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General Non-local Potentials

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I. INTRODUCTION

Non-local central potentials for the Nijmegen soft-core interactions were first treated in [1]. The treatment with the inclusion of a non-local tensor potential was presented at the Graz-conference in 1978 and published in the Proceedings [2]. In this note we include next to the non-local central- and the non-local tensor potential also a non-local spin-orbit potential.

Of course, the case with only a central non-local potential present is the simplest one, and the familiar Green transformation brings the radial Schrödinger equation into its 'normal' form, i.e. the form it has for the usual local NN-potentials.

In the case with a non-local tensor potential one needs a more complicated generalized Green transformation matrix B, henceforth denoted by $A^{-1/2}$. A simplifying feature is that in this case the matrix A has the form $A = f_C(r) + f_T(r)\ S_{12}$, so that it commutes with its derivatives A', A''. In these notes, we add a non-local spin-orbit potential. Then, it will turn out that $A \neq M$, where $M = f_C(r) + f_T(r)\ S_{12} + f_{LS}(r)\ \mathbf{L}\cdot\mathbf{S}$, as one would guess from the case with the non-local tensor potential. Since for the triplet-coupled case $[\mathbf{L}\cdot\mathbf{S}, S_{12}] \neq 0$, the treatment given in the Graz-Proceedings has to be modified, since $[A, A'] \neq 0$ etc. For the 2-dimensional triplet-coupled waves, the correct solution turns out to be $\sqrt{M}$ times an r-dependent rotation. So, the Green transformation is not symmetric in the general case.

We note that adding a non-local quadratic-spin-orbit potential does not bring extra complications beyond the case with the non-local spin-orbit. This, because also the Q_{12}-operator is diagonal like the $\mathbf{L}\cdot\mathbf{S}$-operator and the treatment with the non-local Q_{12}- term is the same as for the case where both a non-local S_{12} and a $\mathbf{L}\cdot\mathbf{S}$-term are present.

II. DERIVATION RADIAL SCHRÖDINGER EQUATION FOR NON-LOCAL POTENTIALS

The Schrödinger equation for a non-local central potential reads (units $\hbar = c = 1$)

$$\left[-\frac{1}{2M_{red}}\boldsymbol{\nabla}^2 + V - \left(\boldsymbol{\nabla}^2\frac{\Phi}{2M_{red}} + \frac{\Phi}{2M_{red}}\boldsymbol{\nabla}^2\right)\right]\ \psi(\mathbf{r}) = E\ \psi(\mathbf{r})\ , \tag{1}$$

where the operator Φ is defined as

$$\Phi = \phi(r) + \chi(r)\ S_{12} + \rho(r)\ \mathbf{L}\cdot\mathbf{S}\ . \tag{2}$$

We write

$$\boldsymbol{\nabla}^2 = \Delta_r - \frac{\mathbf{L}^2}{r^2}\quad ,\quad \text{with } \Delta_r = \frac{2}{r}\frac{d}{dr} + \frac{d^2}{dr^2} \tag{3}$$

We note that

$$\Delta_r S_{12} = \Delta_r \mathbf{L}\cdot\mathbf{S} = 0\quad ,\quad \text{and}\ \left[\mathbf{L}^2, \mathbf{L}\cdot\mathbf{S}\right] = 0\ . \tag{4}$$

Then, for a general LSJ-state we write the wave function in the form

$$\psi(\mathbf{r}) = \frac{u(r)}{r}\ \mathcal{Y}^M_{LSJ}(\hat{\mathbf{r}})\ , \tag{5}$$

and find, because $\Delta_r(u/r) = u''/r$,

$$\boldsymbol{\nabla}^2\ \psi(\mathbf{r}) = \frac{1}{r}\left[u'' - \frac{\mathbf{L}^2}{r^2}u\right]\ \mathcal{Y}^M_{LSJ}(\hat{\mathbf{r}})\ . \tag{6}$$

Now, from

$$\Delta_r\left(\Phi\ \frac{u}{r}\right) = \frac{1}{r}\left[\Phi\ u'' + 2\Phi'\ u' + \Phi''\ u\right]\ , \tag{7}$$

it follows rather straightforwardly that

$$\begin{aligned}\boldsymbol{\nabla}^2\ \left(\Phi\ \frac{u}{r}\ \mathcal{Y}^M_{LSJ}\right) &= \left\{\Delta_r\left(\Phi\ \frac{u}{r}\right) - \frac{\mathbf{L}^2}{r^2}\left(\Phi\ \frac{u}{r}\right) - \frac{1}{r^2}\left[\mathbf{L}^2, S_{12}\right]_-\ \left(\chi\frac{u}{r}\right)\right\}\mathcal{Y}^M_{LSJ} \\ &= \frac{1}{r}\left[\Phi\ u'' + 2\Phi'\ u' + \Phi''\ u - \frac{\mathbf{L}^2}{r^2}\ \Phi\ u - \frac{1}{r^2}\left[\mathbf{L}^2, S_{12}\right]_-\ \chi\ u\right]\ \mathcal{Y}^M_{LSJ}\ .\end{aligned} \tag{8}$$

Now, multiplying (1) by $-2M_{red}$, defining $U = 2M_{red}\ V$, and $k^2 = 2M_{red}E$, obtains with the preparations given above, in a straightforward manner the radial Schrödinger equation

$$(1+2\Phi)\ u_l'' + 2\Phi'\ u_l' + \left[\left(k^2 - U\right) - (1+2\Phi)\frac{\mathbf{L}^2}{r^2} - \frac{\chi}{r^2}\left[\mathbf{L}^2, S_{12}\right]_- + \Phi''\right]\ u_l = 0\ , \tag{9}$$

III. GENERALIZED GREEN TRANSFORMATION

Written in full, equation (9) reads

$$\begin{aligned}&\left\{(1+2\phi) + 2\chi\ S_{12} + 2\rho\ \mathbf{L}\cdot\mathbf{S}\right\}\ u'' + \left(2\phi' + 2\chi'\ S_{12} + 2\rho'\ \mathbf{L}\cdot\mathbf{S}\right)u' + \\ &\left[\left[k^2 - 2m_{red}\ V\right] - \left\{(1+2\phi) + \chi\ S_{12} + \rho\ \mathbf{L}\cdot\mathbf{S}\right\}\ \frac{\mathbf{L}^2}{r^2} - \frac{\mathbf{L}^2}{r^2}\ \chi\ S_{12} + \right. \\ &\left.\left(\phi'' + \chi''\ S_{12} + \rho''\ \mathbf{L}\cdot\mathbf{S}\right)\right]\ u = 0\ .\end{aligned} \tag{10}$$

The generalized Green transformation

$$\begin{aligned}u &= A^{-1/2}\ v\ , \\ u' &= \left(A^{-1/2}\right)'\ v + A^{-1/2}\ v'\ , \\ u'' &= \left(A^{-1/2}\right)''\ v + 2\left(A^{-1/2}\right)'\ v' + A^{-1/2}\ v''\ ,\end{aligned} \tag{11}$$

which, when substituted into (10), gives

$$\begin{aligned}
&\Big(1+2\Phi\Big)\ A^{-1/2}\ v'' + \Big[2\Big(1+2\Phi\Big)\ \Big(A^{-1/2}\Big)' + 2\Phi'\ A^{-1/2}\Big]\ v' + \\
&\Big\{\Big(1+2\Phi\Big)\ \Big(A^{-1/2}\Big)'' + 2\Phi'\Big(A^{-1/2}\Big)' + \Big[\Big[k^2 - 2m_{red}\ V\Big] - \\
&\Big(1+2\Phi\Big)\ \frac{\mathbf{L}^2}{r^2} - \frac{\mathbf{L}^2}{r^2}\ \chi\ S_{12} + \Phi''\Big]\ A^{-1/2}\ \Big\}\ v = 0\ .
\end{aligned} \tag{12}$$

We note that in the last square bracket, we have actually the expression

$$\Big[\dots\Big] = \Big[\Big[k^2 - 2m_{red}\ V\Big] - (1+2\phi)\,\frac{\mathbf{L}^2}{r^2} + \chi\ \Big[S_{12}, \frac{\mathbf{L}^2}{r^2}\Big]_- + \Phi''\Big]\ . \tag{13}$$

Requiring that the first derivatives of the wave function $v(r)$ disappear leads to

$$0 = 2\Big\{(1+2\phi) + 2\chi\ S_{12} + 2\rho\ \mathbf{L}\cdot\mathbf{S}\Big\}\ \Big(A^{-1/2}\Big)' + 2\Big(\phi' + \chi'\ S_{12} + \rho'\ \mathbf{L}\cdot\mathbf{S}\Big)\ A^{-1/2}\ . \tag{14}$$

We rewrite this equation schematically as

$$0 = M\ \Big(A^{-1/2}\Big)' + N\ A^{-1/2}\ , \tag{15}$$

where, obviously,

$$\begin{aligned}
M &= (1+2\phi) + 2\chi\ S_{12} + 2\rho\ \mathbf{L}\cdot\mathbf{S}\ , \\
N &= \phi' + \chi'\ S_{12} + \rho'\ \mathbf{L}\cdot\mathbf{S} = \frac{1}{2}M'\ .
\end{aligned} \tag{16}$$

Of course, $M \equiv 1 + 2\Phi$, but in view of the case of the triplet-coupled states on which space the Φ-operator acts as a 2×2-matrix, we denote this 2×2-matrix by M.

In the following, we deal only with the triplet-coupled waves. This is technically the most complex and difficult case. The singlet and the triplet-uncoupled cases are straightforward and completely analogous to the case where there is only a central non-local interaction. As such a case has been dealt with in [1], we do not treat this here since the adaption to the case with tensor and spin-orbit non-localities is obvious.

IV. DERIVATION NEW DIFFERENTIAL EQUATION

We start the derivation of A in equation (15), with the observation that the 2×2-matrices M, N are symmetric. However, we can not assume that also the matrix A is symmetric. When nevertheless doing so we would find, following the same procedure as in the case of the Graz-Proceedings paper, that $A = M$. But, as it turned out, this is not a correct solution of equation (15). We therefore have to follow a more subtle route to the solution. Equation (15) reads

$$\boxed{\Big(A^{-1/2}\Big)' = -\frac{1}{2}\Big(M^{-1}\ M'\Big)\ A^{-1/2}\ .} \tag{17}$$

Writing $B = A^{-1/2}$, we have the equation

$$B' = -\frac{1}{2}\left(M^{-1}\ M'\right)\ B\ \rightarrow\ M^{1/2}\ B' = -\frac{1}{2}\left(M^{-1/2}\ M'\ M^{-1/2}\right)\ \left(M^{1/2}\ B\right)\ , \tag{18}$$

where in the 'commutative' case, i.e. with no non-local spin-orbit, we have that $M^{1/2}\ B \rightarrow 1$. Using now

$$\left(M^{1/2}\ B\right)' = M^{1/2}\ B' + \left(M^{1/2}\right)'\ B\ , \tag{19}$$

we find for $C \equiv M^{1/2}\ B$, the differential equation

$$C'(r) = \left[-\frac{1}{2}\left(M^{-1/2}\ M'\ M^{-1/2}\right) + \left(M^{1/2}\right)'\ M^{-1/2}\right] \cdot C(r) \tag{20}$$

At this point it is convenient to use the auxiliary matrix $N \equiv M^{1/2}$. Then,

$$\begin{aligned}\left(M^{1/2}\right)'\ M^{-1/2} \equiv N'\ N^{-1} &= \frac{1}{2}\left(N'\ N^{-1} + N^{-1}\ N'\right)\\ &+\frac{1}{2}\left(N'\ N^{-1} - N^{-1}\ N'\right)\ ,\end{aligned} \tag{21}$$

and also

$$\frac{1}{2}\left(M^{-1/2}\ M'\ M^{-1/2}\right) = \frac{1}{2}\left(N^{-1}\ M'\ N^{-1}\right) = \frac{1}{2}\left(N'\ N^{-1} + N^{-1}\ N'\right)\ . \tag{22}$$

From equations (20)-(22) we obtain the surprisingly simple differential equation

$$\boxed{C'(r) = \frac{1}{2}\left[N'\ N^{-1} - N^{-1}\ N'\right]\ C(r)\quad ,\quad N \equiv M^{1/2}\ .} \tag{23}$$

We note at this point that if $[N', N] = 0$, i.e. when $\rho(r) = 0$ in (16), we have from (23) $C' = 0$. Imposing the condition that $C(r) \rightarrow 1$, for $r \rightarrow \infty$, which is the right physical boundary condition, gives $C = 1$. So, in this case we rediscover the Graz-solution:

$$A = M = \Big(1 + 2\Phi\Big) = (1 + 2\phi) + 2\chi\ S_{12}\ . \tag{24}$$

V. SOLUTION OF THE C AND A-EQUATIONS

Before starting with the actual solution, we first assemble some technical material needed in the construction of the solution. The tensor operator

$$S_{12} = 3\,(\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}})\,(\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\ , \tag{25}$$

has on the basis

$$\mathcal{Y}^M_{JLS} = \sum_{m,\mu} C^{L\ S\ J}_{m\ \mu\ M} Y^{(L)}_m(\theta,\phi)\ \chi^{(S)}_\mu\ , \tag{26}$$

for the triplet-coupled states the matrix elements

$$S_{12} = \frac{1}{2J+1}\begin{pmatrix} -2J+2 & 6\sqrt{J(J+1)} \\ 6\sqrt{J(J+1)} & -2J-4 \end{pmatrix}\ . \tag{27}$$

Note that in the definition of the base states (28), we have not included the phase-factor i^L, which is often included for convenient time-reversal properties (see e.g. [4]).
The $\mathbf{L}^2$-operator, and the $\mathbf{L}\cdot\mathbf{S}$-operator have on the same basis the matrix elements

$$\mathbf{L}\cdot\mathbf{S} = \begin{pmatrix} (J-1) & 0 \\ 0 & -(J+2) \end{pmatrix}\ \ ,\ \ \mathbf{L}^2 = \begin{pmatrix} (J-1)J & 0 \\ 0 & (J+1)(J+2) \end{pmatrix}\ . \tag{28}$$

Now, it is clear from the expressions given above together with the fact that $[\mathbf{L}^2, S_{12}] \neq 0$, that

$$[M', M]_- \neq [M'', M]_- \neq 0\ . \tag{29}$$

Using now a technique analogously to the Graz-paper, by writing e.g.

$$A^{1/2} = \alpha + \beta\ S_{12} + \gamma\ \mathbf{L}\cdot\mathbf{S} + \delta\ \ [\mathbf{L}\cdot\mathbf{S}, S_{12}]\ , \tag{30}$$

would not work because the algebra of the operators S_{12} and $\mathbf{L}\cdot\mathbf{S}$ is not closed under multiplication. Therefore, we proceed as follows. We write all 2×2-matrices in terms

$$\tau_0 = I\ \ ,\ \ \tau_1 = \sigma_1\ \ ,\ \ \tau_2 = -i\sigma_2\ \ ,\ \ \tau_3 = \sigma_3\ , \tag{31}$$

where τ_2 is anti-symmetric and all others are symmetric. So, we rewrite

$$\boxed{\begin{aligned} M &= (1+2\phi) + 2\chi\ S_{12} + 2\rho\ \mathbf{L}\cdot\mathbf{S} \\ &= a(r)\ \tau_0 + b(r)\ \tau_1 + c(r)\ \tau_3\ , \end{aligned}} \tag{32}$$

Making the τ-expansions for the tensor and the spin-orbit matrices,

$$\begin{aligned} S_{12} &= \frac{1}{2J+1}\Big(-(2J+1) + 6\sqrt{J(J+1)}\ \tau_1 + 3\tau_3\Big)\ , \\ \mathbf{L}\cdot\mathbf{S} &= \frac{1}{2}\Big(-3 + (2J+1)\ \tau_3\Big)\ , \end{aligned} \tag{33}$$

we find that

$$
\begin{aligned}
& a=(1+2\phi)-2\chi-3\rho \quad , \quad b=12\frac{\sqrt{J(J+1)}}{2J+1}\ \chi \ , \\
& c=(2J+1)\ \rho+\frac{6}{2J+1}\ \chi \ .
\end{aligned} \tag{34}
$$

From the τ-expansion in (32) it is easily seen that

$$
M^{-1}=\left[a-b\ \tau_1-c\ \tau_3\right]/D \quad , \quad \text{where} \quad D=\det M=a^2-b^2-c^2 \ . \tag{35}
$$

Similarly to M and M^{-1}, we get from $N^2=M$ that

$$
\begin{aligned}
N=M^{1/2}&=\alpha(r)+\beta(r)\ \tau_1+\gamma(r)\ \tau_3 \\
N^{-1}=M^{-1/2}&=\left[\alpha(r)-\beta(r)\ \tau_1-\gamma(r)\ \tau_3\right]/\mathcal{D} \ ,
\end{aligned} \tag{36}
$$

with

$$
\begin{aligned}
& \mathcal{D}=\alpha^2-\beta^2-\gamma^2=\sqrt{D} \ , \quad \text{and} \\
& \alpha=\frac{1}{\sqrt{2}}\left(a+\sqrt{D}\right)^{1/2} \quad , \quad \beta=\frac{b}{2\alpha} \quad , \quad \gamma=\frac{c}{2\alpha} \ .
\end{aligned} \tag{37}
$$

From (36) we derive that

$$
\begin{aligned}
N'\ N^{-1} &= \left(\alpha'+\beta'\ \tau_1+\gamma'\ \tau_3\right)\left(\alpha-\beta\ \tau_1-\gamma\ \tau_3\right)/\mathcal{D} \\
&= \Big[\ (\alpha\alpha'-\beta\beta'-\gamma\gamma')+(\alpha\beta'-\beta\alpha')\ \ \tau_1+(\alpha\gamma'-\gamma\alpha')\ \ \tau_3 \\
&\qquad +(\beta\gamma'-\gamma\beta')\ \ \tau_2\ \Big]/\mathcal{D} \ .
\end{aligned} \tag{38}
$$

Equation (38) and using $N^{-1}N'=\left(N'N^{-1}\right)^T$, we obtain

$$
\frac{1}{2}\left(N'\ N^{-1}-N^{-1}\ N'\right)=\mathcal{D}^{-1}\ \ (\beta\gamma'-\gamma\beta')\ \ \tau_2\equiv f(r)\ \tau_2 \ . \tag{39}
$$

Using the expressions in (37) leads to

$$
\begin{aligned}
f(r)=\mathcal{D}^{-1}\ \ (\beta\gamma'-\gamma\beta') &= \frac{1}{2}\left(b\ c'-c\ b'\right)\frac{\sqrt{D}}{a+\sqrt{D}}\cdot\frac{1}{D} \\
&\approx \frac{1}{2}\left(b\ c'-c\ b'\right)=6\sqrt{J(J+1)}\left(\chi\ \rho'-\rho\ \chi'\right) \ .
\end{aligned} \tag{40}
$$

Using these results, we see that the differential equation (23) becomes

$$C'(r) = (f(r)\ \tau_2)\ C(r) \quad , \quad C(r) = \exp\left[-\left(\int_r^\infty\ f(r)dr\right)\ \tau_2\right] \ . \tag{41}$$

In (41) we imposed the boundary condition $C(r) \to 1$, for $r \to \infty$.
Exploiting $\tau_2^2 = -1$, we can rewrite $C(r)$ as follows

$$\boxed{C(r) \equiv e^{-\theta(r)\ \tau_2} = \cos(\theta(r)) - \sin(\theta(r))\ \tau_2 \quad , \quad \text{where } \theta(r) = \int_r^\infty\ f(r)dr \ .} \tag{42}$$

From the solution (42) [1] we obtain the solution for the Green transformation (11).
We have

$$\boxed{A^{-1/2} = M^{-1/2}\ C(r) = M^{-1/2}\left[\cos(\theta(r)) - \sin(\theta(r))\ \tau_2\right] \equiv M^{-1/2}\ R^{-1}(\theta) \ ,} \tag{43}$$

where introduced the notation $R(\theta)$, which is a rotation. The inverse of (43) reads

$$A^{1/2} = \left[\cos(\theta(r)) + \sin(\theta(r))\ \tau_2\right]\ M^{1/2} = R(\theta)\ M^{1/2} \ . \tag{44}$$

In the following we assume that $\theta(r) << 1$, and make the approximation that $A^{-1/2} \approx M^{-1/2}$, and so

$$A \approx M = (1 + 2\phi) + 2\chi\ S_{12} + 2\rho\ \mathbf{L}\cdot\mathbf{S} \ . \tag{45}$$

VI. TRANSFORMED SCHRÖDINGER EQUATION

The radial Schrödinger equation (12) after the elimination of the u'-term reads

$$\boxed{\begin{aligned} & v'' + \left[\left(A^{1/2}\ \left(A^{-1/2}\right)'' + A^{1/2}\ \left(M^{-1}M'\right)\left(A^{-1/2}\right)'\right) + \left\{A^{1/2}\ M^{-1}\left(k^2 - 2m_{red}V\right)\ A^{-1/2}\right.\right. \\ & \left.\left. -A^{1/2}\frac{L^2}{r^2}\ A^{-1/2} - A^{1/2}\ M^{-1}\frac{L^2}{r^2}S_{12}\ \chi\ A^{-1/2} + \frac{1}{2}A^{1/2}\ M^{-1}\ M''\ A^{-1/2}\right\}\right]\ v = 0 \ . \end{aligned}} \tag{46}$$

---

[1] We note from (42) that $\theta'(r) = -f(r)$, which can be solved easily by e.g. making an algorithm based on Adams interpolation formula, see Abramowitz and Stegun [3], formula 25.5.5.

A. Approximate Treatment Schrödinger Equation

In making the approximation (45), the radial Schrödinger equation (46) becomes

$$v'' + \Big[A^{-1/2}\ A\ \left(A^{-1/2}\right)'' + A^{-1/2}\ A'\ \left(A^{-1/2}\right)' + \Big\{A^{-1/2}\ k^2\ A^{-1/2} - 2m_{red}A^{-1/2}\ V\ A^{-1/2}$$
$$-A^{1/2}\frac{L^2}{r^2}\ A^{-1/2} + \frac{1}{2r^2}A^{-1/2}\left[A, L^2\right]_-\ A^{-1/2} + \frac{1}{2}A^{-1/2}\ A''\ A^{-1/2}\Big\}\Big]\ v = 0\ . \tag{47}$$

(i) We notice that

$$A^{-1/2}\ k^2\ A^{-1/2} = A^{-1}\ k^2 = k^2 + \left(A^{-1} - 1\right)\ k^2\ . \tag{48}$$

(ii) We notice that

$$\begin{aligned}
&-A^{1/2}\frac{L^2}{r^2}\ A^{-1/2} + \frac{L^2}{r^2} + \frac{1}{2r^2}A^{-1/2}\left[A, L^2\right]_-\ A^{-1/2} = \\
&-\frac{1}{2r^2}\left[A^{1/2}\ L^2\ A^{-1/2} + A^{-1/2}\ L^2\ A^{1/2}\right] + \frac{L^2}{r^2} = \\
&-\frac{1}{2r^2}\left\{A^{1/2}\ \left[L^2, A^{-1/2}\right]_- + A^{-1/2}\ \left[L^2, A^{1/2}\right]_-\right\}\ .
\end{aligned} \tag{49}$$

We now cast (47) into the standard form

$$\boxed{v'' + \left[k^2 - 2m_{red}\ W - \frac{L^2}{r^2}\right]\ v = 0\ . \qquad (50)}$$

with

$$\begin{aligned}
-2m_{red}\ W \equiv &\left\{A^{-1/2}\ A\ \left(A^{-1/2}\right)'' + A^{-1/2}\ A'\ \left(A^{-1/2}\right)'\right\} + \left(A^{-1} - 1\right) k^2 \\
&-2m_{red}\ A^{-1/2}\ V\ A^{-1/2}B + \frac{1}{2}A^{-1/2}\ A''\ A^{-1/2} \\
&-\left\{\left[A^{1/2}\ L^2\ A^{-1/2} - L^2\right]\frac{1}{r^2} - \frac{1}{2r^2}A^{-1/2}\left[A, L^2\right]\ A^{-1/2}\right\} \\
= &-2m_{red}\ A^{-1/2}\ V\ A^{-1/2} + \left(A^{-1} - 1\right)\ k^2 \\
&-\frac{1}{2r^2}\left\{A^{1/2}\left[L^2, A^{-1/2}\right]_- + A^{-1/2}\left[L^2, A^{1/2}\right]_-\right\} \\
&+\left\{A^{-1/2}\ A\ \left(A^{-1/2}\right)'' + A^{-1/2}\ A'\ \left(A^{-1/2}\right)'\right\} + \frac{1}{2}A^{-1/2}\ A''\ A^{-1/2}\ .
\end{aligned} \tag{51}$$

Or,

$$
\boxed{\begin{aligned}
2m_{red}\ W = 2m_{red}\ A^{-1/2}\ V\ A^{-1/2} - \left(A^{-1}-1\right)\ k^2 - \frac{1}{2}A^{-1/2}\ A''\ A^{-1/2} \\
+\frac{1}{2r^2}\left\{A^{1/2}\left[L^2, A^{-1/2}\right]_- + A^{-1/2}\left[L^2, A^{1/2}\right]_-\right\} \\
-\left\{A^{-1/2}\ A\ \left(A^{-1/2}\right)'' + A^{-1/2}\ A'\ \left(A^{-1/2}\right)'\right\}\ . \qquad (52)
\end{aligned}}
$$

We can simplify equation (52) by using our approximation (45) also in the differential equation (17). The latter reads approximately

$$
\left(A^{-1/2}\right)' \approx -\frac{1}{2}\left(A^{-1}\ A'\right)\ A^{-1/2}\ . \tag{53}
$$

Then,

$$
\left(A^{-1/2}\right)'' \approx -\frac{1}{2}\left[\left(A^{-1}\right)'\ A'\ A^{-1/2} + A^{-1}\ A''\ A^{-1/2} - \frac{1}{2}\ A^{-1}\ A'\ A^{-1}\ A'\ A^{-1/2}\right]\ . \tag{54}
$$

Using that $(A^{-1})' = -A^{-1}i\ A'\ A^{-1}$ we obtain from (54)

$$
A^{-1/2}\ A\ \left(A^{-1/2}\right)'' \approx -\frac{1}{2}\left[-\frac{3}{2}A^{-1/2}A'A^{-1}A'A^{-1/2} + A^{-1/2}\ A''\ A^{-1/2}\right] \tag{55}
$$

B Also, using again (53), one has

$$
A^{-1/2}\ A'\ \left(A^{-1/2}\right)' \approx -\frac{1}{2}\ A^{-1/2}A'A^{-1}A'A^{-1/2}\ . \tag{56}
$$

Then, in (52) using (55)-(56) we can cast the following terms into a compact expression, as follows

$$
\begin{aligned}
&-\frac{1}{2}A^{-1/2}\ A''\ A^{-1/2} - \left\{A^{-1/2}\ A\ \left(A^{-1/2}\right)'' + A^{-1/2}\ A'\ \left(A^{-1/2}\right)'\right\} \approx \\
&-\frac{1}{4}A^{-1/2}\ A'\ A^{-1}\ A'\ A^{-1/2} = -\frac{1}{4}\left(A^{-1/2}\ A'\ A^{-1/2}\right)^2\ .
\end{aligned} \tag{57}
$$

Equation (52) then becomes approximately:

$$
\boxed{\begin{aligned}
2m_{red}\ W \approx 2m_{red}\ A^{-1/2}\ V\ A^{-1/2} - \left(A^{-1}-1\right)\ k^2 - \frac{1}{4}\left(A^{-1/2}\ A'\ A^{-1/2}\right)^2 \\
+\frac{1}{2r^2}\left\{A^{1/2}\left[L^2, A^{-1/2}\right]_- + A^{-1/2}\left[L^2, A^{1/2}\right]_-\right\}\ . \qquad (58)
\end{aligned}}
$$

Note that the 'effective' potential W in (58) is very similar to the expression in the Graz-Proceedings, with however a more general A-matrix.

We note that

$$\mathbf{L}^2 = \left(J^2+J+1\right) - (2J+1)\ \sigma_3\ , \tag{59}$$

and so

$$\left[L^2, A^{-1/2}\right]_- = -(2J+1)\frac{2\beta}{\alpha^2-\beta^2-\gamma^2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\ , \left[L^2, A^{1/2}\right]_- = (2J+1)\cdot\ 2\beta\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\ , \tag{60}$$

Then,

$$\boxed{\left\{A^{1/2}\left[L^2, A^{-1/2}\right]_- + A^{-1/2}\left[L^2, A^{1/2}\right]_-\right\} = -(2J+1)\frac{4\beta\gamma}{\alpha^2-\beta^2-\gamma^2}\left[\frac{\beta}{\gamma}\ \sigma_3 - \sigma_1\right]\ .} \tag{61}$$

B. Exact Treatment Schrödinger Equation

The method used in the approximation of the last subsection, can also be applied to the unapproximated equation (46). This, with only a few modifications.

(i) Non-local terms: From the differential equation (17), we find the analog of equation (54)

$$\begin{aligned}\left(A^{-1/2}\right)'' &= -\frac{1}{2}\left(M^{-1}M'\right)\ \left(A^{-1/2}\right)' - \frac{1}{2}\left((M^{-1})'\ M'\right)\ A^{-1/2} \\ &-\frac{1}{2}\left(M^{-1}\ M''\right)\ A^{-1/2}\ .\end{aligned} \tag{62}$$

In equation (46), this expression is multiplied by $A^{1/2}$. One then sees easily that the last term in (46) is cancelled by the last term in (62). Therefore, we find for the following terms between the square brackets in (46)

$$\begin{aligned}&\left(\ldots\right) + \frac{1}{2}A^{1/2}\ M^{-1}\ M''\ A^{-1/2} = \\ &-\frac{1}{2}\left[A^{1/2}\left(M^{-1}M'\right)\left(A^{-1/2}\right)' + A^{1/2}\left((M^{-1})'\ M'\right)\ A^{-1/2}\right]\ .\end{aligned} \tag{63}$$

Now, using equation (17) again, and $(M^{-1})' = -M^{-1}M'M^{-1}$, we find that the above expression becomes

$$\boxed{-\frac{1}{4}A^{1/2}\ M^{-1}\ M'\ M^{-1}\ M'\ A^{-1/2} = -\frac{1}{4}R\ \left(M^{-1/2}\ M'\ M^{-1/2}\right)^2\ R^{-1}\ .} \tag{64}$$

Notice that for $R \to 1$, this expression becomes identical to (57).

(ii) Kinetic and Potential terms: Next, we derive that

$$A^{1/2}\ M^{-1}\ \left(k^2 - 2m_{red}V\right) A^{-1/2} = R\ M^{-1/2}\ \left(k^2 - 2m_{red}V\right) M^{-1/2}\ R^{-1}\ , \tag{65}$$

(iii) $\mathbf{L}^2$-terms:

$$\begin{aligned} &-A^{1/2}\ \frac{\mathbf{L}^2}{r^2} A^{-1/2} - A^{1/2}\ M^{-1}\ \frac{\mathbf{L}^2}{r^2} S_{12}\ \chi\ A^{-1/2} \Rightarrow \\ &-A^{1/2}\ \frac{\mathbf{L}^2}{r^2} A^{-1/2} - A^{1/2}\ M^{-1}\ \left[\frac{\mathbf{L}^2}{r^2}, S_{12}\right]_-\ \chi\ A^{-1/2}\ , \end{aligned} \tag{66}$$

where we used that $\mathbf{L}^2$ on a scalar function, like χ and v, gives zero. Now, $[\mathbf{L}^2, S_{12}]_-\ \chi = [\mathbf{L}^2, M]_-$, and using $A^{1/2} = R\ M^{1/2}$ etc., we find after some straightforward algebraic manipulations that the expression in (66) becomes

$$\boxed{-\frac{1}{2r^2}\ R\ \left(M^{1/2}\left[\mathbf{L}^2, M^{-1/2}\right]_- + M^{-1/2}\left[\mathbf{L}^2, M^{1/2}\right]_-\right)\ R^{-1} - R\ \frac{\mathbf{L}^2}{r^2}\ R^{-1}\ .} \tag{67}$$

With these results, the transformed Schrödinger equation (46) becomes

$$\boxed{\begin{aligned} v'' + \Big[&RM^{-1/2}\left(k^2 - 2m_{red}V\right) M^{-1/2} R_{-1} - \frac{1}{4} R\ \left(M^{-1/2}\ M'\ M^{-1/2}\right)^2\ R^{-1} \\ &-\frac{1}{2r^2}\ R\ \left(M^{1/2}\left[\mathbf{L}^2, M^{-1/2}\right]_- + M^{-1/2}\left[\mathbf{L}^2, M^{1/2}\right]_-\right)\ R^{-1} - R\ \frac{\mathbf{L}^2}{r^2}\ R^{-1}\ \Big]\ v = 0\ . \end{aligned}} \tag{68}$$

We note that (68) is actually of the form

$$v'' + R(\theta)\left[\ldots\ldots\right]\ R^{-1}(\theta)\ v = 0\ . \tag{69}$$

Bringing (68) into the standard form

$$v'' + \left[k^2 - 2m_{red}\ W - \frac{L^2}{r^2}\right]\ v = 0\ . \tag{70}$$

we have found that

$$\boxed{\begin{aligned} 2m_{red}\ W = R\ \Big[&M^{-1/2}\ 2m_{red}V\ M^{-1/2} + \left(M^{-1} - 1\right)\ k^2 - \frac{1}{4}\left(M^{-1/2}\ M'\ M^{-1/2}\right)^2 + \\ &+\frac{1}{2r^2}\ \left(M^{1/2}\left[\mathbf{L}^2, M^{-1/2}\right]_- + M^{-1/2}\left[\mathbf{L}^2, M^{1/2}\right]\right) + \left(\frac{\mathbf{L}^2}{r^2} - R^{-1}\ \frac{\mathbf{L}^2}{r^2}\ R\right)\Big]\ R^{-1}\ . \end{aligned}} \tag{71}$$

Note, that for $R \to 1$, the expression in (71) goes over into that of (58), because in this case $M = A$.

C. On the Coupled-Channel Solution

In principle, the solution of equation (70) is in the of the triplet-coupled waves more complicated than the usual one. This we discuss in this subsection. For that purpose, we rewrite (70) in the form

$$v'' = A(r)\ v(r) \quad , \quad A(r) = \left[2m_{red}W + \frac{\mathbf{L}^2}{r^2} - k^2\right] \ . \tag{72}$$

and equation (71) as

$$W = R(\theta)\ W_1\ R^{-1}(\theta) + \frac{1}{2m_{red}}\left[R\ \frac{\mathbf{L}^2}{r^2}\ R^{-1} - \frac{\mathbf{L}^2}{r^2}\right] \ . \tag{73}$$

Introducing

$$A_1(r) = \left[2m_{red}W_1 + \frac{\mathbf{L}^2}{r^2} - k^2\right] \ , \tag{74}$$

one easily sees that

$$A(r) = R[\theta(r))]A_1(r)\ R^{-1}[\theta(r)] \ . \tag{75}$$

Now, the off-diagonal elements of the A_1-matrix vanish for $\lim_{r\to 0}$ as r^2, because that is the hehavior of the tensor-potential. However, because of the $R(\theta)$-rotation, this is not the case for the A-matrix. Therefore, the solution of the triplet-coupled waves contains, in principle, logarithmic terms at the origin. This complicates the numerical solution of the general equation (70) for the triplet-coupled waves.

VII. MISCELANEOUS FORMULAE

In the case of no non-local spin-orbit potential, i.e. $\rho(r) = 0$, we get using

$$\begin{aligned}
\left[L^2, S_{12}\right]_- &= 12\sqrt{J(J+1)}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \ , \\
(1+S_{12})\left[L^2, S_{12}\right]_- &= \frac{36\sqrt{J(J+1)}}{2J+1}\begin{pmatrix} 2\sqrt{J(J+1)} & -1 \\ -1 & -2\sqrt{J(J+1)} \end{pmatrix} \\
&= \frac{36\sqrt{J(J+1)}}{2J+1}\left(2\sqrt{J(J+1)}\ \tau_3 - \tau_1\right) \ ,
\end{aligned} \tag{76}$$

that equation (55) becomes

$$\left\{A^{1/2}\left[L^2, A^{-1/2}\right]_- + A^{-1/2}\left[L^2, A^{1/2}\right]_-\right\} = -2\frac{(x-y)^2}{xy}\cdot\frac{\sqrt{J(J+1)}}{2J+1}\begin{pmatrix} 2\sqrt{J(J+1)} & -1 \\ -1 & -2\sqrt{J(J+1)} \end{pmatrix} \ . \tag{77}$$

Here,

$$x = (1 + 2\phi + 4\chi)^{1/2} \quad , \quad y = (1 + 2\phi - 8\chi)^{1/2} \ . \tag{78}$$

Finally, we note that because of $\mathbf{L}\cdot\mathbf{S} = \frac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right))$, and $S = 1$,

$$[\mathbf{L}\cdot\mathbf{S}, S_{12}] = -\frac{1}{2}\left[\mathbf{L}^2, S_{12}\right] \ . \tag{79}$$

APPENDIX A: MISCELANEOUS FORMULAS

From (34) we can solve for σ_1 and σ_2 in terms of S_{12} and $\mathbf{L}\cdot\mathbf{S}$. We get

$$\begin{aligned}
\sigma_1 &= \frac{1}{6(2J+1)\sqrt{J(J+1)}}\left[4(J-1)(J+2) + (2J+1)^2\ S_{12} - 6\ \mathbf{L}\cdot\mathbf{S}\right] \\
\sigma_3 &= \frac{1}{2J+1}\left(3 + 2\mathbf{L}\cdot\mathbf{S}\right) = \frac{1}{2J+1}\left((J^2+J+1) - \mathbf{L}^2\right) \ .
\end{aligned} \tag{A1}$$

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