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The perturbed ladder operator method: closed form expressions of perturbed wavefunctions and matrix elements

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Abstract. By mapping the perturbation scheme onto the ladder operator formalism, the field of application of the Schrödinger–Infeld–Hull factorisation method is enlarged. It is shown how, at each order of the perturbation, perturbed ladder operators can be constructed. Thus, without having to calculate explicitly either the excited unperturbed functions or any matrix element, one obtains analytical expressions of the perturbed eigenvalues in terms of the quantum numbers of the factorisable unperturbed problem. A three-terms recurrence relation, valid at any rank of the perturbation, is derived and leads to closed form expressions of the perturbed eigenfunctions. Consequently, a closed form expression of any matrix element on the basis of the perturbed eigenfunctions is easily obtained from the calculation of one unique particular integral. It is shown how the method can be applied to the resolution of wave equations with the potentials

$$V(x)=[-d^2\exp(2ax)+2ad(m+\tfrac{1}{2})\exp(ax)]+d_3\exp(3ax)+\ldots+d_S\exp(Sax)$$

$$V(x)=\{-[m(m+1)]/x^2-b^2x^2\}+b_2x^4+\ldots+b_Sx^{2S}$$

$$V(x)=[-(bx+d)^2-b(2m+1)]+b_3(bx+d)^3+\ldots+b_S(bx+d)^S$$

$$V(x)=\{-[m(m+1)]/x^2-2q/x\}+b_1x+b_2x^2+\ldots+b_Sx^S$$

which correspond to the unperturbed Infeld–Hull types B, C, D and F, respectively.

1. Introduction

In a previous paper (Bessis *et al* 1978, to be referred to as I) a novel method of resolution of perturbed eigenequations has been proposed. Indeed, by mapping the perturbation scheme onto the ladder operator formalism, one generates the 'perturbed ladder operator' procedure which oversteps the narrow bounds of applicability of the Schrödinger–Infeld–Hull factorisation method (Schrödinger 1940, Infeld and Hull 1951). It has been shown how, when starting from an unperturbed problem leading to a factorisable equation, one can build up 'perturbed ladder operators' together with 'perturbed factorisation functions', allowing the factorisation of the perturbed equation at any rank of the perturbation. Hence, one finds again the well-known advantages of the exact factorisation scheme: one obtains, without having to calculate any matrix element, analytical expressions of the perturbed eigenvalues in terms of the quantum numbers and, also, analytical expressions of the perturbed eigenfunctions by successive application of the perturbed ladder operators. Of course, to each type of factorisation

associated with the unperturbed potential correspond specific expressions for the perturbed ladder and factorisation functions. Thus, for the generalised central field problem, corresponding to the unperturbed Infeld–Hull type F, expressions of the ladder and factorisation functions have been given (see I).

In the present paper, the remaining radial types of factorisation (types B, C and D) are investigated. Moreover, we have reconsidered the determination of perturbed wavefunctions and found a three-terms recurrence relation which allows, for all types (A–F), a straightforward determination of the perturbed wavefunctions at any rank of the perturbation. The advantages of the method are pursued to the determination of closed form expressions of any matrix element of a Hermitian operator between perturbed eigenfunctions in terms of one unique integral which, in most cases, is obtainable from tables. As an illustrative example, our procedure is applied, up to the second order of the perturbation, to the determination of analytical expressions of the generalised central field wavefunctions and closed form expressions of the $\langle r^k \rangle$ matrix elements between these functions.

2. The perturbed ladder operator scheme

Let us consider a second-order differential eigenequation which has been reduced to the standard form

$$\left(\frac{d^2}{dx^2} + \mathcal{U}(x, m) + \Lambda_j\right)\psi_{jm}(x) = 0 \tag{1}$$

associated with the boundary conditions ($x_1 \leqslant x \leqslant x_2$)

$$|\psi(x_1)|^2 = |\psi(x_2)|^2 = 0 \qquad \int_{x_1}^{x_2} |\psi(x)|^2 \, dx = 1 \tag{2}$$

where $m = m_0, m_0+1, m_0+2, \ldots$ is a quantum number which takes successive discrete values labelling the eigenfunctions. In most problems of physical interest, the potential function $\mathcal{U}(x, m)$ in (1) does not belong to any of the six Infeld–Hull factorisable types but one can assume that it is possible to expand it in a perturbation series with a parameter η,

$$\mathcal{U}(x, m) = U^{(0)}(x, m) + \eta U^{(1)}(x, m) + \ldots + \eta^N U^{(N)}(x, m), \tag{3}$$

in such a way that the wave equation (1) with $U^{(0)}(x, m)$ is factorisable. With that condition, it has been shown (see I) how one can build up the two perturbed 'factorisation instruments', i.e. the perturbed ladder function $\mathcal{K}(x, m)$ and the perturbed factorisation function $\mathcal{L}(m)$, allowing the factorisation of the perturbed equation (1) up to any order N of the perturbation:

$$\begin{aligned} \mathcal{K}(x, m) &= K^{(0)}(x, m) + \eta K^{(1)}(x, m) + \ldots + \eta^N K^{(N)}(x, m) \\ \mathcal{L}(m) &= L^{(0)}(m) + \eta L^{(1)}(m) + \ldots + \eta^N L^{(N)}(m) \end{aligned} \tag{4}$$

where $K^{(0)}$ and $L^{(0)}$ are the ladder and factorisation functions of the wave equation (1) with $U^{(0)}$. The expressions of $K^{(\nu)}$, $L^{(\nu)}$ are obtained recursively, i.e. when considering the determination of $K^{(N)}$, $L^{(N)}$ and $U^{(N)}$ it is assumed that all the $K^{(\nu)}$, for $\nu = 1, 2, \ldots, N-1$, have already been found. The generation procedure of these perturbed 'factorisation instruments' has been already outlined and, in particular, applied to

the Coulombic case (type F) in I. Hereafter it is applied to types B, C and D. Since this procedure remains roughly the same as for type F, details of calculations will not be reproduced here *in extenso*. Hence, we just briefly recall the main results for type F completed by the new results for types B, C and D.

2.1. Perturbed type F

Given the unperturbed type F, $U^{(0)}(x, m)$, $K^{(0)}(x, m)$ and $L^{(0)}(m)$ functions (see table 1), let us first focus attention on the m dependence of the current $U^{(\nu)}$, $K^{(\nu)}$ and $L^{(\nu)}(\nu = 1, N)$. One finds that, in order to satisfy the factorisability condition for equation (1), up to a given order N of the perturbation, convenient expressions are

$$U^{(\nu)}(x, m) = \frac{d\gamma_0^{(\nu)}}{dx} + \sum_{v=1}^{S_\nu} \frac{d\gamma_v^{(\nu)}}{dx}[m(m+1)]^v \tag{5}$$

$$K^{(\nu)}(x, m) = \sum_{v=1}^{S_\nu} m^{2v-1} \sum_{u=0}^{S_\nu - v} \binom{v+u}{2u+1} \gamma_{v+u}^{(\nu)}(x) \tag{6}$$

$$L^{(\nu)}(m) = \sum_{v=0}^{S_\nu} \beta_v^{(\nu)} m^{2v} \tag{7}$$

where $\binom{a}{b}$ are binomial coefficients.

Table 1. Radial Infeld–Hull exact factorisation types.

Type	$U^{(0)}(x, m)$	$K^{(0)}(x, m)$	$L^{(0)}(m)$	Range
B	$-d^2\exp(2ar) + ad(2m+1)\exp(ar)$	$-am + d\exp(ar)$	$-a^2m^2$	$]-\infty, +\infty[$
C	$-\frac{m(m+1)}{x^2} - b^2x^2 - b(2m+1)$	$\frac{m}{x} - bx$	$+4bm$	$[0, +\infty[$
D	$-(bx+d)^2 - b(2m+1)$	$-(bx+d)$	$+2bm$	$]-\infty, +\infty[$
F	$-\frac{m(m+1)}{x^2} - \frac{2q}{x}$	$\frac{m}{x} + \frac{q}{m}$	$-q^2/m^2$	$[0, +\infty[$

The $\gamma_v^{(\nu)}(x)$ functions involved in (5) and (6) are then found to be solutions of a linear differential triangular system. Solving this system, one gets for the $\gamma_v^{(\nu)}(x)$ polynomials in x of degree $(S_\nu + 1 - v)$. The set of coefficients of these polynomials depends on the set of the free constants $\beta_i^{(\tau)}$ $(i = 1, S_\tau;\ \tau = 1, \nu)$:

$$\gamma_v^{(\nu)}(x) = -\frac{\beta_v^{(\nu)}}{2v+1}x - \Omega_v^{(\nu)}(x) - \sum_{u=1}^{S_\nu - v} \binom{v+u}{2u} \gamma_{v+u}^{(\nu)}(x) + \sum_{u=1}^{S_\nu - v} \left(\frac{1}{x}\right)^{2v} \int x^{2v}\left[\frac{2u(2v+1)}{(2u+1)x}\binom{v+u}{2u} - 2q\binom{v+u}{2u-1}\right]\gamma_{v+u}^{(\nu)}(x)\,dx. \tag{8}$$

The polynomial $\Omega_v^{(\nu)}(x)$ is given by

$$\Omega_v^{(\nu)}(x) = \left(\frac{1}{x}\right)^{2v} \int x^{2v}\omega_v^{(\nu)}(x)\,dx \tag{9}$$

where the $\omega_v^{(\nu)}(x)$ derive from the data of the preceding orders of the perturbation and are defined by

$$\sum_{\tau=1}^{\nu-1} K^{(\tau)}(x, m)K^{(\nu-\tau)}(x, m) = \sum_{v=1}^{S_\tau+S_{\nu-\tau}-1} \omega_v^{(\nu)}(x)m^{2v}. \tag{10}$$

The $\gamma_v^{(\nu)}(x)$ can be calculated from (8), step by step, downwards for $v = S_\nu, S_\nu - 1, \ldots$. It should be noted that when considering the first order of the perturbation $\omega_v^{(1)}(x) \equiv 0$; thus $\Omega_v^{(1)}(x) \equiv 0$.

Once the first-order truncation S_1 has been arbitrarily chosen, the value of S_ν is not free and is given by

$$S_\nu = \nu S_1 + \nu - 1. \tag{11}$$

Indeed the highest power of x in $\Omega_v^{(\nu)}$ is completely predicted from the results of the preceding orders.

Finally, since at each order ν of the perturbation the $\gamma_v^{(\nu)}(x)$ functions are polynomial in x, the successive $U^{(\nu)}(x)$ are also polynomials in x. Thus, owing to the x dependence of $\mathcal{U}(x, m)$ the 'perturbed type F' ladder method can be applied to eigenequations

$$\left(\frac{d^2}{dx^2} + \mathcal{V}(x, m) + \mathcal{E}_j\right)\psi_{jm}(x) = 0 \tag{12}$$

with

$$\mathcal{V}(x, m) = -\frac{m(m+1)}{x^2} - \frac{2q}{x} + b_1 x + b_2 x^2 + \ldots b_{S_N} x^{S_N}. \tag{13}$$

Nevertheless, let us point out that, although the x dependence of $\mathcal{V}(x, m)$ is obviously the same as that of the perturbed type F $\mathcal{U}(x, m)$, it is not so with the m dependence of the perturbative part of $\mathcal{V}(x, m)$. Indeed, the $U^{(\nu)}$ contain powers of $m(m+1)$ (equation 5) and in order to identify $\mathcal{V}(x, m)$ with $\mathcal{U}(x, m)$, one has to resort to 'artificial' or 'embedded' factorisation (Infeld and Hull 1951). In the same way as within the exact factorisation scheme, one considers the $\mathcal{U}(x, m)$ potential as 'embedded' in a μ-parametric potential function $u(x, m, \mu)$ which depends on a supplementary 'artificial' parameter μ such that $u(x, m, \mu = f(m)) = \mathcal{U}(x, m)$. Thus, the perturbed ladder and factorisation functions associated with $u(x, m, \mu)$ both depend on the parameter μ and lead to μ-parametric eigenvalues and eigenfunctions. Of course, at the end of the process, one merely sets $\mu = f(m)$ and obtains the required eigenvalues and eigenfunctions $\psi_{jm}(x, \mu = f(m))$.

2.2. Perturbed type C

Since any problem which can be treated as type B can also be treated as type C and vice versa, it is convenient to consider first type C problems. Then, these results will be used later for type B.

Starting from the unperturbed type C $U^{(0)}$, $K^{(0)}$ and $L^{(0)}$ (see table 1) the successive adequate expansions in m of the $U^{(\nu)}$, $K^{(\nu)}$ and $L^{(\nu)}$ ($\nu = 1, N$) which enable one to satisfy the factorisability condition for equation (1), up to a given power N of the parameter η, are found to be

$$U^{(\nu)}(x, m) = \frac{d\gamma_0^{(\nu)}}{dx} + \sum_{v=1}^{S_\nu} \frac{d\gamma_v^{(\nu)}}{dx}(2m+1)^v \tag{14}$$

$$K^{(\nu)}(x, m) = \sum_{v=0}^{S_\nu - 1} (2m)^v \sum_{u=0}^{u_\nu} \binom{v+2u+1}{2u+1} \gamma_{v+2u+1}^{(\nu)}(x) \tag{15}$$

$$L^{(\nu)}(m) = \sum_{v=0}^{S_\nu} \beta_v^{(\nu)} (2m)^v \tag{16}$$

where $u_\nu = [\frac{1}{2}(S_\nu - v - 1)]$.

The $\gamma_v^{(\nu)}(x)$ functions involved in (14) and (15) are then found to be solutions of a linear differential triangular system. Solving this system, one gets for the $\gamma_v^{(\nu)}(x)$ polynomials in x of degree $(2S_\nu - 2v + 1)$ obtainable sequentially (for $v = S_\nu, S_\nu - 1, \ldots$) from the following expression:

$$\gamma_v^{(\nu)}(x) = -\frac{1}{(v+1)} \beta_v^{(\nu)}(x) - \Omega_v^{(\nu)}(x) - \sum_{u=1}^{u'_\nu} \binom{v+2u}{2u} \gamma_{v+2u}^{(\nu)}$$
$$- \frac{1}{x^v} \int x^{v+1}\, dx \left\{ 2b(v+1)\gamma_{v+1}^{(\nu)} + \sum_{u=1}^{u'_\nu} \left[-\frac{2uv}{(2u+1)} \binom{v+2u}{2u} \frac{1}{x^2} \gamma_{v+2u}^{(\nu)} \right.\right.$$
$$\left.\left. + 2b \binom{v+2u+1}{2u+1} \gamma_{v+2u+1}^{(\nu)} \right] \right\} \tag{17}$$

where $u'_\nu = [\frac{1}{2}(S_\nu - v)]$.

The polynomial $\Omega_v^{(\nu)}(x)$ is given by

$$\Omega_v^{(\nu)}(x) = \left(\frac{1}{x}\right)^v \int x^v \omega_v^{(\nu)}(x)\, dx \tag{18}$$

where the $\omega_v^{(\nu)}(x)$ derive from the data of the preceding orders of the perturbation and are defined by

$$\sum_{\tau=1}^{\nu-1} K^{(\tau)}(x, m) K^{(\nu-\tau)}(x, m) = \sum_{v=0}^{S_\tau + S_{\nu-\tau} - 2} \omega_v^{(\nu)}(x)(2m)^v. \tag{19}$$

In the same way as for type F, once the first-order truncation S_1 has been arbitrarily chosen, the value of the S_ν associated with the successive orders of the perturbation is now given by

$$S_\nu = \nu S_1 + 1 - \nu. \tag{20}$$

At each order ν of the perturbation the $\gamma_v^{(\nu)}(x)$ functions are odd polynomials in x, the successive $U^{(\nu)}(x)$ are then found to be even polynomials in x. Consequently the perturbed type C ladder operator method can be applied to any problem leading to the resolution of a second-order differential equation (12) with

$$\mathcal{V}(x, m) = -\frac{m(m+1)}{x^2} - b^2 x^2 + \sum_{v=2}^{S_N} b_v x^{2v}. \tag{21}$$

Artificial factorisation is still useful in that case.

2.3. Perturbed type B

As pointed out before, in order to tackle 'type B perturbed' problems, it is convenient to use the connection between type B and C.

Let us consider a second-order differential equation involving an unperturbed potential function type B (see table 1) with an additive perturbative potential

$$\left(\frac{d^2}{dr^2}+\mathcal{W}(r, M)+\Lambda_J\right)\phi_{JM}(r)=0. \tag{22}$$

When introducing the following transformations of function and variable

$$\begin{aligned} x &= e^{ar/2} \\ \phi_{JM} &= x^{-1/2}\psi_{jm} \end{aligned} \tag{23}$$

the eigenequation (22) ($-\infty<r<+\infty$) is transformed into a type C eigenequation ($0\leqslant x<+\infty$). The correspondence between quantum numbers is

$$\begin{aligned} m &= 2J+\tfrac{1}{2}+\epsilon \\ j &= J+M+\tfrac{1}{2}+\epsilon \end{aligned} \tag{24}$$

with $\epsilon=+1$ (or -1) according to whether the type B factorisation function $L^{(0)}(M)$ (see table 1) is an increasing (or decreasing) function of M. Hence, previous results which have been obtained for type C can be used and thus the perturbed ladder operator method can be applied to any problem leading to the resolution of a second-order eigenequation (22) with

$$\mathcal{W}(r, M)=-d^2 e^{2ar}+2ad(M+\tfrac{1}{2})e^{ar}+\sum_{v=3}^{S_N} d_v e^{var}. \tag{25}$$

2.4. Perturbed type D

Starting from the unperturbed type D $U^{(0)}$, $K^{(0)}$ and $L^{(0)}$ (see table 1), it can be shown that the m dependence of the $U^{(\nu)}$, $K^{(\nu)}$ and $L^{(\nu)}$ functions is the same for type D as for type C (equations 14–16). The type D $\gamma_v^{(\nu)}(x)$ functions are given by

$$\begin{aligned} \gamma_v^{(\nu)}(x) = C_v^{(\nu)} &- \beta_v^{(\nu)}(x+d/b)-\Omega_v^{(\nu)}(x)-\sum_{u=1}^{u_\nu}\binom{v+2u}{2u}\gamma_{v+2u}^{(\nu)} \\ &-2\int (bx+d)\,dx\left[(v+1)\gamma_{v+1}^{(\nu)}+\sum_{u=1}^{u_\nu}\binom{v+2u+1}{2u+1}\gamma_{v+2u+1}^{(\nu)}\right] \end{aligned} \tag{26}$$

where $u_\nu=[\frac{1}{2}(S_\nu-v)]$, $C_v^{(\nu)}$ is an integration constant and

$$\Omega_v^{(\nu)}(x)=\int \omega_v^{(\nu)}(x)\,dx. \tag{27}$$

The $\omega_v^{(\nu)}(x)$ are defined by the same expression (19) as for type C. Then the $\gamma_v^{(\nu)}(x)$ functions are polynomials in $(bx+d)$ of degree $(2S_\nu-2v+1)$. The successive values of the S_ν are still defined by (20). Finally, the perturbed type D ladder operator method can be applied to any problem leading to the resolution of a second-order eigenequation (12) with

$$\mathcal{V}(x, m)=-(bx+d)^2-b(2m+1)+\sum_{v=3}^{2S_N} b_v(bx+d)^v. \tag{28}$$

Artificial factorisation is still useful in that case.

3. Determination of perturbed eigenvalues and eigenfunctions

Once the 'factorisation instruments' $\mathscr{K}(x, m)$ and $\mathscr{L}(m)$ have been obtained up to the Nth order of the perturbation (equation 4), one can apply the usual exact factorisation scheme. The total potential $\mathscr{U}(x, m)$ (equation 3) specific to each type of factorisation depends, via the $\gamma_v^{(\nu)}(x)$ functions, on free constants $\beta_v^{(\nu)}$ ($\nu = 1, S_N$; $v = 0, S_\nu$) (see equations (5) and (8) for type F, equations (14) and (17) (or 26) for type C (or D)). One has first to compute these free constants $\beta_v^{(\nu)}$ of $\mathscr{U}(x, m)$ in terms of the b_i constants of $\mathscr{V}(x, m)$ which contain the physical data of the problem under consideration. Since the perturbed parts $U^{(\nu)}(x, m)$ of $\mathscr{U}(x, m)$ involve the quantum number m, one has to resort to 'embedded' factorisation, i.e. to introduce an artificial parameter $\mu = m(m+1)$ for type F (equation 5) or $\mu = 2m+1$ for types C and D (equation 14).

Once the $\beta_v^{(\nu)}$ are calculated in terms of the b_i and μ, the exact factorisation scheme works. The eigenvalue is $\mathscr{E}_j = \mathscr{L}(j+1)$ (or $\mathscr{L}(j)$) for class I (or class II) according to whether $L^{(0)}(m)$ is an increasing (or decreasing) function of m. Then, one directly obtains, at any order N of the perturbation, the analytical expressions of the eigenvalues $\mathscr{E}_j$ in terms of the quantum numbers j and also m (via $\mu = f(m)$).

For type F

$$\mathscr{E}_j(m) = -\frac{q^2}{(j+1)^2} + \sum_{\nu=1}^{N} \sum_{v=0}^{S_\nu} (j+1)^{2v} \beta_v^{(\nu)}(b_i, \mu = m(m+1)). \tag{29}$$

For type C

$$\mathscr{E}_j(m) = 4b(j+1) + \sum_{\nu=1}^{N} \sum_{v=0}^{S_\nu} (2j+2)^v \beta_v^{(\nu)}(b_i, \mu = 2m+1). \tag{30}$$

For type D

$$\mathscr{E}_j(m) = 2b(j+1) + \sum_{\nu=1}^{N} \sum_{v=0}^{S_\nu} (2j+2)^v \beta_v^{(\nu)}(b_i, \mu = 2m+1). \tag{31}$$

These expressions are given for class I problems. For class II problems one has to substitute $(j+1)$ by j.

The eigenfunctions $\psi_{jm}^{(N)}$, at any order N of the perturbation, are solutions of the following pair of difference-differential equations:

$$\begin{aligned} \left(\mathscr{K}(x, m+1) - \frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_{jm}^{(N)} &= [\Lambda_j - \mathscr{L}(m+1)]^{1/2}\psi_{jm+1}^{(N)} \\ \left(\mathscr{K}(x, m) + \frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_{jm}^{(N)} &= [\Lambda_j - \mathscr{L}(m)]^{1/2}\psi_{jm-1}^{(N)} \end{aligned} \tag{32}$$

with $\Lambda_j = \mathscr{L}(j+1)$ (or $\mathscr{L}(j)$) for class I (or class II) problems. The quantification condition $j - m = \text{integer} \geqslant 0$ (or $m - j = \text{integer} \geqslant 0$) for class I (or class II) problems ensures the existence of quadratically integrable solutions up to the Nth order in η.

The equations (32) allow the determination of the Nth order perturbed $\psi_{jm}^{(N)}(x)$ functions, step by step, starting from the 'key function' $\psi_{jj}^{(N)}$ which is the solution of a first-order differential eigenequation:

$$\left(\mathscr{K}(x, j+1) - \frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_{jj}^{(N)}(x) = 0 \qquad \text{(class I)} \tag{33}$$

or

$$\left(\mathcal{H}(x, j)+\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_{jj}^{(N)}(x)=0 \qquad \text{(class II)}. \tag{34}$$

This procedure has been applied, in I, to the determination of analytical expressions of the generalised central field wavefunctions.

Nevertheless, from a practical point of view, the use of a recurrence relation is found to be more efficient for the determination of wavefunctions. Now, from (32), the Nth-order perturbed eigenfunctions $\psi_{jm}^{(N)}$ are seen to satisfy the following three-terms (non-differential) recurrence relation

$$[\mathcal{H}(x, m)+\mathcal{H}(x, m+1)]\psi_{jm}^{(N)}=\mathcal{N}_{jm}\psi_{jm-1}^{(N)}+\mathcal{N}_{jm+1}\psi_{jm+1}^{(N)} \tag{35}$$

with

$$\mathcal{N}_{jm}=[\Lambda_j-\mathcal{L}(m)]^{1/2}. \tag{36}$$

Starting from the key function $\psi_{jj}^{(N)}$ which is a solution of the first-order differential eigenequation (33) or (34), this recurrence relation enables one to determine the Nth-order perturbed wavefunctions without having to calculate explicitly either the excited unperturbed functions or any matrix element. Indeed, as has been shown in I, after matching the given potential of the physical problem under consideration with the theoretical $\mathcal{U}(x, m)$ allowing perturbed factorisation, the 'factorisation instruments' $\mathcal{H}(x, m)$ and $\mathcal{L}(m)$ contain all the essential information following from the preceding orders of the perturbation via the $\beta_{v}^{(\nu)}(b_i, \mu)(\nu=1, 2, \ldots, N-1)$. Furthermore, if one starts from a normalised key function $\psi_{jj}^{(N)}$, then the recurrence relation (35) generates normalised eigenfunctions $\psi_{jm}^{(N)}$. It is worthwhile to note that, according to the 'embedded' factorisation scheme, the parameter μ has to be given its true value $\mu=f(m)$ but only within the final expression $\psi_{jm}^{(N)}(x, b_i, \mu=f(m))$ of the required function, i.e. not during the recurrence process.

Let us introduce the shortened notation

$$\begin{aligned} Q_m &= \mathcal{N}_{j,m+\frac{1}{2}-\frac{\epsilon}{2}(b_i,\,\mu)}^{-1}[\mathcal{H}(x, m; b_i, \mu)+\mathcal{H}(x, m+1; b_i, \mu)] \\ h_m &= -(\mathcal{N}_{jm+1}/\mathcal{N}_{jm})^{\epsilon}(Q_mQ_{m+\epsilon})^{-1} \end{aligned} \tag{37}$$

where $\epsilon=+1$ (or $\epsilon=-1$) for class I (or class II) problems according to the quantification condition $\epsilon(j-m)=v=\text{integer}\geqslant 0$. Then, the recurrence relation (35) is

$$\psi_{jm-\epsilon}^{(N)}=Q_m(\psi_{jm}^{(N)}+h_mQ_{m+\epsilon}\psi_{jm+\epsilon}^{(N)}). \tag{38}$$

For class I problems ($j-m\geqslant 0$), for instance, one gets the following expressions of the successive normalised perturbed eigenfunctions in terms of the normalised perturbed key function:

$$\begin{aligned} \psi_{jj-1}^{(N)} &= Q_j\psi_{jj}^{(N)} \\ \psi_{jj-2}^{(N)} &= Q_{j-1}Q_j(1+h_{j-1})\psi_{jj}^{(N)} \\ &\ldots \\ \psi_{jj-5}^{(N)} &= Q_{j-4}Q_{j-3}Q_{j-2}Q_{j-1}Q_j \\ &\quad\times[1+h_{j-1}+h_{j-2}+h_{j-3}+h_{j-4}+h_{j-3}h_{j-1}+h_{j-4}(h_{j-1}+h_{j-2})]\psi_{jj}^{(N)}. \end{aligned} \tag{39}$$

Finally, any $\psi^{(N)}_{jj-\epsilon v}$ normalised perturbed function is given in terms of the normalised perturbed key function $\psi^{(N)}_{jj}$ by the expression

$$\psi^{(N)}_{jj-\epsilon v} = \psi^{(N)}_{jj}\left[\prod_{u=0}^{v-1} Q_{j-\epsilon u} \sum_{s=0}^{[v/2]} \prod_{i=1}^{s}\left(\sum_{t_i=2i-1}^{t_{\max}} h_{j-\epsilon t_i}\right)\right] \tag{40}$$

where

$$t_{\max} = \min\begin{cases} v-1 \\ t_{i+1}-2 \end{cases}.$$

The $\psi^{(N)}_{jj}$ functions are easily obtained from equation (33) for class I ($\epsilon = +1$) or from equation (34) for class II ($\epsilon = -1$). One gets

$$\psi^{(N)}_{jj} = \psi^{(0)}_{jj} \exp\left[\epsilon \int \sum_{\nu=1}^{N} K^{(\nu)}\left(x, j+\tfrac{1}{2}+\frac{\epsilon}{2}; b_i, \mu\right) \mathrm{d}x\right]. \tag{41}$$

After substituting for the Q_m and h_m functions from equation (37) and retaining the terms up to η^N, any normalised perturbed eigenfunction $\psi^{(N)}_{jm}$ is merely obtained, for each type of factorisation, in terms of the specific zero-order key eigenfunction.

For the 'radial' factorisation types (C, D and F) which have been considered, the expression (40) of any perturbed eigenfunction can be viewed as the known zero-order key function multiplied by a polynomial of x:

$$\psi^{(N)}_{jm}(x) = \psi^{(0)}_{jj}(x) \sum_{u=u_0}^{u_{\max}} A^{(N)}_u(j, m; b_i; \mu = f(m)) x^u. \tag{42}$$

For type F

$$\begin{aligned} &u_0 = m-j \qquad u_{\max} = S_N + 1 \qquad \mu = m(m+1) \\ &\psi^{(0)}_{jj} = \left(\frac{2}{j+1}\right)^{j+3/2} \frac{1}{[(2j+2)!]^{1/2}} x^{j+1} \exp\left[-x(j+1)^{-1}\right]. \end{aligned} \tag{43}$$

For type C ($b > 0$)

$$\begin{aligned} &u_0 = m-j \qquad u_{\max} = 2S_N + 2 \qquad \mu = 2m+1 \\ &\psi^{(0)}_{jj} = \left(\frac{b}{\pi}\right)^{1/4} \left(\frac{2(2b)^{j+1}}{(2j+1)!!}\right)^{1/2} x^{j+1} \exp(-bx^2/2). \end{aligned} \tag{44}$$

For type D ($b > 0$)

$$\begin{aligned} &u_0 = 0 \qquad u_{\max} = 2S_N \qquad \mu = 2m+1 \\ &\psi^{(0)}_{jj} = \left(\frac{b}{\pi}\right)^{1/4} \exp(-d^2/2b) \exp(-bx^2/2 - dx). \end{aligned} \tag{45}$$

4. Closed form expressions of matrix elements between perturbed eigenfunctions

For the radial factorisation types (B, C, D and F) which have been considered, we have now at our disposal closed form expressions of any normalised perturbed eigenfunction. Now let us consider the genral matrix element of a Hermitian operator

$\mathcal{M}(x)$ between two eigenfunctions. Using (42), one obtains the closed form expression

$$\langle \psi_{jm}^{(N)} \mathcal{M} \psi_{j'm'}^{(N)} \rangle = \sum_{u,u'} A_u^{(N)}(j, m; b_i) A_{u'}^{(N)}(j', m'; b_i) \times \int_{x_1}^{x_2} x^u \psi_{jj}^{(0)}(x) \mathcal{M}(x) x^{u'} \psi_{j'j'}^{(0)}(x)\, dx \tag{46}$$

where, following the type F, C or D of factorisation, the summation bounds for u and u' are given, respectively, by (43), (44) or (45). In all cases, when retaining solely the contributions of the perturbation up to η^N one has only to take into account values of u and u' such that $u + u' \leqslant u_{\max}$.

It should be noted that the integral in (46) does not depend upon the order N of the perturbation and moreover has a very simple dependence upon the u and u' index.

Furthermore, in most cases of interest in quantum theory, the analytical expression of this integral can be found in tables. Subsequently, formula (46) defines an analytical closed form expression of any matrix element between perturbed normalised eigenfunctions, and hence, an easy and quick algorithm of computation.

5. Illustrative application

As an illustrative example, let us apply the perturbed ladder scheme, up to the second order ($N = 2$), to the determination of eigenvalues and eigenfunctions of the perturbed type F (class I) wave equation (equations 12 and 13)

$$\left(\frac{d^2}{dx^2} - \frac{m(m+1)}{x^2} - \frac{2q}{x} + b_1 x + b_2 x^2 + b_3 x^3 + \mathscr{E}_j \right) \psi_{jm}(x) = 0. \tag{47}$$

Let us assume that $q = -1$. This is not a restriction since one can always assume $q = -1$ by change of variable $-qx \to x'$.

After choosing $S_1 = 1$ and $S_2 = 3$ (equation 11) and using the recursive relation (8), one gets the following expressions of the perturbed type F potentials (equation 5):

$$\begin{aligned} U^{(1)} &= -\beta_0^{(1)} - \tfrac{1}{3}\beta_1^{(1)}\mu - \tfrac{2}{3}\beta_1^{(1)} x \\ U^{(2)} &= -\tfrac{1}{7}\beta_3^{(2)}(\mu^3 - \mu^2 + \tfrac{1}{3}\mu) - \tfrac{1}{5}\beta_2^{(2)}(\mu^2 - \tfrac{1}{3}\mu) - \tfrac{1}{3}\beta_1^{(2)}\mu - \beta_0^{(2)} \\ &\quad + [-\tfrac{2}{7}\beta_3^{(2)}(\mu^2 - \mu + \tfrac{1}{3}) - \tfrac{2}{5}\beta_2^{(2)}(\mu - \tfrac{1}{3}) - \tfrac{2}{3}\beta_1^{(2)}]x \\ &\quad + [-\tfrac{2}{7}\beta_3^{(2)}(\tfrac{6}{5}\mu - 1) - \tfrac{2}{5}\beta_2^{(2)} - \tfrac{1}{15}(\beta_1^{(1)})^2 \mu]x^2 - [\tfrac{8}{35}\beta_3^{(2)} + \tfrac{2}{45}(\beta_1^{(1)})^2]x^3 \end{aligned} \tag{48}$$

with $\mu = m(m+1)$.

After matching these perturbed potentials (48) with $\mathscr{V}^{(1)} = b_1 x$ and $\mathscr{V}^{(2)} = b_2 x^2 + b_3 x^3$ one gets the $\beta_i^{(1)}$ and $\beta_i^{(2)}$ expressed in terms of the b_i and μ:

$$\begin{aligned} &\beta_1^{(1)} = -\tfrac{3}{2} b_1 \qquad \beta_0^{(1)} = \tfrac{1}{2} b_1 \mu \\ &\beta_3^{(2)} = -\tfrac{7}{16}(10 b_3 + b_1^2) \\ &\beta_2^{(2)} = -\tfrac{5}{8}(5 - 6\mu) b_3 - \tfrac{5}{2} b_2 - \tfrac{5}{16} b_1^2 \\ &\beta_1^{(2)} = -\tfrac{3}{8}\mu(\mu - 2) b_3 + \tfrac{1}{2}(3\mu - 1) b_2 + \tfrac{3}{16}\mu^2 b_1^2 \\ &\beta_0^{(2)} = 0. \end{aligned} \tag{49}$$

Then, one gets the following expressions of the factorisation instruments:

$$\mathscr{L}(m) = -\frac{1}{m^2} + \eta(\beta_0^{(1)} + \beta_1^{(1)} m^2) + \eta^2(\beta_1^{(2)} m^2 + \beta_2^{(2)} m^4 + \beta_3^{(2)} m^6)$$
$$\mathscr{H}(x, m) = \left(\frac{m}{x} - \frac{1}{m}\right) + \eta\left(\frac{b_1}{2} mx\right) + \eta^2(a_1(m)x + a_2(m)x^2 + a_3(m)x^3) \tag{50}$$

with

$$a_1(m) = \tfrac{1}{8}m[b_3(15m^4 + 5m^2 + \mu^2 - 12\mu m^2) + 4b_2(2m^2 - \mu) + \tfrac{1}{2}b_1^2(3m^4 + m^2 - \mu^2)]$$
$$a_2(m) = \tfrac{1}{8}m[2b_3(5m^2 - 3\mu) + 4b_2 + m^2 b_1^2]$$
$$a_3(m) = \tfrac{1}{2}m b_3.$$

Hence, one obtains the expressions of $\mathscr{N}_{jm}$ and Q_m in terms of the b_i:

$$\mathscr{N}_{jm} = [\mathscr{L}(j+1) - \mathscr{L}(m)]^{1/2}$$
$$Q_m = \frac{(2m+1)(j+1)m}{[(j+1)^2 - m^2]^{1/2}}\left[B_0\left(\frac{1}{x} - \frac{1}{m(m+1)}\right) + B_1 x + B_2 x^2 + B_3 x^3\right] \tag{51}$$

with, when introducing the shortened notation $J = j + 1$,

$$B_0 = 1 + \eta^3_4 b_1 J^2 m^2 + \eta^2 \tfrac{1}{4} J^2 m^2 \{7(J^4 + J^2 m^2 + m^4)(5b_3 + \tfrac{1}{2}b_1^2)$$
$$+ 5(J^2 + m^2)[(5 - 6\mu)b_3 + 4b_2 + \tfrac{1}{2}b_1^2]$$
$$+ 3\mu^2(b_3 - \tfrac{1}{2}b_1^2) - 6\mu(b_3 + 2b_2) + b_2 + \tfrac{27}{8}b_1^2 J^2 m^2\}$$
$$B_1 = \eta\tfrac{1}{2}b_1 + \eta^2 \tfrac{1}{8}\{3(m^4 + 2m^3 + 4m^2 + 3m + 1)(5b_3 + \tfrac{1}{2}b_1^2)$$
$$+ (m^2 + m + 1)[(5 - 12\mu)b_3 + 8b_2 + \tfrac{1}{2}b_1^2] \tag{52}$$
$$+ \mu^2(b_3 - \tfrac{1}{2}b_1^2) - 4\mu b_2 + 3b_1^2 J^2 m^2\}$$
$$B_2 = \eta^2 \tfrac{1}{8}[(m^2 + m + 1)(10b_3 + b_1^2) + 4b_2 - 6\mu b_3]$$
$$B_3 = \eta^2 \tfrac{1}{2}b_3.$$

Now, the expression (40), with $\epsilon = +1$ (class I), gives the expression of any normalised eigenfunction ψ_{jm} of the wave equation (47) in terms of the key function ψ_{jj} and then (equation 41) in terms of the zero-order key function $\psi_{jj}^{(0)}$.

Let us apply these results to the determination of the generalised central field energies and wavefunctions. After introducing the usual quantum numbers (n, l) and after setting $rR_{nl}(r) = Z^{1/2}\psi_{jm}(x; \mu = l(l+1))$, $Zr = x$, the Coulombic problem is a type F (class I) case with $j = n - 1$ and $m = l$. One finds, for instance,

$$R_{1S}(r) = R_{1S}^{(0)}[1 - \tfrac{1}{4}(3b_1 + 11b_2 + \tfrac{155}{4}b_3 + 5b_1^2) + \tfrac{1}{4}(b_1 + 2b_2 + 5b_3 - \tfrac{1}{4}b_1^2)(Zr)^2$$
$$+ \tfrac{1}{24}(4b_2 + 10b_3 + b_1^2)(Zr)^3 + \tfrac{1}{8}(b_3 + \tfrac{1}{4}b_1^2)(Zr)^4]$$
$$R_{2p}(r) = R_{2p}^{(0)}[1 - 15b_1 - 20(8b_2 + 77b_3 + \tfrac{97}{8}b_1^2) + 3(\tfrac{1}{6}b_1 + b_2 + 7b_3 - \tfrac{3}{2}b_1^2)(Zr)^2$$
$$+ \tfrac{1}{3}(b_2 + 7b_3 + b_1^2)(Zr)^3 + \tfrac{1}{4}(b_3 + \tfrac{1}{2}b_1^2)(Zr)^4]$$
$$R_{3d}(r) = R_{3d}^{(0)}[1 - \tfrac{189}{8}(4b_1 + 84b_2 + 1539b_3 + \tfrac{459}{2}b_1^2) + \tfrac{3}{4}(b_1 + 12b_2 + 162b_3 - \tfrac{135}{2}b_1^2)(Zr)^2$$
$$+ \tfrac{1}{2}(b_2 + \tfrac{27}{2}b_3 + \tfrac{9}{4}b_1^2)(Zr)^3 + \tfrac{3}{8}(b_3 + \tfrac{3}{4}b_1^2)(Zr)^4]$$

$$R_{2S}(r) = R_{2P}^{(0)} \sum_{u=-1}^{4} A_u (Zr)^u$$

with

$$A_{-1} = 2\sqrt{3}(1 - 12b_1 - 164b_2 - 1880b_3 - 260b_1^2)$$

$$A_0 = -\tfrac{1}{2}A_{-1}$$

$$A_1 = 2\sqrt{3}(b_1 + 7b_2 + 55b_3 - \tfrac{13}{2}b_1^2)$$

$$A_2 = -\frac{\sqrt{3}}{2}(b_1 + \tfrac{14}{3}b_2 + \tfrac{110}{3}b_3 - \tfrac{25}{3}b_1^2)$$

$$A_3 = -\frac{1}{\sqrt{3}}(b_2 + \tfrac{11}{2}b_3 - \tfrac{5}{4}b_1^2)$$

$$A_4 = -\frac{\sqrt{3}}{4}(b_3 + \tfrac{1}{2}b_1^2).$$

The zero-order key functions are the well-known normalised hydrogenic key functions, with $m = j \to l = n - 1$,

$$R_{nl=n-1} = Z^{3/2}\left(\frac{2}{n}\right)^{n+1/2} \frac{1}{\sqrt{(2n)!}} (Zr)^{n-1} \exp(-Zr/n).$$

From (29) and (49), one gets the following analytical expression of the generalised central field associated energies:

$$2E_{nl} = -Z^2\Big(\frac{1}{n^2} + \tfrac{1}{2}b_1(3n^2 - \lambda) + \tfrac{1}{2}b_2 n^2(5n^2 - 3\lambda + 1)$$
$$+ \tfrac{1}{8}b_3 n^2[-35n^4 + 5n^2(5 - 6\lambda) - 3\lambda(2 - \lambda)] + \tfrac{1}{16}b_1^2 n^2(7n^4 + 5n^2 - 3\lambda^2)\Big)$$

with $\lambda = l(l+1)$.

A closed form expression for matrix elements of r^k between generalised central field wavefunctions is easily obtained:

$$\langle nl|r^k|n'l'\rangle = \sum_{u,u'} A_u^{(N)}(n, l) A_{u'}^{(N)}(n', l') \langle r^{k+u+u'}\rangle$$

where $l - n + 1 \leqslant u \leqslant S_N + 1$, $l' - n' + 1 \leqslant u' \leqslant S_N + 1$ and $u + u' \leqslant S_N + 1$. The shortened notation $\langle r^{k+u+u'}\rangle$ stands for the matrix element between the hydrogenic key functions:

$$\langle r^{k+u+u'}\rangle = Z^{u+u'} \int_0^\infty R_{nn-1}^{(0)*} R_{n'n'-1}^{(0)} r^{k+u+u'+2}\, \mathrm{d}r.$$

One gets

$$\langle r^{k+u+u'}\rangle = Z^{-k}\left(\frac{2}{n}\right)^{n+\frac{1}{2}}\left(\frac{2}{n'}\right)^{n'+\frac{1}{2}} [(2n)!(2n')!]^{-1/2}$$
$$\times \left(\frac{nn'}{n+n'}\right)^{n+n'+k+u+u'+1} (n+n'+k+u+u')!$$

This key matrix element vanishes unless $n + n' + k + u + u' \geqslant 0$. Owing to the condition $u + u' \leqslant S_N + 1$ with $S_N = NS_1 + N - 1$, one obtains for the generalised central field

problem the following selection rule:

$$-k \leqslant n + n' + S_N + 1.$$

One could question if the application of the well-known Pasternack–Sternheimer (1962) selection rules, $2 \leqslant -(k+u+u') \leqslant l - l' + 1$, $n = n'$, $l > l'$ and $l + l' + (k+u+u') + 2 \geqslant 0$, for matrix elements of $r^{k+u+u'}$ between hydrogenic radial functions can give an additional selection rule for $n = n'$. Since $\langle r^{k+u+u'} \rangle$ is a matrix element between 'key' hydrogenic functions it follows therefrom that $n = n' \rightarrow l = l'$. Consequently, only the second Pasternack–Sternheimer rule holds but it is merely a particular case of the selection rule already found.

6. Conclusion

The perturbed ladder operator method can be viewed as an improved hybrid of the factorisation and perturbation schemes which combines the advantageous features of the two schemes. Finally, all these features are essentially embedded in the factorisation and the ladder perturbed functions. Once these 'factorisation instruments' have been expressed in terms of the physical data of the problem, one obtains directly, without prior knowledge of the unperturbed spectrum and without having to calculate any matrix element, analytical expressions of the eigenvalues in terms of the quantum numbers, for any order of the perturbation. In the present paper, it has been shown how the use of the three-terms recurrence relation between perturbed eigenfunctions allows a straightforward determination of any perturbed eigenfunction as well as closed form expressions of any matrix element of a Hermitian operator between these functions in terms of one unique integral. One may add that the treatment of the Nth order of the perturbation is not significantly more difficult than the first order. As a particular illustrative example, results are given for the generalised central field problem (perturbed type F). The same treatment is relevant for studying the Stark effect either by considering it as a 'perturbed type F' or, after some manipulations (Hehenberger *et al* 1974), by considering it as a 'perturbed type C'. The perturbed ladder procedure works nicely also for calculating rotation–vibration wavefunctions and intensities of diatomic molecules. For instance, the diatomic nuclear equation, when it involves a perturbed Morse potential with additional perturbations describing rotational energy (Huffaker 1976), is relevant to the 'perturbed type B' treatment while, when it involves a Dunham potential (Dunham 1932, Kilpatrick 1959), the 'perturbed type D' (anharmonic oscillator) scheme applies. Results of this last investigation will be given elsewhere.

References

Bessis N, Bessis G, Dakhel B and Hadinger G 1978 *J. Phys. A: Math. Gen.* **11** 467
Dunham J L 1932 *Phys. Rev.* **41** 721
Hehenberger M, McIntosh H V and Brändas E 1974 *Phys. Rev.* A **10** 1494
Huffaker J N 1976 *J. Chem. Phys.* **64** 3175
Infeld L and Hull T E 1951 *Rev. Mod. Phys.* **23** 21
Kilpatrick J E 1959 *J. Chem. Phys.* **30** 801
Pasternack S and Sternheimer R M 1962 *J. Math. Phys.* **3** 1280
Schrödinger E 1940 *Proc. R. Irish Acad.* A **46** 183