N$ gives freedom to tune the dressed potential to that obtained from *ab initio* calculations. However, one should be aware that a certain proportion of these constants leads to singular behavior at particular $r > 0$ that we consider unreasonable and which should be eliminated. Namely, for a single Darboux transformation this consideration leads to the restriction $B_1/A_1 \geq -1$.

The dressed potential can be adjusted by matching the partial shifts η_l governing the continuous spectrum solutions.

In the Born approximation we have [16]:

$$\eta_l \approx -\frac{2\mu}{\hbar^2} k \int_0^\infty j_l^2(kr) U(r) r^2 dr \tag{24}$$

Hence, in this case, the problem of matching phase shifts resorts to consequent minimization of functions at high values of k and large l (such that the Born approximation is valid):

$$F_l(A_1, B_1, \ldots, A_N, B_N) = \frac{2\mu}{\hbar^2} k \left| \int_0^\infty j_l^2(kr) \left[U(r) - u^{[N]}(r) \right] r^2 dr \right| \tag{25}$$

where $U(r)$ is the averaged radial potential obtained from *ab initio* computations.

Evidently, the best results should be obtained for nearly isotropic molecules for which the most reasonable action is averaging over angles to obtain the radial potential. Typical examples of these structures are fullerenes, and such averaged radial potential has been dealt with in [17].

As an example of the application of the described dressing procedure, in Figure 1 we demonstrate the finite range solvable potential obtained for the following set of parameters: $\kappa_1 = 1.66$, $\kappa_2 = 1.57$, $\kappa_3 = 1.39$, $\kappa_4 = 1.29$, $A_1 = -2$, $B_1 = -5$, $A_2 = 1$, $B_2 = 4$, $A_3 = -3$, $B_3 = 2$, $A_4 = 7$, $B_4 = 9$ [18].

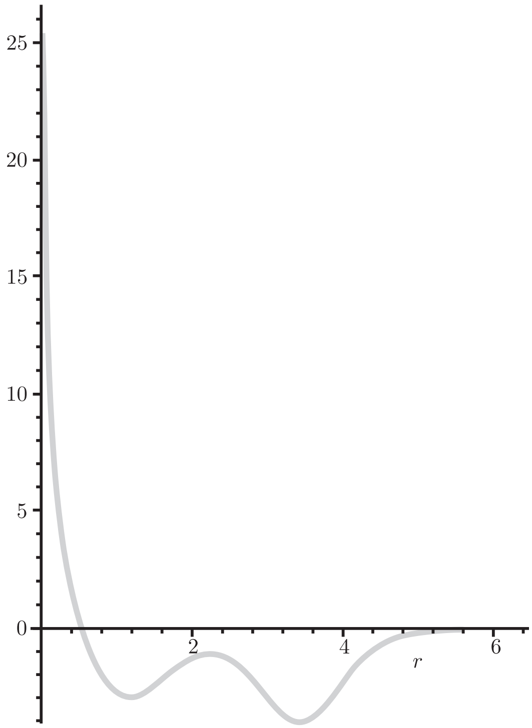

Figure 1. An example of solvable finite range potential obtained by dressing procedure

4. Conclusions

The approach described in the present work offers an alternative to the gZRP description. The final potential obtained by the chain of DT applied to ZRP is of a finite range and may be adjusted to possess physically meaningful properties. This can be achieved by matching discrete spectrum levels and partial waves phase shifts with those obtained by *ab initio* computational methods. The effective potential obtained in such way, preserving the spectral structure of the molecule, can be used in further calculations where the material constituents are molecules, not atoms, that will significantly simplify the computation cost.

The algorithm is expected to be beneficially applied for isotropic molecules. A typical application might be a description of fullerenes.

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