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# The perturbed ladder operator method—analytical determination of the generalised central field energies and wavefunctions

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**Abstract.** In order to extend the original range of applicability of the ladder operator formalism, a novel method of resolution of perturbed equations is presented. This method, capable of handling any order of the perturbation, allows an easy determination of 'perturbed ladder operators' and hence gives analytical expressions for the perturbed eigenvalues and eigenfunctions in terms of the quantum numbers of the unperturbed factorisable problem. The case of a wave equation with a Coulomb potential (factorisable type F) perturbed by an additive Hamiltonian expanded in a positive power series of  $r$ , i.e.  $V(r) = -[l(l+1)/r^2] - (2q/r) + b_0 + b_1r + \dots + b_sr^s$ , is worked out in detail. Application to the screened (static or cosine) Coulombic problem is given as an illustrative example.

## 1. Introduction

The Schrödinger–Infeld–Hull factorisation method (Schrödinger 1940, Infeld and Hull 1951) is known to be an elegant method of solving fundamental equations of mathematical physics which admit solutions of hypergeometric form (Duff 1949, Hadinger *et al* 1974). The concept of 'ladder operators' (for instance, the  $J^\pm$  operators of angular momentum theory) is now a familiar one, and there is interest in the principle and computational point of view of the method. When a given equation is factorisable the complete set of normalised eigenfunctions can be generated by repeated application of the ladder operators to the 'key function', which is the solution of a first-order differential equation. Moreover, the eigenvalues are readily obtained from knowledge of the factorisation type to which the equation belongs. In fact, the original range of applicability of the method can be extended within the perturbation scheme, in order to treat problems which are beyond its primè and original scope.

One of these possible extensions, i.e. the 'perturbed factorisation' technique was recognised early (Schrödinger 1940, Infeld and Hull 1951, Infeld 1942). Summarising '*grosso modo*' the principle of this technique: one tries to build up perturbed ladder operators associated with successive orders of the perturbation. Once the perturbed ladder operator is found, the usual factorisation scheme applies. Hence, one could obtain analytical expressions for both the perturbed eigenvalues and eigenfunctions to the required accuracy.

At this early stage, it should be emphasised that the straightforward extension of the 'unperturbed scheme' (i.e. trying to determine the perturbed ladder right from the

beginning) unfortunately leads to rather intricate calculations. This is probably why Infeld and Hull (1951) have limited their pioneering use of this procedure to second-order Stark effect calculations and this is why we have to work out a novel procedure capable of handling any order of perturbation and possessing a wider range of applicability.

After an essential review of the basic theory of the 'exact' ladder operator in § 2, our new perturbed factorisation scheme is presented in § 3 and particular attention is paid to the fundamental radial factorisation types E and F. For the Coulombic case (F), detailed computations are carried out in § 4. Finally, eigen-energies and eigenfunctions of the screened Coulombic problem are given as an illustrative application.

## 2. Exact factorisation

In order to set up the notation, it is necessary first to briefly recall how the ladder operator works when it is applied to solve a so called factorisable equation.

Many problems of fundamental interest in quantum mechanics lead to equations of the Sturm–Liouville type. Without restricting the generality of the problem, by an appropriate transformation of variable and function, these equations can be reduced to the standard form (see appendix 1):

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

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

$$|\psi(x_1)|^2 = |\psi(x_2)|^2 = 0; \quad \int_{x_1}^{x_2} |\psi(x)|^2 dx = 1 \quad (2)$$

where  $m = m_0, m_0 + 1, m_0 + 2 \dots$  is assumed to take successive discrete values labelling the eigenfunctions.

Such an equation (1) is factorisable when it can be replaced by each of the following two differential equations:

$$\begin{aligned} H_{m+1}^- H_{m+1}^+ \Psi_{jm} &= (\Lambda_j - L(m+1))\Psi_{jm} \\ H_m^+ H_m^- \Psi_{jm} &= (\Lambda_j - L(m))\Psi_{jm} \end{aligned} \quad (3)$$

where  $j$  is the quantum number associated with the eigenvalue  $\Lambda_j$ ,  $L(m)$  is a function which does not depend on  $x$  and  $H_m^\pm$  are ladder operators

$$H_m^\pm = K(x, m) \mp \frac{d}{dx}. \quad (4)$$

Then, the eigenfunctions  $\Psi_{jm}$  are solutions of the following pair of difference-differential equations (see Infeld and Hull 1951, Hadinger *et al* 1974):

$$\begin{aligned} H_{m+1}^+ \Psi_{jm} &= (\Lambda_j - L(m+1))^{1/2} \Psi_{jm+1} \\ H_m^- \Psi_{jm} &= (\Lambda_j - L(m))^{1/2} \Psi_{jm-1}. \end{aligned} \quad (5)$$

That is to say, the ladder operators  $H_m^\pm$  generate the eigenfunctions step by step, downward or upward, and allow the determination of any  $\Psi_{jm}(x)$  function from the knowledge of the 'key function'  $\Psi_{jj}$  which is the solution of a first-order differential

equation. Furthermore one very interesting property is that if one starts from a normalised key function  $\Psi_{jj}$ , then the ladder operation (5) generates normalised eigenfunctions  $\Psi_{jm}$ .

When  $L(m)$  is an increasing function of  $m$  (class 1 problems), the necessary condition for the existence of quadratically integrable solutions, i.e. the quantification condition, is given by

$$j - m = v = \text{integer} \geq 0. \tag{6}$$

The eigenvalues are

$$\Lambda_j = L(j + 1). \tag{7}$$

The 'key function' is the solution of the first-order differential equation

$$\left( K(x, j + 1) - \frac{d}{dx} \right) \Psi_{jj}(x) = 0. \tag{8}$$

When  $L(m)$  is a decreasing function of  $m$  (class 2 problems) the quantisation condition is  $m - j = v = \text{integer} \geq 0$ . The eigenvalues are  $\Lambda_j = L(j)$  and the eigenfunctions are obtained in an analogous way to class 1 problems.

From the comparison of equations (1) and (3), it is easily shown that the necessary and sufficient condition to be satisfied by  $K(x, m)$  and  $L(m)$  allowing the factorisation of equation (1) is:

$$\begin{aligned} (K(x, m + 1))^2 + \frac{d}{dx} K(x, m + 1) + L(m + 1) &= -U(x, m) \\ (K(x, m))^2 - \frac{d}{dx} K(x, m) + L(m) &= -U(x, m). \end{aligned} \tag{9}$$

As is well known (Infeld and Hull 1951), there are six fundamental factorisable cases which are summarised in table 1. However, when direct factorisation is not possible solely because of the inadequate  $m$ -dependence of the potential  $U(x, m)$  under consideration, one can resort to 'artificial' or 'embedded' factorisation, i.e. one can consider  $U(x, m)$  as 'embedded' in a new potential function  $u(x, m, \mu)$  which belongs to table 1 (if one considers  $\mu$  as a supplementary parameter) such that  $u(x, m, m) = U(x, m)$ . Then, equation (1) is factorised using  $u(x, m, \mu)$ , and class 1 (or class 2) eigenvalues  $\Lambda_j = L(j + 1, \mu)$  (or  $\Lambda_j = L(j, \mu)$ ) are determined as well as the eigenfunctions  $\Psi_{jm}(x, \mu)$ , both depending on the parameter  $\mu$ . At the end of the ladder procedure, one sets  $\mu = m$  and merely obtains the required solutions.

Nevertheless, as will be shown in the present paper, when neither direct nor embedded factorisation applies, it is still possible to widen out the narrow limits of the six Infeld-Hull cases of factorisability by mapping the perturbation scheme onto the ladder operator formalism.

### 3. The perturbed ladder operator method

#### 3.1. Method

Now let us consider the second-order differential equation (1) involving a potential function  $\mathcal{U}(x, m)$  which does not belong to any of the six factorisable types of table 1

**Table 1.** Infeld–Hull factorisation types.

Type	$U(x, m)$	$K(x, m)$	$L(m)$
A	$-\frac{a^2}{\sin^2 ax} (m(m+1) + d^2 + d(2m+1) \cos ax)$	$ma \cot ax + \frac{ad}{\sin ax}$	$a^2 m^2$
B	$-d^2 \exp(2ax) + ad(2m+1) \exp(ax)$	$-ma + d \exp(ax)$	$-a^2 m^2$
C	$-\frac{m(m+1)}{x^2} - b^2 x^2 + b(2m+1)$	$\frac{m}{x} + bx$	$-4bm$
D	$-(bx+d)^2 + b(2m+1)$	$bx+d$	$-2bm$
E	$-\frac{a^2}{\sin^2 ax} m(m+1) - 2aq \cot ax$	$ma \cot ax + \frac{q}{m}$	$a^2 m^2 - \frac{q^2}{m^2}$
F	$-\frac{m(m+1)}{x^2} - \frac{2q}{x}$	$\frac{m}{x} + \frac{q}{m}$	$-\frac{q^2}{m^2}$

and let us assume that this potential function, as well as the associated factorisation functions  $\mathcal{K}(x, m)$  and  $\mathcal{L}(m)$  to be found, can be expanded in a perturbation series with a parameter  $\eta$ :

$$\begin{aligned}
 \mathcal{U}(x, m) &= U^{(0)}(x, m) + \eta U^{(1)}(x, m) + \eta^2 U^{(2)}(x, m) + \dots \\
 \mathcal{K}(x, m) &= K^{(0)}(x, m) + \eta K^{(1)}(x, m) + \eta^2 K^{(2)}(x, m) + \dots \\
 \mathcal{L}(m) &= L^{(0)}(m) + \eta L^{(1)}(m) + \eta^2 L^{(2)}(m) + \dots
 \end{aligned}
 \tag{10}$$

where  $K^{(0)}(x, m)$  and  $L^{(0)}(m)$  are the factorisation functions allowing an exact factorisation of the wave equation (1) with  $U^{(0)}(x, m)$ .

Then one has to satisfy the factorisability condition (9) up to a given power of the parameter  $\eta$ . The required  $K^{(N)}$ ,  $L^{(N)}$  and  $U^{(N)}$  are found to be solutions of the following equations:

$$\begin{aligned}
 \sum_{\nu=0}^N K^{(\nu)}(x, m+1) K^{(N-\nu)}(x, m+1) + \frac{d}{dx} K^{(N)}(x, m+1) + L^{(N)}(m+1) &= -U^{(N)}(x, m) \\
 \sum_{\nu=0}^N K^{(\nu)}(x, m) K^{(N-\nu)}(x, m) - \frac{d}{dx} K^{(N)}(x, m) + L^{(N)}(m) &= -U^{(N)}(x, m).
 \end{aligned}
 \tag{11}$$

These equations (11) will be solved recursively, i.e. when considering the determination of  $K^{(N)}$  and  $U^{(N)}$ , it is assumed that all the  $K^{(\nu)}$  for  $\nu = 1, 2 \dots N-1$  have already been found.

As we pointed out before, our procedure at this stage will differ from the Infeld–Hull one: we determine first  $U^{(N)}(x, m)$  instead of  $K^{(N)}(x, m)$ . In order to eliminate  $K^{(N)}(x, m)$  from (11), it is best to consider the two equivalent combinations

$$\begin{aligned}
 \frac{d}{dx} K^{(N)}(x, m) &= \frac{1}{2}(U^{(N)}(x, m) - U^{(N)}(x, m-1)) \\
 2K^{(0)}(x, m) K^{(N)}(x, m) + \frac{1}{2}(U^{(N)}(x, m) + U^{(N)}(x, m-1)) & \\
 + L^{(N)}(m) + \sum_{\nu=1}^{N-1} K^{(\nu)}(x, m) K^{(N-\nu)}(x, m) &= 0.
 \end{aligned}
 \tag{12}$$

Integrating the first equation of (12) by setting

$$U^{(N)}(x, m) = \frac{d}{dx} W^{(N)}(x, m) \tag{13}$$

gives

$$K^{(N)}(x, m) = \frac{1}{2}(W^{(N)}(x, m) - W^{(N)}(x, m - 1)) + k(m) \tag{14}$$

where  $k(m)$  is an integration constant which, of course, could depend on  $m$ .

Then, from (12) and (14), one obtains the following difference-differential equation:

$$\begin{aligned} \frac{1}{2} \frac{d}{dx} (W^{(N)}(x, m) + W^{(N)}(x, m - 1)) + K^{(0)}(x, m)(W^{(N)}(x, m) - W^{(N)}(x, m - 1)) \\ + 2K^{(0)}(x, m)k(m) + L^{(N)}(m) + \sum_{\nu=1}^{N-1} K^{(\nu)}(x, m)K^{(N-\nu)}(x, m) = 0. \end{aligned} \tag{15}$$

The finite-difference aspect of (15) determines the  $m$ -dependence of the functions  $W^{(N)}(x, m)$  and  $L^{(N)}(m)$  while its differential aspect determines the  $x$ -dependence of  $W^{(N)}(x, m)$ . Once the  $W^{(N)}(x, m)$  is found, the perturbing potential  $U^{(N)}(x, m)$  and the associated ladder function  $K^{(N)}(x, m)$  are given by (13) and (14) respectively. Then the perturbed problem (up to the  $N$ th order) may be handled in the same way as the exact factorisable (unperturbed) problems.

### 3.2. $m$ -dependence of the factorisation functions and potential

The kind of  $m$ -dependence of the perturbing  $U^{(N)}$ ,  $K^{(N)}$  and  $L^{(N)}$  functions follows (see equations (12) or (15)) from the  $m$ -dependence of the zeroth-order ladder function  $K^{(0)}(x, m)$  which is (table 1):

$$K^{(0)}(x, m) = f(x)m + g(x), \quad \text{for types A to D} \tag{16}$$

or

$$K^{(0)}(x, m) = f(x)m + (q/m), \quad \text{for types E and F.} \tag{17}$$

By analogy with the exact factorisation scheme, a finite expansion of powers of  $m$  is assumed for  $U^{(1)}(x, m)$ , and hence for  $W^{(1)}(x, m)$ . Nevertheless, when substituting both expressions of  $W^{(1)}$  and  $K^{(0)}$  (equations (16) or (17)) into (15), it is easily shown that, for all factorisation types (A-F),  $W^{(1)}(x, m)$  involves only positive powers of  $m$ . Step by step it could be shown that this result holds for any order.

In order to investigate thoroughly the  $m$ -dependence of  $W^{(N)}(x, m)$ , one has to distinguish between the  $K^{(0)}(x, m)$  which are linear functions in  $m$  (equation (16)) and the  $K^{(0)}(x, m)$  which are non-linear in  $m$  (equation (17)). In the present paper, we shall focus our attention on this last case.

For general types E and F ( $q \neq 0$ ) and for any order  $N$  of the perturbation, the following  $m$ -parity relationships hold:  $K^{(N)}(x, -m) = -K^{(N)}(x, m)$ ;  $L^{(N)}(-m) = L^{(N)}(m)$  and  $U^{(N)}(x, m)$  is found to be a series of  $m(m+1)$ . These are indeed properties already verified by  $K^{(0)}(x, m)$ ,  $L^{(0)}(m)$  and  $U^{(0)}(x, m)$  (see table 1).

Therefore, an adequate expansion of the  $W^{(N)}$  and  $U^{(N)}$  functions is as follows:

$$W^{(N)}(x, m) = \gamma_0^{(N)}(x) + \sum_{v=1}^{S_N} \gamma_v^{(N)}(x)[m(m+1)]^v \tag{18}$$

$$U^{(N)}(x, m) = \frac{d\gamma_0^{(N)}}{dx} + \sum_{v=1}^{S_N} \frac{d\gamma_v^{(N)}}{dx} [m(m+1)]^v. \tag{19}$$

From (18) one gets

$$W^{(N)}(x, m) + W^{(N)}(x, m-1) = 2\gamma_0^{(N)}(x) + 2 \sum_{v=1}^{S_N} m^{2v} \sum_{u=0}^{S_N-v} \binom{v+u}{2u} \gamma_{v+u}^{(N)}(x) \tag{20}$$

$$W^{(N)}(x, m) - W^{(N)}(x, m-1) = 2 \sum_{v=1}^{S_N} m^{2v-1} \sum_{u=0}^{S_N-v} \binom{v+u}{2u+1} \gamma_{v+u}^{(N)}(x)$$

where  $\binom{n}{m}$  are binomial coefficients.

From (14), one obtains the perturbing ladder function

$$K^{(N)}(x, m) = \sum_{v=1}^{S_N} m^{2v-1} \sum_{u=0}^{S_N-v} \binom{v+u}{2u+1} \gamma_{v+u}^{(N)}(x) + \sum_{v=0}^{S_N} k_v m^{2v-1} \tag{21}$$

where  $k_v$  are constants (with respect to  $x$  and  $m$ ).

An adequate expansion of the factorisation function is

$$L^{(N)}(m) = \sum_{v=-1}^{S_N} \beta_v m^{2v}. \tag{22}$$

Anticipating the results demonstrated in the next section, and also for convenience, the effective bounds of summations in (22) and in the last term of (21) have been written out.

### 3.3. Perturbing potentials and ladders (E) and (F)

3.3.1. *First order of perturbation* ( $N = 1$ ). Using (20), (22), (17) and (15), that is to say putting the  $m$ -dependence of  $W^{(1)}$  into the factorisability condition (15), one obtains:

$$\begin{aligned} & \left[ \binom{v}{v} \frac{d}{dx} + 2 \binom{v}{v-1} f(x) \right] \gamma_v^{(1)}(x) \\ &= -\beta_v^{(1)} - 2qk_{v+1}^{(1)} - 2k_v^{(1)} f(x) \\ & \quad - \sum_{u=1}^{S_1-v} \left[ 2 \binom{v+u}{2u+1} f(x) + \binom{v+u}{2u} \frac{d}{dx} + 2q \binom{v+u}{2u-1} \right] \gamma_{v+u}^{(1)}(x) \end{aligned} \tag{23}$$

where (see table 1)

$$f(x) = \begin{cases} a \cot ax & \text{for type E} \\ 1/x & \text{for type F.} \end{cases} \tag{24}$$

The general solution of this triangular linear differential system in the  $\gamma_v^{(1)}(x)$  is easily found. Setting

$$F_v(x) = \exp\left(-2v \int f(x) dx\right) = \begin{cases} (1/\sin ax)^{2v} & \text{for type E} \\ (1/x)^{2v} & \text{for type F,} \end{cases} \tag{25}$$

one gets ( $1 \leq v \leq S_1$ ):

$$\gamma_v^{(1)}(x) = C_v^{(1)}F_v(x) - F_v(x) \int \frac{dx}{F_v(x)} \left\{ \beta_v^{(1)} + 2qk_{v+1}^{(1)} + 2k_v^{(1)}f(x) + \sum_{u=1}^{S_1-v} \left[ 2 \binom{v+u}{2u+1} f(x) + \binom{v+u}{2u} \frac{d}{dx} + 2q \binom{v+u}{2u-1} \right] \gamma_{v+u}^{(1)}(x) \right\}. \tag{26}$$

For any choice of the truncation bound  $S_1$ , the  $\gamma_v^{(1)}(x)$  can be calculated from (26), step by step, downwards for  $v = S_1, S_1 - 1 \dots 1$ . The ladder function  $K^{(1)}(x, m)$  involving the free constants  $C_v^{(1)}, k_v^{(1)}$  and  $\beta_v^{(1)}$ , is then obtained from (21) and the perturbing potential  $U^{(1)}(x, m)$  from (19) where (see equation (23) for  $v = 0$ )

$$\frac{d\gamma_0^{(1)}}{dx} = -\beta_0^{(1)} - 2qk_1^{(1)} - 2k_0^{(1)}f(x) - 2q\gamma_1^{(1)}(x). \tag{27}$$

Let us point out that, for type F,  $U^{(1)}$  is merely a series of positive and negative powers of  $x$  while for type E,  $U^{(1)}$  is a rather intricate function of  $x$  (see equations (25) and (26)).

Finally, the vanishing conditions, when  $v = -1, -2, \dots$  or  $v = S + 1, S + 2, \dots$ , of the binomial coefficients involved in (23) lead to the following identities:

$$\begin{aligned} \beta_{-1} &= -2qk_0 \\ k_{-1}^{(1)} &= k_{-2}^{(1)} = \dots = 0; & k_{S+1}^{(1)} &= k_{S+2}^{(1)} = \dots = 0 \\ \beta_{-2}^{(1)} &= \beta_{-3}^{(1)} = \dots = 0; & \beta_{S+1}^{(1)} &= \beta_{S+2}^{(1)} = \dots = 0. \end{aligned} \tag{28}$$

This is the justification of the values of the summation bounds in (21) and (22).

3.3.2. *Nth order of the perturbation.* When considering the determination of the  $N$ th-order functions, it is assumed that those of the lower orders have already been found. Then in equation (15) one can write

$$\sum_{\nu=1}^{N-1} K^\nu(x, m)K^{(N-\nu)}(x, m) = \sum_{\nu} \omega_\nu^{(N)}(x)m^{2\nu} \tag{29}$$

where the  $\omega_\nu^{(N)}(x)$  are completely known.

Consequently, the  $N$ th-order differential system which determines the  $\gamma_v^{(N)}(x)$  is merely obtained from the first-order equation (23) by the formal change  $\beta_v^{(1)} \rightarrow \beta_v^{(N)} + \omega_v^{(N)}(x)$ , i.e. one gets  $\gamma_v^{(N)}(x)$  by use of expression (26), and subtracting the following term from this:

$$\Omega_v^{(N)}(x) = F_v(x) \int \frac{dx}{F_v(x)} \omega_v^{(N)}(x). \tag{30}$$

Finally, the  $K^{(N)}$  and  $U^{(N)}$  functions can be calculated, to any order  $N$ , without significant difficulty (equations (21) and (19)) and the general type E (or type F) factorising (up to the  $N$ th order) potential  $\mathcal{U}(x, m)$  is obtained (equation (10)). Its general expression involves free constants  $C_\nu^{(\nu)}, k_\nu^{(\nu)}$  and  $\beta_\nu^{(\nu)}$  ( $\nu = 1, N; v = 1, S_\nu$ ) to be adjusted in order to match with a given physical potential function in equation (1).

The same procedure applies to determine types A–D perturbed potentials. It has been found that, in these cases,  $K^{(N)}(x, m)$  does not have a definite parity in  $m$  and



that an adequate expansion of  $U^{(N)}$ , and hence of  $W^{(N)}$ , involves powers of  $m(m + 1)$  as well as odd powers of  $(2m + 1)$ . These cases will be investigated in a further paper together with some illustrative applications.

**4. Generalised central field energies and wavefunctions**

*4.1. Determination of the factorisation and ladder functions*

In view of many possible applications and as an illustrative example, it is worthwhile to work out in detail a special type F case corresponding to the particular choice of the free constants in (26), i.e.  $C_v^{(\nu)} = k_v^{(\nu)} = 0$  ( $\nu = 1, N$ ). In that case the expression of the  $\gamma_v^{(N)}(x)$  reduces to

$$\gamma_v^{(N)}(x) = -\frac{\beta_v^{(N)}}{2v+1}x - \Omega_v^{(N)}(x) - \sum_{u=1}^{S_N-v} \binom{v+u}{2u} \gamma_{v+u}^{(N)}(x) + \sum_{u=1}^{S_N-v} \left(\frac{1}{x}\right)^{2v} \int x^{2v} \left[ \frac{2u(2v+1)}{(2u+1)x} \binom{v+u}{2u} - 2q \binom{v+u}{2u-1} \right] \gamma_{v+u}^{(N)}(x) dx. \tag{31}$$

From this expression it can be inferred recursively that the  $\gamma_v^{(N)}$  are polynomials of  $x$  of degree  $(S_N + 1 - v)$  whose coefficients depend on the free constants  $\beta_i^{(\nu)}$  ( $\nu = 1, N - 1; i = 1, S_\nu$ ). It should be noted that, once the first-order truncation bound  $S_1$  has been arbitrarily chosen, the choice (i.e. the minimal values) of  $S_2, S_3 \dots S_N$  is not free. Indeed, when calculating  $\gamma_v^{(N)}$ , the polynomial  $\Omega_v^{(N)}(x)$  in (31) is already fixed as data following from the results of the preceding orders. Subsequently, the highest power of  $x$  on the right-hand side of (31) is fixed and associated to  $S_N = S_\nu + S_{N-\nu} + 1$  for  $\nu = 1, N - 1$ . Hence the value of  $S_N$  depends recursively on  $S_1$ , and one finds

$$S_N = NS_1 + N - 1. \tag{32}$$

Finally, after calculating the set of the  $\gamma_v^{(\nu)}(x)$  polynomials, the factorising perturbed potential is obtained:

$$\mathcal{U}(x, m) = -\frac{m(m+1)}{x^2} - \frac{2q}{x} + \sum_{\nu=1}^N \eta^\nu U^{(\nu)}(x, m)$$

with (33)

$$U^{(\nu)}(x, m) = -\beta_0^{(\nu)} - 2q\gamma_1^{(\nu)} + \sum_{v=1}^{S_\nu} \frac{d\gamma_v^{(\nu)}}{dx} [m(m+1)]^v,$$

i.e. the perturbing part of  $\mathcal{U}(x, m)$  is merely a polynomial in  $x$  of degree  $S_N$ , the coefficients of which depend on  $m(m + 1)$  and  $\beta_v^{(\nu)}$ .

The associated ladder function is

$$\mathcal{K}(x, m) = \frac{m}{x} + \frac{q}{m} + K_N(x, m)$$

where (cf equation (21) with  $k_v = 0$ ) (34)

$$K_N(x, m) = \sum_{\nu=1}^N \eta^\nu \sum_{v=1}^{S_\nu} m^{2v-1} \sum_{u=0}^{S_\nu-v} \binom{v+u}{2u+1} \gamma_{v+u}^{(\nu)}(x).$$

The associated energy function is (cf equation (22) with  $\beta_{-1} = -2qk_0 = 0$ ):

$$\mathcal{L}(m) = -\frac{q^2}{m^2} + \sum_{\nu=1}^N \eta^\nu \sum_{\nu=0}^{s_\nu} \beta_\nu^{(\nu)} m^{2\nu}. \tag{35}$$

We have thus manufactured the necessary mathematical tools to factorise any wave equation (1) involving a Coulomb potential (type F) with an additive perturbative Hamiltonian which is (or can be expanded in) a positive power series of  $x$ .

Indeed, let us consider a given equation

$$\left( \frac{d^2}{dx^2} + \mathcal{V}(x) + b_0 + \mathcal{E} \right) \Psi = 0 \tag{36}$$

with

$$\mathcal{V}(x) = -\frac{m(m+1)}{x^2} - \frac{2q}{x} + b_1x + b_2x^2 + \dots + b_{s_N}x^{s_N}. \tag{37}$$

The values of  $q$  and  $b_i$  are, of course, specific to the physical problem under consideration.

In order to identify  $\mathcal{V}(x)$  with  $\mathcal{U}(x, m)$  (equation (33)), it is convenient to write

$$\mathcal{V}(x) = -\frac{m(m+1)}{x^2} - \frac{2q}{x} + \sum_{\nu=1}^N \mathcal{V}^{(\nu)}(x)$$

with

$$\mathcal{V}^{(\nu)}(x) = \sum_{\mu=s_{\nu-1}+1}^{s_\nu} b_\mu x^\mu. \tag{38}$$

From successive identifications of  $\mathcal{V}^{(\nu)}$  with  $U^{(\nu)}$ , the  $\beta_\nu^{(\nu)}$  may be expressed in terms of  $b_i$  and  $\mu = m(m+1)$  so consequently analytical expressions of the factorisation function  $\mathcal{L}(m; b_i, \mu)$  and the ladder function  $\mathcal{K}(x, m; b_i, \mu)$  are found depending on  $b_i$  and  $\mu$ . Hence, using the factorisation scheme (with  $\mu$  considered as an artificial parameter) one obtains analytical expressions of the eigenvalues (class 1):

$$\mathcal{E}_j = \mathcal{E}_j^{(0)} + \mathcal{E}_j^{(1)} + \dots + \mathcal{E}_j^{(N)} = \mathcal{L}(j+1; b_i, \mu) - b_0. \tag{39}$$

The ‘key perturbed’ function is the solution of the first-order differential equation

$$\left( K^{(0)}(x, j+1) + K_N(x, j+1; b_i, \mu) - \frac{d}{dx} \right) \Psi_{jj} = 0 \tag{40}$$

and one gets the following expression of the ‘key perturbed eigenfunction’ ( $m = j$ )

$$\Psi_{jj} \approx \Psi_{jj}^{(0)} \exp\left( \int K_N(x, j+1; b_i, \mu) dx \right) \tag{41}$$

where the artificial parameter  $\mu$  has to be set to its actual value  $\mu = j(j+1)$  and

$$\Psi_{jj}^{(0)} = \mathcal{N}_j x^{j+1} \exp[qx/(j+1)] \tag{42}$$

is the zero-order normalised key function, the solution of equation (5) for type F (class 1):

$$\left( K^{(0)}(x, j+1) - \frac{d}{dx} \right) \Psi_{jj}^{(0)} = \left( \frac{j+1}{x} + \frac{q}{j+1} - \frac{d}{dx} \right) \Psi_{jj}^{(0)} = 0. \tag{43}$$

Then, starting from the 'key perturbed' eigenfunction (41), the complete set of eigenfunctions is generated by successive application of the ladder operator

$$\left( K^{(0)}(x, m) + K_N(x, m; b_i, \mu) + \frac{d}{dx} \right) \Psi_{jm} = (\mathcal{E}_j - \mathcal{L}(m; b_i, \mu))^{1/2} \Psi_{jm-1}. \quad (44)$$

Once the  $\Psi_{jm}(x; b_i, \mu)$  function is obtained, the artificial parameter  $\mu$  is set to its true value  $m(m+1)$ . For instance, applying the ladder operation (44) once to (41) gives

$$\Psi_{j-1} = \left( \frac{(2j+1)^{1/2}}{j(j+1)} \Psi_{j-1}^{(0)} + (K_N(j) + K_N(j+1)) \Psi_{jj}^{(0)} \right) \exp\left( \int K_N(j+1) dx \right). \quad (45)$$

where  $K_N(j) = K_N(x, j; b_i, \mu)$  and  $m = j-1 \rightarrow \mu = j(j-1)$ .

$$\Psi_{j-1}^{(0)} = (2j+1)^{1/2} \mathcal{N}_j [qx + j(j+1)] x^j \exp[qx/(j+1)] \quad (46)$$

is the zero-order normalised wavefunction and  $\mathcal{N}_j$  is the normalised constant of the key, since the ladder operation (5) preserves the normalisation of the functions.

#### 4.2. Illustrative application

Let us apply the method to a special case, i.e. let us take  $S_1 = 2$  and  $q = -1^\dagger$ . One has first to work out the expression of  $U^{(1)}$ .

Since  $\Omega_v^{(1)}(x) = 0$ , from equation (31):

$$\begin{aligned} \gamma_2^{(1)} &= -\frac{1}{5} \beta_2^{(1)} x \\ \gamma_1^{(1)} &= \left( -\frac{1}{3} \beta_1^{(1)} + \frac{1}{15} \beta_2^{(1)} \right) x - \frac{1}{5} \beta_2^{(1)} x^2. \end{aligned} \quad (47)$$

Then from equation (33), setting  $m(m+1) = \mu$ :

$$\begin{aligned} U^{(1)}(x, m) &= -\beta_0^{(1)} + \left( -\frac{1}{3} \beta_1^{(1)} + \frac{1}{15} \beta_2^{(1)} \right) \mu - \frac{1}{5} \beta_2^{(1)} \mu^2 \\ &\quad + \left( -\frac{2}{3} \beta_1^{(1)} + \frac{2}{15} \beta_2^{(1)} - \frac{2}{5} \beta_2^{(1)} \mu \right) x - \frac{2}{5} \beta_2^{(1)} x^2. \end{aligned} \quad (48)$$

Equating coefficients of equal powers of  $x$  in  $U^{(1)} = \mathcal{V}^{(1)} = b_1 x + b_2 x^2$ , one gets:

$$\begin{aligned} \beta_2^{(1)} &= -\frac{5}{2} b_2 \\ \beta_1^{(1)} &= -\frac{3}{2} b_1 - \frac{1}{2} b_2 (1 - 3\mu) \\ \beta_0^{(1)} &= \frac{1}{2} b_1 \mu \end{aligned} \quad (49)$$

and, from (35), for the first order ( $N = 1$ ):

$$\mathcal{L}(m) = -\frac{1}{m^2} + \frac{1}{2} b_1 \mu - \left( \frac{3}{2} b_1 + \frac{1}{2} b_2 (1 - 3\mu) \right) m^2 - \frac{5}{2} b_2 m^4. \quad (50)$$

In order to obtain the first-order perturbed eigenvalue one can now apply the factorisation scheme (with  $\mu$  considered as an artificial parameter). Since, in terms of the usual quantum numbers ( $n, l$ ), and after setting  $R_{nl}(r) = \Psi_{jm}/r$  and  $x = Zr$ , the Coulombic problem is a class 1 case with  $j = n-1$ ,  $m = l$ , the following analytical expression of the first-order perturbed energy (cf equations (39) and (50)) is obtained:

$$\mathcal{E}_n^{(0)} + \mathcal{E}_n^{(1)} = -\frac{1}{n^2} - b_0 - \frac{1}{2} b_1 [3n^2 - l(l+1)] - \frac{1}{2} b_2 n^2 [5n^2 - 3l(l+1) + 1]. \quad (51)$$

$^\dagger$  This is not a restriction. One can always assume  $q = -1$  by change of variable  $-qx \rightarrow x'$ .

Let us now consider the determination of the second-order energy with  $S_2 = 2S_1 + 1 = 5$  (equation (32)). In order to obtain the  $\gamma_v^{(2)}$ , one has first to calculate the increments  $\Omega_v^{(2)}$  arising from the first-order contribution ( $K^{(1)}$ )<sup>2</sup> (see equations (29) and (30)). Since, from equation (21)

$$K^{(1)}(x, m) = \gamma_1^{(1)}(x)m + 2\gamma_2^{(1)}(x)m^3, \tag{52}$$

where  $\gamma_v^{(1)}$  are already known functions of  $x$ ,  $b_i$  and  $\mu$ , after a few elementary manipulations, one arrives at:

$$\begin{aligned} \Omega_5^{(2)} &= \Omega_4^{(2)} = 0 \\ \Omega_3^{(2)} &= \frac{1}{9}b_2^2x^3 \\ \Omega_2^{(2)} &= \frac{1}{7}b_2(b_1 - \mu b_2)x^3 + \frac{1}{8}b_2^2x^4 \\ \Omega_1^{(2)} &= \frac{1}{20}(\mu b_2 - b_1)^2x^3 + \frac{1}{12}(\mu b_2 - b_1)b_2x^4 + \frac{1}{28}b_2^2x^5. \end{aligned} \tag{53}$$

After calculating the  $\gamma_v^{(2)}(x)$  (see appendix 2), in the same way as the first-order calculation, one obtains the second-order energy

$$\begin{aligned} \mathcal{E}_n^{(0)} + \mathcal{E}_n^{(1)} + \mathcal{E}_n^{(2)} &= -\frac{1}{n^2} - b_0 - \frac{1}{2}b_1(3n^2 - \lambda) - \frac{1}{2}b_2n^2(5n^2 - 3\lambda + 1) \\ &\quad - \frac{1}{8}b_3n^2[35n^4 + 5n^2(5 - 6\lambda) - 3\lambda(2 - \lambda)] - \frac{1}{16}b_1^2n^2(7n^4 + 5n^2 - 3\lambda^2) \\ &\quad - \frac{1}{8}b_4n^4[63n^4 + 35n^2(3 - 2\lambda) + 12 - 50\lambda + 15\lambda^2] \\ &\quad - \frac{1}{16}b_5n^4[231n^6 + 105n^4(7 - 3\lambda) + 21n^2(14 - 25\lambda + 5\lambda^2) \\ &\quad - 5\lambda(12 - 8\lambda + \lambda^2)] - \frac{1}{16}b_1b_2n^4[45n^4 + 7n^2(9 - 2\lambda) - 5\lambda(2 + 3\lambda)] \\ &\quad - \frac{1}{32}b_2^2n^6[143n^4 + 15n^2(23 - 6\lambda) + 7(4 - 18\lambda - 3\lambda^2)] \end{aligned} \tag{54}$$

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

One can also calculate the third-order ( $N = 3$ ) energy corresponding to the same truncation of the perturbing potential (up to  $x^5$ ). Taking  $S_1 = 1$ ,  $S_2 = 3$  and  $S_3 = 5$ , one finds that the third-order energy is given by expression (54) with the last term replaced by the two following ones:

$$\begin{aligned} &-\frac{3}{32}b_1b_3n^4[77n^6 + 15n^4(13 - 3\lambda) + 7n^2(4 - 9\lambda - 3\lambda^2) - 5\lambda(2 - \lambda)] \\ &\quad - \frac{1}{64}b_1^3n^4(33n^6 + 75n^4 - 7n^2\lambda^2 - 10\lambda^3). \end{aligned} \tag{55}$$

Let us point out that expression (54) generalises previous results of Iafate and Mendelsohn (1969, 1970, 1973). Indeed, when re-arranging their expression (cf equation (28) of Iafate and Mendelsohn 1970) in terms of  $\lambda = l(l + 1)$  one finds again expression (54) cut off from the four last terms, i.e. their result is found to correspond, with our perturbed scheme, to a second-order calculation with  $S_1 = 1 \rightarrow S_2 = 3$ .

Let us now obtain the wavefunctions. As pointed out before, it is sufficient to view the perturbative ladder function  $K$  as a polynomial in  $x$ . For our illustrative example  $S_1 = 2$ , and for the first order

$$K_1 = \eta K^{(1)} = \frac{1}{2}\eta\{[b_1 - b_2\mu]m + 2b_2m^3\}x + b_2mx^2. \tag{56}$$

When using the general results of the preceding section for  $m = l$ ,  $j = n - 1$ ,  $\mu = \lambda = l(l + 1)$ ,  $x = Zr$  and  $\Psi_{jm} = Z^{-1/2}rR_{nl}$  and on retaining the linear term in  $\eta$ , one finds

for instance, the following first-order perturbed wavefunctions:

$$\begin{aligned} R_{1s}^{(1)} &\approx [1 + \frac{1}{4}(b_1 + 2b_2)Z^2 r^2 + \frac{1}{6}b_2 Z^3 r^3] R_{1s}^{(0)} \\ R_{2p}^{(1)} &\approx [1 + \frac{1}{2}(b_1 + 6b_2)Z^2 r^2 + \frac{1}{3}b_2 Z^3 r^3] R_{2p}^{(0)} \end{aligned} \quad (57)$$

$$R_{2s}^{(1)} \approx [1 + (\frac{1}{2}b_1 + 4b_2)Z^2 r^2 + \frac{1}{3}b_2 Z^3 r^3] R_{2s}^{(0)} + 3^{1/2}[(b_1 + 6b_2)Zr + b_2 Z^2 r^2] R_{2p}^{(0)}$$

where the  $R_{nl}^{(0)}$  are the well known radial hydrogenic normalised functions.

Expressions for  $\gamma_v^{(2)}(x)$  and  $K^{(2)}$ , which are needed in order to determine the second-order perturbed wavefunctions ( $N=2, S_1=2 \rightarrow S_2=5$ ), are given in appendix 2.

## 5. Analytical determination of the screened Coulombic energies and wavefunctions

Let us focus our attention on the determination of the bound state energies of the screened Kepler problem. Its importance has been widely recognised (see for instance Rogers *et al* 1970, Bessis *et al* 1975, McEnnan *et al* 1976 and the references given therein). It is known that the static screened Coulomb potential

$$V_{SSCP}(r) = -(Z e^{-\alpha_0 r})/r \quad (58)$$

or the exponential cosine screened Coulomb potential

$$V_{ECSP}(r) = -(Z e^{-\alpha_0 r}/r) \cos(\alpha_0 r) \quad (59)$$

where  $\alpha_0$  is a screening parameter, occurs in several fields of physics (solid state physics, nuclear physics, statistical thermodynamics, etc). Instead of (58) or/and (59), it is convenient to use one unique expression

$$V_{SC}(r) = -(Z e^{-\alpha_0 r}/r) \cos(\epsilon \alpha_0 r) \quad (60)$$

which for  $\epsilon = 0$  and  $\epsilon = 1$  reduces to  $V_{SSCP}$  and  $V_{ECSP}$  respectively.

After setting  $R_{nl}(r) = \psi_{nl}(r)/r$ , the radial Schrödinger equation involving the screened potentials writes (in au)

$$\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} e^{-\alpha_0 r} \cos(\epsilon \alpha_0 r) + 2E_n \right) \psi_{nl}(r) = 0. \quad (61)$$

Let us consider the screened potentials  $V_{SC}$  as a Coulomb potential with an additive perturbative potential. Setting  $x = Zr$ ,  $\alpha = \alpha_0/Z$  and introducing the Taylor expansion of this perturbative potential near  $r = 0^+$ , the equation (61) is reduced to the standard form (36) with

$$\mathcal{E} = \frac{2}{Z^2} E_n; \quad q = -1 \quad (62)$$

$$b_u = \frac{2}{u!} \left[ \frac{d^u}{dx^u} \left( \frac{e^{-\alpha x} \cos(\epsilon \alpha x) - 1}{x} \right) \right]_{x=0}$$

or

$$b_u = 2 \frac{(-\alpha)^{u+1}}{(u+1)!} \sum_{j=0}^{\lfloor \frac{u+1}{2} \rfloor} (-1)^j \binom{u+1}{2j} \epsilon^{2j}. \quad (63)$$

† One could also choose, without introducing any difficulty, another origin of the Taylor expansion: for instance, the Bohr radius (see Bessis *et al* 1975).

Particularly

$$\begin{aligned}
 b_0 &= -2\alpha \\
 b_1 &= \alpha^2(1 - \epsilon^2) \\
 b_2 &= -\frac{1}{3}\alpha^3(1 - 3\epsilon^2) \\
 b_3 &= \frac{1}{12}\alpha^4(1 - 6\epsilon^2 + \epsilon^4) \\
 b_4 &= -\frac{1}{60}\alpha^5(1 - 10\epsilon^2 + 5\epsilon^4) \\
 b_5 &= \frac{1}{360}\alpha^6(1 - 15\epsilon^2 + 15\epsilon^4 - \epsilon^6).
 \end{aligned}
 \tag{64}$$

When substituting these expressions for  $b_i$  into expression (54) ( $S_1 = 2 \rightarrow S_2 = 5$ ) one gets† for the static case ( $\epsilon = 0$ ):

$$\begin{aligned}
 E_{nl} &= \frac{Z^2}{2} \left( -\frac{1}{n^2} + 2\alpha - \frac{1}{2}(3n^2 - \lambda)\alpha^2 + \frac{1}{6}n^2(5n^2 - 3\lambda + 1)\alpha^3 \right. \\
 &\quad - \frac{n^2}{96}[77n^4 + 5n^2(11 - 6\lambda) - 3\lambda(2 + 5\lambda)]\alpha^4 \\
 &\quad + \frac{n^4}{160}[171n^4 + 35n^2(7 - 2\lambda) - 5\lambda(10 + 9\lambda^2) + 4]\alpha^5 \\
 &\quad \left. - \frac{n^4}{5760}[3091n^6 + 15n^4(509 - 141\lambda) + 7n^2(122 - 435\lambda - 45\lambda^2) \right. \\
 &\quad \left. - 5\lambda(12 - 8\lambda + \lambda^2)]\alpha^6 \right).
 \end{aligned}
 \tag{65}$$

The third-order static energy ( $N = 3$  with  $S_1 = 1 \rightarrow S_3 = 5$ ) is given by expression (65) when the last ( $\sim \alpha^6$ ) term is replaced by the following:

$$\begin{aligned}
 &-\frac{n^4}{5760}[6666n^6 + 60n^4(271 - 39\lambda) + 42n^2(37 - 80\lambda - 35\lambda^2) \\
 &\quad - 5\lambda(102 - 53\lambda + 181\lambda^2)]\alpha^6.
 \end{aligned}
 \tag{66}$$

For the cosine case ( $\epsilon = 1$ )

$$\begin{aligned}
 E_{nl} &= \frac{Z^2}{2} \left( -\frac{1}{n^2} + 2\alpha + \frac{2}{3}n^2(5n^2 - 3\lambda + 1)\alpha^3 + \frac{1}{24}n^2[35n^4 + 5n^2(5 - 6\lambda) - 3\lambda(2 - \lambda)]\alpha^4 \right. \\
 &\quad - \frac{1}{120}n^4[63n^4 + 35n^2(3 - 2\lambda) + 12 - 50\lambda + 15\lambda^2]\alpha^5 \\
 &\quad \left. - \frac{1}{72}n^6[143n^4 + 15n^2(23 - 6\lambda) + 7(4 - 18\lambda - 3\lambda^2)]\alpha^6 \right).
 \end{aligned}
 \tag{67}$$

In this case, the third-order energy ( $S_3 = 5$ ) is given by the expression (67) cut off from the last ( $\sim \alpha^6$ ) term. Since the main purpose of this paper is to present the method rather than to give extensive tables, only two illustrative test results, i.e. second-order perturbed energies corresponding to successive choices  $S_1 = 2 \rightarrow S_2 = 5$  and  $S_1 = 3 \rightarrow S_2 = 7$  are given in table 2 ( $\epsilon = 0$ ) and table 3 ( $\epsilon = 1$ ).

Our results are in good agreement with the most accurate ones obtained elsewhere (Rogers *et al* 1970, Lam *et al* 1971, 1972, Bessis *et al* 1975).

†It should be noted that our result stands for a more general cosine potential  $V_{\text{ECSP}} = (-Z e^{-\alpha_0 r}/r) \cos(\alpha'_0 r)$  with  $\alpha'_0 \neq \alpha_0$  by choosing  $\epsilon = \alpha'_0/\alpha_0$  in (63).

Table 2. Comparative results for the eigenstate energies ( $-2E_{nl}$ ) in a static screened potential ( $\epsilon = 0$ ).

$Z/\alpha_0$	1s	2s	3s	4s	5s	2p	3p	3d	4p	4d
$\infty$	1.0000	0.2500	0.1111	0.06250	0.04000	0.2500	0.1111	0.1111	0.06250	0.06250
500	0.9960	0.2460	0.1072	0.05859	0.03615	0.2460	0.1072	0.1072	0.05859	0.05858
100	0.9801	0.2306	0.09240	0.04471	0.02332	0.2305	0.09231	0.09212	0.04463	0.04446
50	0.9606	0.2123	0.07604	0.03072 <sup>a</sup>	0.01182 <sup>a</sup>	0.2119	0.07570	0.07503	0.03043 <sup>a</sup>	0.02984 <sup>a</sup>
				0.03075 <sup>b</sup>	0.01204 <sup>b</sup>				0.03406 <sup>b</sup>	0.02987 <sup>b</sup>
				0.03076 <sup>c</sup>	0.01206 <sup>c</sup>				0.03047 <sup>c</sup>	0.02988 <sup>c</sup>
30	0.9350	0.1895	0.05739 <sup>a</sup>	0.01649 <sup>a</sup>	0.00121 <sup>a</sup>	0.1886	0.05656 <sup>a</sup>	0.05490 <sup>a</sup>	0.01585 <sup>a</sup>	0.01456 <sup>a</sup>
			0.05743 <sup>b</sup>	0.01699 <sup>b</sup>	0.00410 <sup>b</sup>		0.05660 <sup>b</sup>	0.05493 <sup>b</sup>	0.01633 <sup>b</sup>	0.01498 <sup>b</sup>
			0.05744 <sup>c</sup>	0.01701 <sup>c</sup>	0.00337 <sup>c</sup>		0.05662 <sup>c</sup>	0.05494 <sup>c</sup>	0.01638 <sup>c</sup>	0.01507 <sup>c</sup>
20	0.9036	0.1635	0.03827 <sup>a</sup>	0.00326 <sup>a</sup>		0.1615	0.03670 <sup>a</sup>	0.03348 <sup>a</sup>	0.00211 <sup>a</sup>	
			0.03866 <sup>b</sup>	0.00708 <sup>b</sup>			0.03705 <sup>b</sup>	0.03372 <sup>b</sup>	0.00584 <sup>b</sup>	
			0.03870 <sup>c</sup>	0.00618 <sup>c</sup>			0.03712 <sup>c</sup>	0.03348 <sup>c</sup>	0.00520 <sup>c</sup>	
10	0.8141	0.09922 <sup>a</sup>	0.00588 <sup>a</sup>			0.09250 <sup>a</sup>	-0.00249 <sup>a</sup>			
		0.09979 <sup>b</sup>	0.01193 <sup>b</sup>			0.09294 <sup>b</sup>	0.00670 <sup>b</sup>			
		0.09986 <sup>c</sup>	0.00642 <sup>c</sup>			0.09307 <sup>c</sup>	0.00318 <sup>c</sup>			
7	0.7424	0.05651 <sup>a</sup>				0.04516 <sup>a</sup>				
		0.06025 <sup>b</sup>				0.04808 <sup>b</sup>				
		0.05994 <sup>c</sup>				0.04845 <sup>c</sup>				
5	0.6535 <sup>a</sup>	0.01215 <sup>a</sup>				-0.00593 <sup>a</sup>				
	0.6536 <sup>b,c</sup>	0.03209 <sup>b</sup>				0.00991 <sup>b</sup>				
		0.02421 <sup>c</sup>				0.00820 <sup>c</sup>				
2	0.2853 <sup>a</sup>									
	0.2994 <sup>b</sup>									
	0.2962 <sup>c</sup>									

<sup>a</sup> Second-order  $N = 2$  with  $S_1 = 2 \rightarrow S_2 = 5$ . <sup>b</sup> Second-order  $N = 2$  with  $S_1 = 3 \rightarrow S_2 = 7$ . <sup>c</sup> Exact numerical (Rogers *et al.* 1970). Unreferenced when all methods converge to the same result.

**Table 3.** Comparative results for the eigenstate energies ( $-2E_n$ ) in a cosine screened potential ( $\epsilon = 1$ ).

$Z/\alpha_0$	1s	2s	3s	4s	5s	2p	3p	3d	4p	4d	4f	5p
$\infty$	1.0000	0.2500	0.1111	0.06250	0.04000	0.2500	0.1111	0.1111	0.06250	0.06250	0.06250	0.04000
500	0.9960	0.2460	0.1071	0.05850	0.03601	0.2460	0.1071	0.1071	0.05850	0.05850	0.05850	0.03601
100	0.9800	0.2300	0.09124	0.04287	0.02085 <sup>ab</sup> 0.02084 <sup>c</sup>	0.2300	0.09122	0.09119	0.04285	0.04280 <sup>ab</sup> 0.04279 <sup>c</sup>	0.04272	0.02081 <sup>ab</sup> 0.02080 <sup>c</sup>
50	0.9600	0.2102	0.07205	0.02512 <sup>a</sup> 0.02514 <sup>bc</sup>	0.00548 <sup>a</sup> 0.00574 <sup>b</sup> 0.00534 <sup>c</sup>	0.2101	0.07193	0.07170	0.02496 <sup>a</sup> 0.02497 <sup>b</sup> 0.02491 <sup>c</sup>	0.02461 <sup>a</sup> 0.02462 <sup>b</sup> 0.02457 <sup>c</sup>	0.02407 <sup>a</sup> 0.02408 <sup>b</sup> 0.02404 <sup>c</sup>	0.00528 <sup>a</sup> 0.00553 <sup>b</sup> 0.00518 <sup>c</sup>
30	0.9334	0.1842	0.04837 <sup>a</sup> 0.04839 <sup>b</sup>			0.1840	0.04791 <sup>a</sup> 0.04793 <sup>b</sup>	0.04697 <sup>a</sup> 0.04698 <sup>b</sup>	0.00532 <sup>a</sup> 0.00594 <sup>b</sup>			
20	0.9002	0.1529				0.1521	0.02148 <sup>a</sup> 0.02185 <sup>b</sup> 0.02118 <sup>c</sup>	0.01886 <sup>a</sup> 0.01910 <sup>b</sup> 0.01858 <sup>c</sup>				
10	0.8018	0.06930 <sup>a</sup> 0.06987 <sup>bc</sup>				0.06452 <sup>a</sup> 0.06492 <sup>b</sup> 0.06408 <sup>c</sup>						
7	0.7192											
5	0.61261 <sup>a</sup> 0.61266 <sup>b</sup> 0.61267											
2	0.1469 <sup>a</sup> 0.15454 <sup>b</sup> 0.1552 <sup>c</sup>											

<sup>a</sup> Second-order  $N = 2$  with  $S_1 = 3 \rightarrow S_2 = 7$ . <sup>b</sup> First-order on the bases of the Hulthen functions (Bessis *et al* 1975). <sup>c</sup> Perturbative Hamiltonian in terms of  $y = 1 - e^{-\alpha r}$  (Lam and Varshni 1972). Unreferenced when all methods converge to the same result.



**6. Conclusion**

Following the original suggestions of Schrödinger, Infeld and Hull, we have enlarged the field of application of the factorisation method. Indeed, by mapping the perturbation scheme onto the ladder operator formalism ‘perturbed factorisation and ladder functions’ have been built up. Consequently, one is able to obtain, in a straightforward way, analytical expressions of eigenvalues and eigenfunctions. These expressions are given in terms of the quantum numbers of the properly chosen factorisable unperturbed problem. Since the perturbed ladders contain all the essential information, the perturbed eigenvalues are obtained without having to calculate explicitly either the excited unperturbed functions or any matrix element. One may add that the treatment of the *N*th order is not significantly more difficult than the first order.

In this paper, special attention has been paid to type F factorisation and the generalised central field problem has been thoroughly investigated. Our calculations of the screened Coulombic eigen-energies, which have been chosen among other possible interesting applications, lead to results in good agreement with the most accurate ones.

The remaining other types of factorisation are under study and will be presented in a further paper.

**Appendix 1**

Consider a one-dimensional differential equation of the Sturm–Liouville type

$$\left[ \frac{d}{dy} \left( P(y) \frac{d}{dy} \right) + Q(y, m) + \Lambda \rho(y) \right] \phi(y) = 0. \tag{A.1}$$

It can be transformed into the standard form

$$\left( \frac{d^2}{dx^2} + U(x, m) + \Lambda \right) \psi(x) = 0. \tag{A.2}$$

The transformation connecting equations (A.1) and (A.2) is

$$\psi = (P\rho)^{1/4} \phi, \quad dx = (\rho/P)^{1/2} dy. \tag{A.3}$$

Indeed, the possibility of such a transformation implies that the functions *P*(*y*) and  $\rho(y)$  are never negative and  $\rho(y)/P(y)$  exists everywhere.

**Appendix 2. Second-order (*N* = 2, *S*<sub>2</sub> = 5) perturbative potential and ladder functions**

From (31), one gets

$$\begin{aligned} \gamma_5 &= -\Omega_5(x) - \frac{1}{11}\beta_5 x \\ \gamma_4 &= -\Omega_4(x) - \frac{1}{9}(\beta_4 - \frac{30}{11}\beta_5)x - \frac{1}{11}\beta_5 x^2 \\ \gamma_3 &= -\Omega_3(x) - \left(\frac{1}{7}\beta_3 - \frac{2}{9}\beta_4 + \frac{17}{33}\beta_5\right)x - \frac{1}{9}(\beta_4 - \frac{30}{11}\beta_5)x^2 - \frac{8}{99}\beta_5 x^3 \\ \gamma_2 &= -\Omega_2(x) - \left(\frac{1}{5}\beta_2 - \frac{1}{7}\beta_3 + \frac{1}{5}\beta_4 - \frac{5}{11}\beta_5\right)x - \left(\frac{1}{7}\beta_3 - \frac{2}{9}\beta_4 + \frac{17}{33}\beta_5\right)x^2 - \left(\frac{2}{21}\beta_4 - \frac{28}{99}\beta_5\right)x^3 - \frac{2}{33}\beta_5 x^4 \end{aligned} \tag{A.4}$$

$$\gamma_1 = -\Omega_1(x) - \frac{1}{3}(\beta_1 - \frac{1}{5}\beta_2 + \frac{1}{7}\beta_3 - \frac{1}{5}\beta_4 + \frac{5}{11}\beta_5)x - (\frac{1}{5}\beta_2 - \frac{1}{7}\beta_3 + \frac{1}{5}\beta_4 - \frac{5}{11}\beta_5)x^2 \\ - 4(\frac{1}{35}\beta_3 - \frac{1}{21}\beta_4 + \frac{19}{165}\beta_5)x^3 - \frac{4}{9}(\frac{1}{7}\beta_4 - \frac{5}{11}\beta_5)x^4 - \frac{8}{231}\beta_5x^5$$

where the shortened notation  $\gamma_v = \gamma_v^{(2)}$ ;  $\Omega_v = \Omega_v^{(2)}$  and  $\beta_v = \beta_v^{(2)}$  has been introduced.

After substituting the expressions (53) of the  $\beta_v^{(2)}$  and identifying  $U^{(2)} = \gamma^{(2)} = b_3x^3 + b_4x^4 + b_5x^5$ , one gets:

$$\beta_5 = -\frac{11}{32}(42b_5 + 13b_2^2) \\ \beta_4 = -\frac{63}{8}b_4 - \frac{105}{16}(7 - 3\mu)b_5 - \frac{45}{16}b_1b_2 - \frac{15}{32}(23 - 6\mu)b_2^2 \\ \beta_3 = -\frac{35}{8}b_3 - \frac{35}{8}(3 - 2\mu)b_4 - \frac{21}{16}(14 - 25\mu + 5\mu^2)b_5 - \frac{7}{16}b_1^2 - \frac{7}{16}(9 - 2\mu)b_1b_2 \\ - \frac{7}{32}(4 - 18\mu - 3\mu^2)b_2^2 \tag{A.5} \\ \beta_2 = -\frac{5}{8}(5 - 6\mu)b_3 - \frac{1}{8}(12 - 50\mu + 15\mu^2)b_4 + \frac{5}{16}(12 - 8\mu + \mu^2)\mu b_5 - \frac{5}{16}b_1^2 \\ + \frac{1}{16}(10 + 3\mu)\mu b_1b_2 \\ \beta_1 = \frac{3}{8}(2 - \mu)\mu b_3 + \frac{3}{16}\mu^2 b_1^2.$$

Then from the second-order perturbative ladder function (see equation (34)):

$$K^{(2)} = \gamma_1 m + (2\gamma_2 + \gamma_3)m^3 + (3\gamma_3 + 4\gamma_4 + \gamma_5)m^5 + (4\gamma_4 + 10\gamma_5)m^7 + 5\gamma_5 m^9. \tag{A.6}$$

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