Full three-dimensional Equivalent Local Potential by an extension of the Wronskian method

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Abstract

A generalization of the Wronskian relation for the Schrödinger equation in three dimensions is found. This generalization is used to calculate an equivalent local potential for arbitrary, non-rotationally invariant non-local potentials, by an extension of Fiedeldey's Wronskian method. The final equations are given in a matrix notation, and the differences to Fiedeldey's results are discussed. For the special cases of mirror and cylindrical symmetry, the resulting simplifications are examined.

1 Introduction

In order to describe scattering of a projectile by a many-body target in a one-particle picture, one generally uses non-local potentials, often also called optical potentials [1–7]. However, a *local* picture of the scattering and of the nuclear, atomic or molecular potential is often desirable in order to make the physical processes more clear. To this end, one can try to find a so-called equivalent local potential (ELP) which is constructed in a way so that the asymptotic behaviour of the wave function and the spectrum of the original Hamilton operator (which included the non-local potential) are reproduced.

In nuclear as well as in atomic physics, the non-local potentials are in general rotationally invariant, and the resulting ELP is taken to be spherically symmetric. Several well-established methods are known for finding such a potential - see e.g. [4, 8–12] for applications in nuclear physics and [13, 14] for atomic physics; for a review which compares different methods, see [15]. However, in applications in molecular physics, the non-local potentials (optical potentials) are in general not rotationally invariant, and the ELP can not be spherically symmetric. Additionally, even in nuclear physics one sometimes has to deal with potentials which are only cylindrically symmetric (prolate and oblate nuclei). To our knowledge, no attempt was made so far to extend the well-established methods mentioned above to a treatment of full three-dimensional problems.

Our approach here is based on the Wronskian method, which was first presented by Fiedeldey in [9]. After introducing our terminology in section 2, we present in section 3 a three-dimensional analogue to the well-known fact that the Wronskian for two linearly independent solutions of the one-dimensional Schrödinger equation is constant. Using this generalized Wronskian relation leads us in section 4 to matrix equations for the ELP as well as the Perey factor [16]. Section 5 deals with

the simplifications which arise in the presence of mirror and cylindrical symmetry. Finally section 6 contains our summary and some concluding remarks.

2 Terminology and basic equations

Let us begin by stating the problem more precisely: Given is a wave function $\psi(\vec{r})$ satisfying the Schrödinger equation with a non-local potential $\Sigma(\vec{r},\vec{r}')$:

$$-\frac{1}{2}\Delta\psi(\vec{r}) + \int d^3r'\Sigma(\vec{r},\vec{r}')\psi(\vec{r}') = E\psi(\vec{r}). \tag{1}$$

The goal now is to find an ELP $V(\vec{r})$ and a so-called local wave function $\phi(\vec{r})$ satisfying

$$-\frac{1}{2}\Delta\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) = E\phi(\vec{r}) \tag{2}$$

such that

$$\psi(\vec{r}) = f(\vec{r})\phi(\vec{r}) \tag{3}$$

with

$$f(\vec{r}) \to 1 \quad \text{for } |\vec{r}| \to \infty. \tag{4}$$

The function f is called the Perey factor [16].

In order to reduce this problem to a set of coupled one-dimensional equations, we now make a partial wave expansion (PWE) of the functions as well as the potentials:

$$\begin{aligned}
\psi(\vec{r}) &= \frac{1}{r}\sum_{lm}\psi_{lm}(r)Y_{lm}(\theta,\varphi) \\
\phi(\vec{r}) &= \frac{1}{r}\sum_{lm}\phi_{lm}(r)Y_{lm}(\theta,\varphi) \\
V_{lml'm'}(r) &= 2\int d\Omega Y^*_{lm}(\theta,\varphi)V(\vec{r})Y_{l'm'}(\theta,\varphi) \\
\Sigma_{lml'm'}(r,r') &= 2\int d\Omega\int d\Omega' Y^*_{lm}(\theta,\varphi)rr'\Sigma(\vec{r},\vec{r}')Y_{l'm'}(\theta',\varphi')
\end{aligned}$$

and introduce the usual abbreviation $k^2 = 2E$. This yields now the following equations for the coefficients of the non-local and the local wave functions:

$$\psi''_{lm}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\psi_{lm}(r) - \sum_{l'm'}\int dr'\Sigma_{lml'm'}(r,r')\psi_{l'm'}(r') = 0 \tag{5}$$

$$\phi''_{lm}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\phi_{lm}(r) - \sum_{l'm'}V_{lml'm'}(r)\phi_{l'm'}(r) = 0. \tag{6}$$

Additionally, we introduce a partial wave expansion for the Perey factor:

$$f_{lml'm'}(r) = \int d\Omega Y^*_{lm}(\theta,\varphi)f(\vec{r})Y_{l'm'}(\theta,\varphi) \to \delta_{ll'}\delta_{mm'} \quad \text{for } r\to\infty. \tag{7}$$

Inserting this into the equations (5,6), one is lead to the following relation between

the non-local potential and the ELP:

$$\begin{aligned}
&\sum_{l'm'l''m''} f_{lml'm'}(r)V_{l'm'l''m''}(r)\phi_{l''m''}(r) \\
= &\sum_{l'm'} f_{lml'm'}(r)\phi_{l'm'}(r)\left(\frac{l(l+1)}{r^2}-\frac{l'(l'+1)}{r^2}\right) \\
- &\ 2\sum_{l'm'} f'_{lml'm'}(r)\phi'_{l'm'}(r) - \sum_{l'm'} f''_{lml'm'}(r)\phi_{l'm'}(r) \\
+ &\sum_{l'm'l''m''}\int \Sigma_{lml'm'}(r,r')f_{l'm'l''m''}(r')\phi_{l''m''}(r')dr'. \qquad (8)
\end{aligned}$$

We now define the abbreviation

$$f^L_{lml'm'}(r) = f_{lml'm'}(r)\left(\frac{l(l+1)}{r^2}-\frac{l'(l'+1)}{r^2}\right)$$

and introduce a matrix notation for V, Σ, f and f^L, and, correspondingly, a vector notation for ϕ. Then the equation above takes the simple form

$$\mathbf{f}(r)\mathbf{V}(r)\vec{\phi}(r) = \mathbf{f}^L(r)\vec{\phi}(r) - 2\mathbf{f}'(r)\vec{\phi}'(r) - \mathbf{f}''(r)\vec{\phi}(r) + \int \mathbf{\Sigma}(r,r')\mathbf{f}(r')\vec{\phi}(r')dr'. \quad (9)$$

This equation, which is analogous to eq. (6) in [9], will be our starting point for constructing the ELP.

3 The three-dimensional Wronskian relation

In order to proceed as in [9], we now have to express $\vec{\phi}(r')$ in eq. (9) by a suitable linear combination of $\vec{\phi}(r)$ and $\vec{\phi}'(r)$. To this end, we introduce functions ω_{lm} which solve the following equations:

$$\omega''_{lm}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\omega_{lm}(r) - \sum_{l'm'} V_{l'm'lm}(r)\omega_{l'm'}(r) = 0 \qquad (10)$$

Note the change in the order of the indices of V, compared to (6). If one defines

$$\omega(\vec{r}) = \frac{1}{r}\sum_{lm}\omega_{lm}(r)Y^*_{lm}(\theta,\varphi) = \frac{1}{r}\sum_{lm}\omega_{lm}(r)Y_{lm}(\theta,-\varphi)$$

(note the complex conjugation of the spherical harmonic), then $\omega(\vec{r})$ fulfills the same equation (2) as $\phi(\vec{r})$. Using these functions, we now get:

$$\begin{aligned}
&\frac{d}{dr}\sum_{lm}\left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) \\
= &\sum_{lm}\left(\omega_{lm}(r)\phi''_{lm}(r) - \omega''_{lm}(r)\phi_{lm}(r)\right) \\
= &\sum_{lml'm'}\left(\omega_{lm}(r)V_{lml'm'}(r)\phi_{l'm'}(r) - \phi_{lm}(r)V_{l'm'lm}(r)\omega_{l'm'}(r)\right) \\
= &\ 0
\end{aligned}$$

and hence

$$\sum_{lm}\left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) = const.$$

These results for the PWE coefficients can also be expressed by the full functions:

$$\begin{aligned}
&\sum_{lm} \left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) \\
= \;& r^2 \int d\Omega \left[\omega(\vec{r}) \left(\frac{d}{dr} + \frac{1}{r}\right) \phi(\vec{r}) - \phi(\vec{r}) \left(\frac{d}{dr} + \frac{1}{r}\right) \omega(\vec{r})\right] \\
= \;& r^2 \int d\Omega \left[\omega(\vec{r}) \frac{d}{dr}\phi(\vec{r}) - \phi(\vec{r}) \frac{d}{dr}\omega(\vec{r})\right]
\end{aligned}$$

and hence

$$\begin{aligned}
&\frac{d}{dr} \sum_{lm} \left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) \\
= \;& r^2 \int d\Omega \left[\omega(\vec{r}) \left(\frac{d^2}{dr^2} + \frac{2}{r}\right) \phi(\vec{r}) - \phi(\vec{r}) \left(\frac{d^2}{dr^2} + \frac{2}{r}\right) \omega(\vec{r})\right] \\
= \;& r^2 \int d\Omega \left[\omega(\vec{r})\Delta\phi(\vec{r}) - \phi(\vec{r})\Delta\omega(\vec{r})\right] \\
= \;& 0,
\end{aligned}$$

where it was used that the square of the angular momentum operator is hermitean, and that both ϕ and ω fulfill (2). It follows that

$$r^2 \int d\Omega \left[\omega(\vec{r}) \frac{d}{dr}\phi(\vec{r}) - \phi(\vec{r}) \frac{d}{dr}\omega(\vec{r})\right] = const.,$$

in complete accordance with the results above. This expresses a generalization of the well-known fact that for two linear independent solutions of the one-dimensional Schrödinger equation, the Wronskian is constant. We will discuss later under which circumstances one can prove that two functions exist for which this constant is non-zero, and give the proof in the appendix.

4 Matrix equations for ELP and Perey factor

Here we simply assume that two sets of functions which satisfy (3) with a non-zero constant exist, and choose their normalizations in a way so that

$$\begin{aligned}
\sum_{lm} \left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) &= r^2 \int d\Omega \left[\omega(\vec{r}) \frac{d}{dr}\phi(\vec{r}) - \phi(\vec{r}) \frac{d}{dr}\omega(\vec{r})\right] \\
&= 1. \qquad (11)
\end{aligned}$$

We then define

$$\begin{aligned}
\alpha_{l'm'lm}(r', r) &= \phi'_{lm}(r)\omega_{l'm'}(r') - \omega'_{lm}(r)\phi_{l'm'}(r') = -\frac{d}{dr}\beta_{l'm'lm}(r', r) \\
\beta_{l'm'lm}(r', r) &= \omega_{lm}(r)\phi_{l'm'}(r') - \phi_{lm}(r)\omega_{l'm'}(r'). \qquad (12)
\end{aligned}$$

This implies:

$$\sum_{lm} \left(\alpha_{l'm'lm}(r', r)\phi_{lm}(r) + \beta_{l'm'lm}(r', r)\phi'_{lm}(r)\right) = \phi_{l'm'}(r'), \qquad (13)$$

or, by introducing a matrix notation for α and β:

$$\vec{\phi}(r') = \boldsymbol{\alpha}(r', r)\vec{\phi}(r) + \boldsymbol{\beta}(r', r)\vec{\phi}'(r). \qquad (14)$$

Inserting all of the PWEs again, this leads to

$$\phi(\vec{r}\,') = r^2 \int d\Omega \left[\alpha(\vec{r}\,', \vec{r}) \phi(\vec{r}) + \beta(\vec{r}\,', \vec{r}) \left(\partial_r + \frac{1}{r} \right) \phi(\vec{r}) \right]$$

with

$$\begin{aligned} \alpha(\vec{r}\,', \vec{r}) &= \left(\partial_r + \frac{1}{r} \right) \left[\phi(r, \theta, -\varphi) \omega(r', \theta', -\varphi') - \omega(r, \theta, \varphi) \phi(r', \theta', \varphi') \right] \\ &= -\left(\partial_r + \frac{1}{r} \right) \beta(\vec{r}\,', \vec{r}) \\ \beta(\vec{r}\,', \vec{r}) &= \omega(r, \theta, \varphi) \phi(r', \theta', \varphi') - \phi(r, \theta, -\varphi) \omega(r', \theta', -\varphi'). \end{aligned}$$

Hence now we have managed to express ϕ at the point $\vec{r}\,'$ by the values of ϕ and its normal derivative $\partial_r \phi$ on a whole surface. This is reminiscent of the Cauchy boundary conditions which are necessary to specify a solution of the Schrödinger equation uniquely.

Inserting (14) into our equation (9) for the ELP, we get:

$$\begin{aligned} \mathbf{f}(r)\mathbf{V}(r)\vec{\phi}(r) &= \mathbf{f}^L(r)\vec{\phi}(r) - 2\mathbf{f}'(r)\vec{\phi}\,'(r) - \mathbf{f}''(r)\vec{\phi}(r) \qquad (15) \\ &+ \int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\alpha}(r', r) dr' \vec{\phi}(r) + \int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\beta}(r', r) dr' \vec{\phi}\,'(r). \end{aligned}$$

If we now require that

$$\int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\beta}(r', r) dr' \vec{\phi}\,'(r) - 2\mathbf{f}'(r)\vec{\phi}\,'(r) = 0, \qquad (16)$$

analogously to [9], this results in

$$\mathbf{f}(r)\mathbf{V}(r)\vec{\phi}(r) = \mathbf{f}^L(r)\vec{\phi}(r) - \mathbf{f}''(r)\vec{\phi}(r) + \int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\alpha}(r', r) dr' \vec{\phi}(r). \qquad (17)$$

Sufficient conditions for (16) and (17) to be satisfied are

$$\mathbf{f}'(r) = \frac{1}{2} \int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\beta}(r', r) dr' \qquad (18)$$

$$\mathbf{V}(r) = \mathbf{f}^{-1}(r)\mathbf{f}^L(r) - \mathbf{f}^{-1}(r)\mathbf{f}''(r) + \mathbf{f}^{-1}(r) \int \mathbf{\Sigma}(r, r')\mathbf{f}(r')\boldsymbol{\alpha}(r', r) dr'. \qquad (19)$$

These equations are now almost completely analogous to the eqs. (11) and (12) in [9] (note the different conventions for the order of the arguments of α and β). The additional term $\mathbf{f}^L$ which appears here expresses the fact that the angular momentum barrier changes when the particle is scattered from an l''-state into an l-state.

Exactly like the equations given in [9], this system of coupled differential equations can be solved by an iterative procedure: choose an initial approximation for $V(\vec{r})$ and $f(\vec{r})$ resp. their PWEs, solve (6) for $\phi_{lm}(r)$ and (10) for $\omega_{lm}(r)$, calculate $\alpha_{l'm'lm}(r', r)$ and $\beta_{l'm'lm}(r', r)$ from them and use these results to obtain a new, improved approximation to the PWEs of $V(\vec{r})$ and $f(\vec{r})$ by solving (18) and (19). Repeat this procedure until convergence is obtained. When solving (18), pay attention to the boundary conditions for $f_{lml'm'}(r)$ given in (7).

One can also obtain equations for the functions f and V themselves by contracting (18) and (19) with vectors of spherical harmonics from the left and the right. The results are:

$$\left(\partial_r + \frac{1}{r} \right) f(r, \theta_1, \varphi_1) \delta(\Omega_1 - \Omega_2) = \frac{1}{2} \int d^3r' \Sigma(\vec{r}\,', r, \theta_1, \varphi_1) f(\vec{r}\,') \beta(\vec{r}\,', r, \theta_2, \varphi_2) \qquad (20)$$

and

$$\begin{aligned} & \Big[f(r,\theta_1,\varphi_1)V(r,\theta_1,\varphi_1) - \Delta_r f(r,\theta_1,\varphi_1)\Big]\delta(\Omega_1-\Omega_2) \\ = & \int d^3r' \Sigma(r,\theta_1,\varphi_1,\vec{r}\,')f(\vec{r}\,')\alpha(\vec{r}\,',r,\theta_2,\varphi_2), \end{aligned} \tag{21}$$

where Δ_r denotes the radial part of the Laplacian. Note that the term with f^L has cancelled out here. Because of the delta function $\delta(\Omega_1 - \Omega_2)$ for the solid angles which appears in these equations, they are rather impractial to solve directly; it is easier to solve the coupled systems of equations (18) and (19) for the partial wave coefficients iteratively, and compute the full three-dimensional ELP only after the calculation has converged.

5 Special symmetries

In the presence of certain symmetries, our results can be simplified. First we discuss the C_s symmetry (which is rather common at least for small molecules) - specifically, a mirror symmetry at the x-z-plane:

$$\begin{aligned} \Sigma(r,\theta,-\varphi,r',\theta',-\varphi') &= \Sigma(r,\theta,\varphi,r',\theta',\varphi') \\ V(r,\theta,-\varphi) &= V(r,\theta,\varphi). \end{aligned}$$

In this case, the PWE coefficients of the ELP are symmetric with respect to an interchange of (l,m) and (l',m'). Then (10) becomes identical to (6), i.e. the ω_{lm} obey the same equations as the ϕ_{lm}. For this special case, we prove in the appendix that there always exist two solutions ϕ_{lm} and ω_{lm} which satisfy (3) with a constant different from zero.

Additionally, the wavefunctions can be chosen to be symmetric or antisymmetric with respect to this reflection:

$$\psi(r,\theta,-\varphi) = \pm\psi(r,\theta,\varphi).$$

(and analogously for ϕ). This implies that the nodes of the wavefunctions also lie symmetric to the x-z-plane. Since the Perey factor was originally introduced in [9] in order to avoid the nodes of ψ (and therefore the poles of the 'trivial' ELP), one can choose the Perey factor to have also this mirror symmetry:

$$f(r,\theta,-\varphi) = f(r,\theta,\varphi).$$

This implies that the PWE coefficients of the Perey factor are also symmetric with respect to an interchange of (l,m) and (l',m'), like the ELP. Hence it suffices to calculate only the upper or lower half of $\mathbf{f}$ and $\mathbf{V}$ in every iteration step, which saves approximately half of the necessary computation time. Alternatively, one could calculate the whole matrices and use the requirement of symmetry as a check for the calculation.

Even further simplifications occur in the rather special case of cylindrical symmetry, which is present in linear molecules, and also relevant for prolate and oblate nuclei. What we want to consider here is a non-local potential which is invariant under simultaneous rotation of φ and φ':

$$\Sigma(r,\theta,\varphi+\alpha,r',\theta',\varphi'+\alpha) = \Sigma(r,\theta,\varphi,r',\theta',\varphi') \quad \forall\,\alpha$$

and a corresponding rotationally invariant ELP:

$$V(r,\theta,\varphi+\alpha) = V(r,\theta,\varphi) \quad \forall\,\alpha.$$

Both of these potentials conserve the z component of angular momentum, so that their PWEs expansions take the special form

$$\begin{aligned} \Sigma_{lml'm'}(r,r') &= \Sigma^{(m)}_{ll'}(r,r')\delta_{mm'} \\ V_{lml'm'}(r) &= V^{(m)}_{ll'}(r)\delta_{mm'}. \end{aligned}$$

Since cylindrical symmetry implies mirror symmetry at the x-z-plane, the ELP is symmetric in the indices l and l'. The wavefunctions can now be chosen to be eigenfunctions of the z component of the angular momentum. If ψ is an eigenfunction with eigenvalue m, it has the property

$$\psi(r,\theta,\varphi+\alpha) = \psi(r,\theta,\varphi)e^{im\alpha} \quad \forall\, \alpha.$$

This implies that if $\psi(r,\theta,\varphi) = 0$ for particular values of r, θ and φ, then $\psi(r,\theta,\varphi) = 0$ for *all* values of φ, i. e. the nodes of the wavefunctions are independent of φ. Again one can argue that since the Perey factor was introduced in order to avoid the nodes of ψ, it suffices to make the following ansatz here:

$$f(\vec{r}) = f(r,\theta),$$

i.e., choose the Perey factor as a cylindrically symmetric function, like the ELP itself. This implies that its PWE also conserves the z component of angular momentum:

$$f_{lml'm'}(r) = f^{(m)}_{ll'}(r)\delta_{mm'}.$$

Because of the symmetry in the indices of $\mathbf{V}$, ϕ and ω obey the same equation:

$$\phi''_{lm}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\phi_{lm}(r) - \sum_{l'} V^{(m)}_{ll'}(r)\phi_{l'm}(r) = 0,$$

and, correspondingly, in the generalized Wronskian relation, there is no sum over m - in contrast, there is now an infinite amount of such relations, which have to be true for *all* m:

$$\sum_l \left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) = const. \quad \forall\, m$$

Defining

$$\begin{aligned} \alpha^{(m)}_{l'l}(r',r) &= \phi'_{lm}(r)\omega_{l'm}(r') - \omega'_{lm}(r)\phi_{l'm}(r') = -\frac{d}{dr}\beta^{(m)}_{l'l}(r',r) \\ \beta^{(m)}_{l'l}(r',r) &= \omega_{lm}(r)\phi_{l'm}(r') - \phi_{lm}(r)\omega_{l'm}(r') \end{aligned}$$

and introducing matrices and vectors again, but here with an extra index m, we can proceed now exactly as in the general case. Our final results look almost equal to the former ones:

$$\mathbf{f}'^{(m)}(r) = \frac{1}{2}\int \mathbf{\Sigma}^{(m)}(r,r')\mathbf{f}^{(m)}(r')\boldsymbol{\beta}^{(m)}(r',r)dr' \tag{22}$$

$$\begin{aligned} \mathbf{V}^{(m)}(r) &= \left(\mathbf{f}^{(m)}\right)^{-1}(r)\mathbf{f}^{(m)L}(r) - \left(\mathbf{f}^{(m)}\right)^{-1}(r)\mathbf{f}''^{(m)}(r) \\ &\quad + \left(\mathbf{f}^{(m)}\right)^{-1}(r)\int \mathbf{\Sigma}^{(m)}(r,r')\mathbf{f}^{(m)}(r')\boldsymbol{\alpha}^{(m)}(r',r)dr'. \end{aligned} \tag{23}$$

The crucial simplification compared to the coupled system of differential equations (18,19) is that the cylindrical symmetry enabled us to decouple that system into several smaller ones (one for each value of m investigated), which can be independently solved.

6 Summary and concluding remarks

We have generalized Fiedeldey's one-dimensional approach to the problem of finding an ELP by using a Wronskian relation to the general three-dimensional case. The generalized Wronskian is expected to be non-zero. This is proven in the appendix for the special cases of mirror and cylindrical symmetry. We used the derived generalized Wronskian relation to find matrix equations for the ELP as well as the Perey factor, which closely resemble Fiedeldey's original equations [9]. The main difference is that in the three-dimensional case, where angular momentum is in general not conserved, an additional factor appears which takes account of the change in the angular momentum barrier due to scattering into another angular momentum channel. We have also shown which simplifications occur in the special cases of C_s symmetry and cylindrical symmetry - both are relevant in molecular physics and the second also in nuclear physics.

For completeness it would be desirable to express the Perey factor exclusively by the solutions of the non-local Schrödinger equation (1) (like eq. (17) in [9]). Unfortunately this can not be done as straightforwardly as in [9], since $f(\vec{r})\omega(\vec{r})$ is not again a solution to (1), in contrast to the spherically symmetric case. This is due to the changed order of indices in (10), compared to (6).

Even in the case of mirror symmetric ELPs, where the ω_{lm} obey the same equation as the ϕ_{lm} and hence $\lambda(\vec{r}) := f(\vec{r})\omega(\vec{r})$ *is* a solution to (1), multiplying (18) from the right with $\mathbf{f}(r)$ leads only to an equation with $\mathbf{f}'(r)\mathbf{f}(r)$ on the left hand side, which can not be written as the derivative of $\mathbf{f}^2(r)$ directly, since the matrices in general do not commute. This problem can be remedied by taking the trace on both sides of the equation after multiplying it - but the resulting equation

$$\frac{d}{dr}\mathrm{Tr}\left(\mathbf{f}^2(r)\right) = \frac{d}{dr}\left(\vec{\psi}'(r)\cdot\vec{\lambda(r)} - \vec{\lambda}'(r)\cdot\vec{\psi(r)}\right)$$

is not very helpful in determining $\mathbf{f}(r)$ either. Perhaps it could be used as a check on the calculation, if one has both of the non-local solutions already available.

But even without being able to express $f(\vec{r})$ exclusively in terms of the solutions of the non-local Schrödinger equation, the formulas derived here should be a valuable tool for finding ELPs even for the non-spherically symmetric potentials common in molecular and other areas of physics.

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Appendix

Here we prove that for a system of differential equations like (6), with a symmetrical matrix $\mathbf{V}$ (which corresponds to a C_s symmetry and hence also applies in the case of cylindrical symmetry), one can find at least two solutions ϕ_{lm} and ω_{lm} which satisfy

$$\sum_{lm}\left(\omega_{lm}(r)\phi'_{lm}(r) - \omega'_{lm}(r)\phi_{lm}(r)\right) \neq 0. \qquad \text{(A-1)}$$

If we define

$$\pi_{lm}(r) = \phi'_{lm}(r),$$

the system (6) is equivalent to the system of differential equations of first order

$$\begin{aligned}\phi'_{lm}(r) &= \pi_{lm}(r) \\ \pi'_{lm}(r) &= \left(\frac{l(l+1)}{r^2} - k^2\right)\phi_{lm}(r) + \sum_{l'm'} V_{lml'm'}(r)\phi_{l'm'}(r). \end{aligned} \tag{A-2}$$

Now we look at the approximation where only N components of the PWE are used. The system (A-2) then consists of $2N$ differential equations of first order for $2N$ functions. For each solution of this system, we introduce the $2N$-dimensional column vector

$$\vec{\Phi}(r) = (\phi_{00}(r), \pi_{00}(r), \phi_{01}(r), \pi_{01}(r), \phi_{11}(r), \pi_{11}(r), \ldots)^T.$$

From the theory of ordinary differential equations, we know that such a system has $2N$ linearly independent solutions $\vec{\Phi}^{(j)}$, $1 \le j \le 2N$ [17], i.e. the determinant of the Wronskian matrix

$$\mathbf{\Phi} = (\vec{\Phi}^{(1)}, \vec{\Phi}^{(2)}, \ldots, \vec{\Phi}^{(2N)})$$

is different from zero.

The statement (A-1) we want to prove can now be rewritten as: there exists at least one pair (j,k) of solutions to (A-2) with $j \neq k$ so that

$$\sum_{lm} \left(\phi^{(j)}_{lm}(r)\pi^{(k)}_{lm}(r) - \phi^{(k)}_{lm}(r)\pi^{(j)}_{lm}(r)\right) \neq 0. \tag{A-3}$$

As an abbreviation for this expression, we introduce the notation

$$\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(k)}.$$

The product $\odot$ of two vectors $\vec{\Phi}^{(j)}$ and $\vec{\Phi}^{(k)}$ is essentially a sum of commutators and therefore bilinear and antisymmetric.

For a set $M = \{1, 2, \ldots 2N\} \subset \mathbf{N}$, we now define the set $\mathcal{C}_M$ consisting of all $(2N-1)!!$ partitions of M into ordered pairs of elements of M; e.g. for $N = 2$, we have $M = \{1,2,3,4\}$ and $\mathcal{C}_M = \{((1,2),(3,4)),((1,3),(2,4)),((1,4),(2,3))\}$. For $p \in \mathcal{C}_M$, we define: p_{n1} gives the first and p_{n2} the second element of the pair n in the partition p, e.g. for $p = ((1,3),(2,4))$, $p_{12} = 3$. Additionally, we define for every p the corresponding permutation π_p by

$$\pi_p = \begin{pmatrix} 1 & 2 & 3 & 4 & \ldots & 2N-1 & 2N \\ p_{11} & p_{12} & p_{21} & p_{22} & \cdots & p_{N1} & p_{N2} \end{pmatrix},$$

and use this to assign a signum to p:

$$\mathrm{sgn}(p) = \mathrm{sgn}(\pi_p).$$

For example, for $p = ((1,3),(2,4))$, $\mathrm{sgn}(p) = -1$, since for the permutation

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 4 \end{pmatrix},$$

$\mathrm{sgn}(\pi) = -1$. Finally we define the following function of the matrix $\mathbf{\Phi}$ of solutions to (A-2):

$$D(\mathbf{\Phi}) = \sum_{p \in \mathcal{C}_M} \mathrm{sgn}(p) \prod_{n=1}^{N} \vec{\Phi}^{(p_{n1})} \odot \vec{\Phi}^{(p_{n2})}.$$

Again e.g. for $N = 2$, this function is given by

$$\begin{aligned} D(\mathbf{\Phi}) &= \left(\vec{\Phi}^{(1)} \odot \vec{\Phi}^{(2)}\right)\left(\vec{\Phi}^{(3)} \odot \vec{\Phi}^{(4)}\right) \\ &- \left(\vec{\Phi}^{(1)} \odot \vec{\Phi}^{(3)}\right)\left(\vec{\Phi}^{(2)} \odot \vec{\Phi}^{(4)}\right) \\ &+ \left(\vec{\Phi}^{(1)} \odot \vec{\Phi}^{(4)}\right)\left(\vec{\Phi}^{(2)} \odot \vec{\Phi}^{(3)}\right). \end{aligned}$$

Using the bilinearity of the product $\odot$, it is easy to see that the function $D(\mathbf{\Phi})$ is multilinear (linear in all $\vec{\Phi}^{(j)}$). Additionally, for the unit matrix $\mathbf{E}$ we get

$$D(\mathbf{E}) = 1,$$

hence the function is normalized. We now show that $D(\mathbf{\Phi})$ is also alternating, i. e. it is zero if for two indices j and k with $j \neq k$, $\vec{\Phi}^{(j)} = \vec{\Phi}^{(k)}$). In the sum over all $(2N-1)!!$ partitions, there are $(2N-3)!!$ addends in which $\vec{\Phi}^{(j)}$ and $\vec{\Phi}^{(k)}$ are directly multiplied by $\odot$. Because of the antisymmetry of the product, these addends are zero. In the other $((2N-1)!! - (2N-3)!!) \in 2\mathbb{N}$ addends, $\vec{\Phi}^{(j)}$ and $\vec{\Phi}^{(k)}$ appear in different pairs. Without loss of generality, we can assume $j < k$. We now look at a particular partition p. Let the other element of the pair in which $\vec{\Phi}^{(j)}$ appears be $\vec{\Phi}^{(j')}$ and the other element of the pair in which $\vec{\Phi}^{(k)}$ appears be $\vec{\Phi}^{(k')}$. Then there are four possible cases:

1. $j < j'$, $k < k'$
2. $j < j'$, $k > k'$
3. $j > j'$, $k < k'$
4. $j > j'$, $k > k'$

In case 1, the partition p looks like

$$p = (\ldots(j, j')\ldots(k, k')\ldots),$$

where the dots stand for the remaining pairs. For every such partition p, exactly one partition p' exists in which j is paired with k' and k with j', and all the other pairs are equal to the ones in p. Here one has to distinguish two cases (the other two can not appear because of our assumption $j < k$):

a. $j < k'$, $k < j'$

b. $j < k'$, $k > j'$

In case 1a, the partition p' looks like

$$p' = (\ldots(j, k')\ldots(k, j')\ldots).$$

Here we have $\mathrm{sgn}(p') = -\mathrm{sgn}(p)$, and therefore we get for the two corresponding addends in $D(\mathbf{\Phi})$:

$$\begin{aligned} & \mathrm{sgn}(p)\left[\ldots\left(\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(j')}\right)\ldots\left(\vec{\Phi}^{(k)} \odot \vec{\Phi}^{(k')}\right)\ldots\right] \\ & +\mathrm{sgn}(p')\left[\ldots\left(\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(k')}\right)\ldots\left(\vec{\Phi}^{(k)} \odot \vec{\Phi}^{(j')}\right)\ldots\right] \\ = \; & \mathrm{sgn}(p)\Big[\ldots\left(\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(j')}\right)\ldots\left(\vec{\Phi}^{(k)} \odot \vec{\Phi}^{(k')}\right)\ldots \\ & -\ldots\left(\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(k')}\right)\ldots\left(\vec{\Phi}^{(k)} \odot \vec{\Phi}^{(j')}\right)\ldots\Big] \\ = \; & 0 \qquad\qquad \text{for } \vec{\Phi}^{(j)} = \vec{\Phi}^{(k)}. \end{aligned}$$

In case 1b, the partition p' looks like

$$p' = (\ldots(j,k')\ldots(j',k)\ldots).$$

Here we have $\mathrm{sgn}(p') = \mathrm{sgn}(p)$ and therefore we get for the two corresponding addends in $D(\mathbf{\Phi})$:

$$\begin{aligned}
& \mathrm{sgn}(p)\left[\ldots\left(\vec{\Phi}^{(j)}\odot\vec{\Phi}^{(j')}\right)\ldots\left(\vec{\Phi}^{(k)}\odot\vec{\Phi}^{(k')}\right)\ldots\right] \\
& +\mathrm{sgn}(p')\left[\ldots\left(\vec{\Phi}^{(j)}\odot\vec{\Phi}^{(k')}\right)\ldots\left(\vec{\Phi}^{(j')}\odot\vec{\Phi}^{(k)}\right)\ldots\right] \\
= \; & \mathrm{sgn}(p)\Big[\ldots\left(\vec{\Phi}^{(j)}\odot\vec{\Phi}^{(j')}\right)\ldots\left(\vec{\Phi}^{(k)}\odot\vec{\Phi}^{(k')}\right)\ldots \\
& -\ldots\left(\vec{\Phi}^{(j)}\odot\vec{\Phi}^{(k')}\right)\ldots\left(\vec{\Phi}^{(k)}\odot\vec{\Phi}^{(j')}\right)\ldots\Big] \\
= \; & 0 \qquad\qquad \text{for } \vec{\Phi}^{(j)} = \vec{\Phi}^{(k)},
\end{aligned}$$

where the antisymmetry of the product $\odot$ was used. The other cases (2-4) can be treated analogously. Hence we have proven now that, if $\vec{\Phi}^{(j)} = \vec{\Phi}^{(k)}$ $(j \neq k)$, for every partition p, there exists exactly one partition p' such that the corresponding addends in the sum in $D(\mathbf{\Phi})$ add up to zero - and this implies that for $\vec{\Phi}^{(j)} = \vec{\Phi}^{(k)}$ $(j \neq k)$, $D(\mathbf{\Phi}) = 0$.

We have shown now that D is a multilinear, normalized and alternating function of $\mathbf{\Phi}$. These are exactly the properties of the determinant, hence we conclude

$$D(\mathbf{\Phi}) = \det \mathbf{\Phi}.$$

Now the proof of our statement becomes quite easy - we use a proof by contradiction: Assume that for every pair of indices (j,k) with $j \neq k$

$$\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(k)} = 0.$$

This would imply

$$D(\mathbf{\Phi}) = 0,$$

and hence

$$\det \mathbf{\Phi} = 0.$$

But this is a contradiction, because the determinant of the Wronskian for the $2N$ solutions of (A-2) is non-zero.

Hence we can conclude that there is at least one pair of indices (j,k) with $j \neq k$ for which

$$\vec{\Phi}^{(j)} \odot \vec{\Phi}^{(k)} \neq 0,$$

which completes our proof.

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