Perturbed ladder-operator method: An algebraic recursive solution of the perturbed Morse-oscillator eigenequation

N. Bessis and G. Bessis
Laboratoire de Physique des Lasers, URA 282, Université Paris-Nord, avenue J. B. Clement, 93430 Villetaneuse, France
(Received 4 May 1994)

The perturbed ladder-operator method is applied to the solution of the perturbed Morse-oscillator eigenequation, i.e., the radial Schrödinger equation with a total potential $U(r)=D_e(1-e^{-\beta(r-r_e)})^2+D_e\sum_t g_t(1-e^{-\beta(r-r_e)})^t$. This method, which is an extension of the original Schrödinger-Infeld-Hull factorization method within the perturbative scheme, allows an analytical solution of perturbed eigenequations in almost the same way as factorizable ones. After expanding each perturbation term in a series of $y_s(r)=e^{-s\beta(r-r_e)}$, analytical expressions of the perturbed Morse energies are obtained in terms of the anharmonicity constant and of the vibrational quantum number without having to calculate either the excited unperturbed spectra or any matrix element. Analytical expressions of the perturbed Morse eigenfunctions are then obtainable by iterated application of the perturbed ladder operator on the key eigenfunction, or on any one of them. Illustrative examples are given.

PACS number(s): 03.65.Fd

I. INTRODUCTION

The radial harmonic-oscillator, radial Coulomb, and radial Morse-oscillator eigenequations have been the subject of considerable interest in the development of theoretical physics, since they correspond to physical problems and they are exactly solvable. Nevertheless, as soon as a more elaborate description of real problems is required, solutions of these equations with an additional perturbation are needed. Recently, it has been shown that the perturbed ladder-operator method [1], i.e., an extension of the original Schrödinger-Infeld-Hull factorization [2,3] method within the perturbative scheme, allows an analytical solution of the perturbed Coulomb as well as of the symmetric anharmonic-oscillator equations by means of algebraic manipulations [4,5]. The perturbed Morse-oscillator model is used widely to describe chemical bonds and the vibration-rotation spectra of diatomic molecules, and, particularly, to provide the theoretical centrifugal contributions to the rotational spectra of diatomic molecules [6,7] or to extract the internuclear distance dependence of diatomic structure constants from the experimental centrifugal data [8] (fine structure, Λ-doubling, spin-rotation constants, etc.). In most cases, analytical solutions of the perturbed Morse-oscillator equation are required.

In the present paper, after a brief and necessary review of the perturbed ladder-operator method, it is shown how an algebraic recursive solution of the perturbed radial Morse-oscillator eigenequation can be carried out by means of the perturbed factorization process.

II. PERTURBED LADDER-OPERATOR METHOD

After exact or approximate separation of variables and appropriate transformations of variables and functions, many Sturm-Liouville eigenequations of current interest in quantum physics can be reduced to the standard form

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

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

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

where $m=m_0,\ m_0+1,\ m_0+2\ldots$ is a quantum number that takes successive discrete values labeling the eigenfunctions.

A. Exact factorization

Such an equation (1) is factorizable when it can be replaced by each of the following pair of difference-differential equations,

$$\begin{aligned}H^-_{m+1}H^+_{m+1}\Psi_{jm}(x)&=[\Lambda_j-L(m+1)]\Psi_{jm}(x)\ ,\\ H^+_mH^-_m\Psi_{jm}(x)&=[\Lambda_j-L(m)]\Psi_{jm}(x)\ ,\end{aligned} \tag{3}$$

where $L(m)$ is the "factorization function," which does not depend on x, and H^+_m and H^-_m are mutually adjoint "ladder operators": $H^{\pm}_m=K(x,m)\mp d/dx$.

Owing to the mutual adjointness of the ladder operators H^+_m and H^-_m, the necessary condition for the existence of quadratically integrable solutions of Eq. (1), i.e., the quantization condition, is $\varepsilon(j-m)=v$, where v is a non-negative integer and $\varepsilon=+1$ (or $\varepsilon=-1$) according to whether $L(m)$ is an increasing (or decreasing) function of m.

The interest and advantages of the factorization method are well known [3]

(i) Closed-form expressions of the eigenvalues Λ_j are readily obtainable from the knowledge of the factorization function $L(m)$,

$$\Lambda_j=L(\tilde{j})\ , \tag{4}$$

where $\tilde{j}=j+\varepsilon/2+\frac{1}{2}$.

(ii) The normalized eigenfunctions are solutions of the following pair of difference-differential equations,

$$\left\{K(x,m)+\frac{d}{dx}\right\}\Psi_{jm}=N_j(m)\Psi_{j,m-1}\ ,$$
$$\left\{K(x,m+1)-\frac{d}{dx}\right\}\Psi_{jm}=N_j(m+1)\Psi_{j,m+1}\ , \tag{5}$$

where $N_j(m)=[\Lambda_j-L(m)]^{1/2}$.

These "ladder equations" allow the determination of any $\Psi_{jm}(x)$ function from the knowledge of any one of them, particularly from the knowledge of the normalized "key eigenfunction" $\Psi_{jj}(x)$, which is a solution of the first-order differential equation

$$\left\{K(x,\tilde{j})-\varepsilon\frac{d}{dx}\right\}\Psi_{jj}(x)=0\ . \tag{6}$$

In fact, when an eigenequation is exactly factorizable, closed-form expressions of the eigenfunctions, involving classical polynomials, are known [9].

There are six fundamental types of potential functions $U^{(0)}(x,m)$ (denoted types A to F, within the Infeld-Hull [3] nomenclature) leading to factorizable equations. Moreover, as pointed out by Infeld and Hull, when direct factorization is not possible solely because of the inadequate m dependence of the potential function $U(x,m)$ under consideration, one can resort to "artificial factorization": one considers $U(x,m)$ as "embedded" in a new potential function $u(x,m;\mu)$ that depends on a supplementary "artificial parameter μ" such that $u(x,m;\mu)$ can be identified in m with a factorizing potential $U^{(0)}(x,m)$ and that $u(x,m;\mu=m)=U(x,m)$. Then Eq. (1) is factorized using $u(x,m;\mu)$ and the associated μ-dependent ladder and factorization functions $K(x,m;\mu)$ and $L(m;\mu)$. The eigenvalues $\Lambda_j(\mu)=L(\tilde{j};\mu)$ are determined as well as the eigenfunctions $\Psi_{jm}(x;\mu)$, both depending on the parameter μ. At the end of the ladder procedure (5), one merely sets $\mu=m$ and obtains the required eigenvalues $\Lambda_j(m)=\Lambda_j(\mu=m)$, and eigenfunctions $\Psi_{jm}(x)=\Psi_{jm}(x;\mu=m)$. This "artificial" or "embedded" factorization device is widely used all along the "perturbed factorization" scheme.

B. Perturbed factorization

Let us now consider an eigenequation (1) where the potential function $U(x,m)$ does not belong to any of the six Infeld-Hull factorization types, and let us assume that this potential function, as well as the associated ladder and factorization functions $K(x,m)$ and $L(m)$ to be found, can be expanded in a perturbation series with a parameter η,

$$U(x,m)=U^{(0)}(x,m)+\eta U^{(1)}(x,m)+\eta^2U^{(2)}(x,m)+\cdots\ ,$$
$$K(x,m)=K^{(0)}(x,m)+\eta K^{(1)}(x,m)+\eta^2K^{(2)}(x,m)+\cdots\ , \tag{7}$$
$$L(m)=L^{(0)}(m)+\eta L^{(1)}(m)+\eta^2L^{(2)}(m)+\cdots\ ,$$

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

As already pointed out [1], the critical point of this extension of the factorization method within the perturbation scheme relies on the choice of suitable x basis functions $y_s(x)$ and $Y_s(x)$ for expanding the required factorizing perturbations $U^{(N)}(x,m)$ and associated perturbed ladder functions $K^{(N)}(x,m)$, respectively. These basis functions, which are specific to each factorization type, have to satisfy the following "ladderlike" relations:

$$2K^{(0)}(x,m)Y_s(x)=A_s(m)y_s(x)+B_s(m)y_{s+1}(x)\ ,$$
$$\frac{dY_s}{dx}=\alpha_sy_s(x)+\beta_sy_{s+1}(x)\ , \tag{8}$$
$$Y_s(x)Y_t(x)=\sum_r h(s,t,r)y_r(x)\ .$$

Hence, when working out the solution of the factorizability condition for the perturbed eigenequation, it can be shown [1] that, at each order N of the perturbation, the perturbed ladder function to be found is

$$K^{(N)}(x,m)=\sum_{s=0}^{S_N}Y_s(x)Q_s(m)\{k_s^{(N)}+F_s^{(N)}(m)\}\ , \tag{9}$$

where $k_s^{(N)}$ is an arbitrary summation constant, $F_s^{(N)}(m)=0$ for $s=S_N$, and

$$Q_s(m)=\prod_{j=1}^{m-1}\frac{[B_s(j)-\beta_s]}{[B_s(j+1)+\beta_s]}\ . \tag{10}$$

The $F_s^{(N)}(m)$ function to be found is the solution of the recursive finite-difference equation

$$F_{s-1}^{(N)}(m)=-\Delta^{-1}\left\{\frac{\Delta W_s^{(N)}+[\Delta(A_s(m)+\alpha_s)+2\alpha_s]Q_s(m)[k_s^{(N)}+F_s^{(N)}(m)]}{Q_{s-1}(m+1)[B_{s-1}(m+1)+\beta_{s-1}]}\right\}, \tag{11}$$

where, at each order N of the perturbation, the $W_s^{(N)}(m)$ function, originated from the preceding orders of the perturbation, is known and is defined by the relation [10],

$$\Theta^{(N)}(x,m)=\sum_{\nu=1}^{N-1} K^{(\nu)}(x,m)K^{(N-\nu)}(x,m)$$
$$=\sum_{s=0}^{S_N} W_s^{(N)}(m)y_s(x) \ . \quad (12)$$

Starting from $s=S_N$, descending down to $s=1$, and keeping in mind that $F_s^{(N)}(m)=0$ for $s=S_N$, Eq. (11) allows a recursive determination of closed-form expressions of the $F_s^{(N)}(m)$ functions. Then, the required ladder function $K^{(N)}(x,m)$ is given by Eq. (9) and, as well as the $F_s^{(N)}(m)$ functions, it contains the arbitrary constants $k_s^{(N)}$. The associated factorizing potential $U^{(N)}(x,m)$ is also obtained [1]. Thus, using the artificial factorization device with an artificial parameter μ, one can solve physico-mathematical problems with a potential function $V(x,m)$, such as

$$V(x,m)=U^{(0)}(x,m)+\eta V^{(1)}(x)+\eta^2 V^{(2)}(x)+\cdots \ , \quad (13)$$

provided the $V^{(N)}(x)$ have the same dependence in x as the $U^{(N)}(x,m)$, i.e., they can be written

$$V^{(N)}(x)=\sum_{s=1}^{S_N+1} b_s^{(N)}y_s(x) \ . \quad (14)$$

When matching the given perturbation $V^{(N)}(x)$ with the factorizing perturbation $U^{(N)}(x,m)$, via the artificial device, it is convenient to keep in mind that $F_s^{(N)}(m)$ is defined within an arbitrary summation constant and to impose the vanishing condition

$$F_s^{(N)}(m=\mu)=0 \ . \quad (15)$$

Then, we obtain the following relations allowing the determination of the arbitrary summation constants in terms of the data,

$$k_{S_N}^{(N)}=-\frac{b_{S_N+1}^{(N)}}{Q_{S_N}(\mu)(B_{S_N}(\mu)-\beta_{S_N})} \ ,$$
$$k_{s-1}^{(N)}=-\frac{b_s^{(N)}+W_s^{(N)}(\mu)+[A_s(\mu)-\alpha_s]Q_s(\mu)k_s^{(N)}}{Q_{s-1}(\mu)[B_{s-1}(\mu)-\beta_{s-1}]} \ , \quad (16)$$

and, consequently, the determination of the $F_s^{(N)}(m)$ functions in terms of the expansion coefficients of the given perturbation $V^{(N)}(x)$. Once the $F_s^{(N)}(m)$ functions known, the perturbed factorization function $L^{(N)}(m;\mu)$ is obtained from the solution of the finite-difference equation [1]

$$L^{(N)}(m)=-\Delta^{-1}(\Delta W_0^{(N)}+\{\Delta[A_0(m)+\alpha_0]+2\alpha_0\}$$
$$\times Q_0(m)[k_0^{(N)}+F_0^{(N)}(m)]) \ , \quad (17)$$

with the associated condition to be fulfilled,

$$L^{(N)}(m=\mu)=-W_0^{(N)}(\mu)-[A_0(\mu)-\alpha_0]$$
$$\times Q_0(\mu)[k_0^{(N)}+F_0^{(N)}(\mu)] \ . \quad (18)$$

Finally, once the perturbed ladder functions $K^{(\nu)}(x,m;\mu)$ and the factorization functions $L^{(\nu)}(m;\mu)$, both depending on the artificial parameter μ, have been found recursively from $\nu=1$ up to $\nu=N$, the perturbed problem (up to the Nth order of the perturbation) may be handled in the same way as the exact factorizable (unperturbed) problem. The perturbed eigenvalue $\Lambda_j^{(\nu)}(m)$ associated with the perturbation $V^{(\nu)}(x)$ is

$$\Lambda_j^{(\nu)}(m)=L^{(\nu)}(m=\tilde{j};\mu=m) \ . \quad (19)$$

The total perturbed eigenvalue and associated ladder function are

$$\Lambda_j(m)=L^{(0)}(\tilde{j})+\sum_{\nu=1}^{N}\eta^\nu L^{(\nu)}(m=\tilde{j};\mu=m) \ , \quad (20)$$

$$K(x,m;\mu)=K^{(0)}(x,m)+\sum_{\nu=1}^{N}\eta^\nu K^{(\nu)}(x,m;\mu) \ . \quad (21)$$

Summarizing the results, a given equation (1) is relevant to the perturbed ladder-operator method as soon as one can display the given potential $U(x,m)$ into an unperturbed "kernel potential" $U^{(0)}(x,m)$ leading to an exactly factorizable equation with an additional perturbation $V(x)$. This perturbation has to be expandable in a series of suitable basis functions $y_s(x)$, which satisfy the ladderlike properties (8). The critical point of the method is the solution of the finite-difference equation (11).

III. EXACT FACTORIZATION OF THE (UNPERTURBED) MORSE-OSCILLATOR EQUATION

Let us consider the radial Morse-oscillator wave equation [11], i.e., the second-order differential equation $(0\le r<\infty)$

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+D_e(1-e^{-\beta(r-r_e)})^2\right\}\phi^{(0)}(r)=E^{(0)}\phi^{(0)}(r) \ , \quad (22)$$

where μ is the reduced mass, D_e is the depth of the potential well, β is the range parameter, and r_e is the equilibrium distance. When introducing the dimensionless coordinate $x=(\mu w_e/\hbar)^{1/2}(r-r_e)$, the Morse-oscillator equation (22) becomes

$$\left\{\frac{d^2}{dx^2}-\frac{1}{2\zeta_e}e^{-2(2\zeta_e)^{1/2}x}+\frac{1}{\zeta_e}e^{-(2\zeta_e)^{1/2}x}-\frac{1}{2\zeta_e}+\frac{2}{\hbar w_e}E^{(0)}\right\}\psi^{(0)}(x)=0 \ , \quad (23)$$

where $w_e=(2D_e/\mu)^{1/2}\beta$ and $\zeta_e=\hbar w_e/4D_e$ are, respectively, the vibrational and anharmonicity constants.

As already known, the (unperturbed) Morse-oscillator equation (23) is exactly solvable and, particularly, can be matched with an exact Infeld-Hull type-B factorizable equation [3], i.e, it can be written again,

$$\left\{\frac{d^2}{dx^2}-a^2d^2e^{2ax}+2a^2d(m+\tfrac{1}{2})e^{ax}+\Lambda^{(0)}\right\}\Psi_{jm}^{(0)}(x)=0 \ , \quad (24)$$

with $a=-(2\zeta_e)^{1/2}$, $d=1/2\zeta_e$, $m=-\frac{1}{2}+1/2\zeta_e$, and $\Lambda^{(0)}=2E^{(0)}/hw_e-1/2\zeta_e$, and the associated Ter Haar boundary conditions [12],

$$|\Psi_{jm}^{(0)}(-\infty)|^2=|\Psi_{jm}^{(0)}(+\infty)|^2=0\ ,$$
$$\int_{-\infty}^{+\infty}|\Psi_{jm}^{(0)}(x)|^2dx=1\ .$$

The associated ladder and factorization functions are

$$\begin{aligned}K^{(0)}(x,m)&=-am+ade^{ax}\ ,\\ L^{(0)}(m)&=-a^2m^2\ .\end{aligned}\tag{25}$$

Closed-form expressions of the eigenfunctions are known [9],

$$\Psi_{jm}^{(0)}(x)=N_{jm}\exp[\tfrac{1}{2}(\tau_1ax-\tau_2e^{ax})]L_v^{\tau_1}(\tau_2e^{ax})\ ,\tag{26}$$

where N_{jm} is a normalization constant, $L_v^{\tau}(\cdots)$ is a Laguerre polynomial of degree $v=\varepsilon(j-m)$, $\tau_1=-2\varepsilon j$, $\tau_2=-2\varepsilon d$, and $\varepsilon=+1$ (or $\varepsilon=-1$) according to whether $L^{(0)}(m)$ is an increasing (or decreasing) function of m.

The Morse-oscillator eigenequation (23) is a (class-II, $\varepsilon=-1$) type-B factorizable equation with the associated quantization condition $m-j=v$. Indeed, since $a=-(2\zeta_e)^{1/2}$ is a real constant, $L^{(0)}(m)$ is a decreasing function of m and the Morse-oscillator eigenvalue is $\Lambda^{(0)}=-a^2j^2=-a^2(m-v)^2$. Setting $m=-\frac{1}{2}+1/2\zeta_e$, we get the expected expression of the energies

$$E_v^{(0)}=\hbar w_e[v+\tfrac{1}{2}-\zeta_e(v+\tfrac{1}{2})^2]\ .\tag{27}$$

At this level, let us remark that the quantum number m plays a central role within the factorization scheme, while it does not appear within the Morse-oscillator equations (22) or (23), general results following from the exact (or perturbed) factorization process have to be expressed in terms of $v=\varepsilon(j-m)$ and m before being applied to the Morse-oscillator problem or any other particular problem.

Since the (unperturbed) Morse-oscillator equation is a type-B factorization equation, an analytical solution of the eigenequation (23) with an additional perturbation $V(x)$ can be carried out by means of perturbed type-B factorization.

IV. PERTURBED TYPE-*B* FACTORIZATION

Let us consider the perturbed type-B eigenequation,

$$\left\{\frac{d^2}{dx^2}-a^2d^2e^{2ax}+2a^2d(m+\tfrac{1}{2})e^{ax}+V(x)+\Lambda\right\}\Psi_{jm}(x)=0\ ,\tag{28}$$

where $V(x)=\eta V^{(1)}(x)+\eta^2V^{(2)}(x)+\cdots$ is a perturbation.

The following x basis functions and associated data can be chosen [see Eq. (8)]:

$$\begin{aligned}&y_s(x)=a^2e^{sax},\quad Y_s(x)=ae^{sax}\ ,\\ &A_s(m)=-2m,\quad B_s(m)=2d,\quad \alpha_s=s,\quad \beta_s=0\ ,\\ &Y_s(x)Y_t(x)=y_{s+t}(x)\ .\end{aligned}\tag{29}$$

The perturbation terms are [13]

$$V^{(N)}(x)=a^2\sum_{s=1}^{S_N+1}b_s^{(N)}e^{sax}\ .\tag{30}$$

A. Determination of the perturbed ladder function

Using Eqs. (10) and (29), it is found that $Q_s(m)=1$ and, at each order N of the perturbation, the perturbed ladder function is [see Eq. (9)]

$$K^{(N)}(x,m)=a\sum_{s=0}^{S_N}e^{sax}[k_s^{(N)}+F_s^{(N)}(m)]\ .\tag{31}$$

The $F_s^{(N)}(m)$ function is found to be the solution of the following finite-difference equation [see Eqs. (11) and (29)]:

$$F_{s-1}^{(N)}(m)=-\frac{1}{2d}\{W_s^{(N)}(m)+[(s-2m)+2s\Delta^{-1}]\times[k_s^{(N)}+F_s^{(N)}(m)]\}\ ,\tag{32}$$

where the $W_s^{(N)}(m)$ functions are defined by Eq. (12), i.e.,

$$\Theta^{(N)}(x,m)=\sum_{\nu=1}^{N-1}K^{(\nu)}(x,m)K^{(N-\nu)}(x,m)=a^2\sum_{s=0}^{S_N}W_s^{(N)}(m)e^{sax}\ .\tag{33}$$

As a consequence of the expression (29) of Y_sY_t, it is easily checked that

$$S_N=S_\nu+S_{N-\nu}=NS_1\ .\tag{34}$$

The determination of the perturbed Morse $F_s^{(N)}(m)$ function can be worked out in the same way as the determination of the anharmonic oscillator $F_s^{(N)}(m)$ function. Since, for $s=S_N$, we have $F_{S_N}^{(N)}(m)=0$, it is checked that $F_s^{(N)}(m)$ is of degree (S_N-s) in m [see Eq. (32)] and that, consequently, $W_s^{(N)}(m)$ is also of degree (S_N-s) in m [see Eqs. (33), (31), and (34)]. Therefore, we set

$$F_s^{(N)}(m;\mu)=\sum_{t=1}^{S_N-s}C_s^{(N)}(t)\begin{bmatrix}\mu-m\\ t\end{bmatrix}\ ,\tag{35}$$

so that the vanishing condition (15) is fulfilled, and

$$W_s^{(N)}(m;\mu)=\sum_{k=0}^{S_N-s}w_s^{(N)}(k)\begin{bmatrix}\mu-m\\ k\end{bmatrix}\ .\tag{36}$$

At any order N of the perturbation, the $C_s^{(N)}(t)$ coefficients are to be found while the $w_s^{(N)}(t)$ coefficients are known functions of the $C_r^{(\nu)}(k)$ of the preceding orders of the perturbation ($\nu=1,N-1$).

Now, in order to obtain the expansion of $F_{s-1}^{(N)}(m;\mu)$ in a series of binomials $\binom{\mu-m}{t}$, we use Eq. (32) together with the above expressions (35) and (36) of $F_s^{(N)}(m;\mu)$ and $W_s^{(N)}(m;\mu)$. Since [14]

$$m\begin{bmatrix}\mu-m\\ t\end{bmatrix}=\mu\begin{bmatrix}\mu-m\\ t\end{bmatrix}-t\begin{bmatrix}\mu-m\\ t\end{bmatrix}-(t+1)\begin{bmatrix}\mu-m\\ t+1\end{bmatrix}\ ,$$
$$\Delta^{-1}\begin{bmatrix}\mu-m\\ t\end{bmatrix}=-\begin{bmatrix}\mu-m\\ t+1\end{bmatrix}-\begin{bmatrix}\mu-m\\ t\end{bmatrix}\ ,$$

we get

$$[s-2m+2s\Delta^{-1}]\begin{bmatrix}\mu-m\\t\end{bmatrix}=-(2\mu+s-2t)\begin{bmatrix}\mu-m\\t\end{bmatrix}-2(s-t-1)\begin{bmatrix}\mu-m\\t+1\end{bmatrix}.$$

Keeping in mind that the expression (32) of $F_{s-1}^{(N)}(m;\mu)$ holds within an arbitrary summation constant that can be chosen so that $F_{s-1}^{(N)}(m)$ keeps the same form (35) as $F_s^{(N)}(m)$, from the comparison of the expression (32) of $F_{s-1}^{(N)}(m)$ with its standard expression (35), we obtain the following relations:

$$C_{s-1}^{(N)}(1)=-\frac{1}{2d}\{w_s^{(N)}(1)-2(s-1)k_s^{(N)}-(s+2\mu-2)C_s^{(N)}(1)\},$$
$$C_{s-1}^{(N)}(t)=-\frac{1}{2d}\{w_s^{(N)}(t)-2(s-t)C_s^{(N)}(t-1)-(s+2\mu-2t)C_s^{(N)}(t)\}\quad\text{for } t\geq 2\,. \tag{37}$$

Starting from $s=S_N+1$ down to $s=1$, and from $t=S_N-s+1$ down to $t=1$, these relations allow a recursive determination of the $C_s^{(N)}(t)$ in terms of the arbitrary constants $k_s^{(N)}$. One has now to obtain analytical expressions of the $k_s^{(N)}$ in terms of the data, i.e., in terms of the expansion coefficients $b_s^{(N)}$ of the given perturbation $V^{(N)}(x)$.

From Eqs. (16) and (29), we get

$$k_{s-1}^{(N)}=-\frac{1}{2d}\{b_s^{(N)}+w_s^{(N)}(0)-(s+2\mu)k_s^{(N)}\}\,. \tag{38}$$

Setting $k_s^{(N)}=C_s^{(N)}(0)$, it is easily seen that the determination of the $C_s^{(N)}(t)$ for $t=S_N-s+1$ down to $t=0$ can be performed in terms of the expansion coefficients $b_s^{(N)}$ of the perturbation $V^{(N)}(x)$ by means of the single recurrence formula,

$$C_{s-1}^{(N)}(k)=-\frac{1}{2d}\{b_s^{(N)}(k)-2(s-k)C_s^{(N)}(k-1)-(s+2\mu-2k)C_s^{(N)}(k)\}\,, \tag{39}$$

where

$$b_s^{(N)}(0)=b_s^{(N)}+w_s^{(N)}(0)\,,\qquad b_s^{(N)}(k)=w_s^{(N)}(k)\quad\text{for } k\neq 0\,. \tag{40}$$

When applying this recurrence formula, it can be inferred that we can write

$$C_{S_N-\sigma}^{(N)}(k)=-\sum_{j=0}^{k}\sum_{u=j}^{j+\sigma-k}\left[\frac{1}{2d}\right]^{\sigma+1-\mu}d_j(\sigma-u,k,S_N-u)\times b_{S_N+1-u}^{(N)}(j)\,, \tag{41}$$

where the $d_j(\sigma,k,s)$ coefficients obey the recurrence formula

$$d_j(\sigma+1,k,s)=2(s-\sigma-k)d_j(\sigma,k-1,s)+(2\mu+s-\sigma-2k)d_j(\sigma,k,s)\,, \tag{42}$$

with $d_k(0,k,s)=1$ and the nonvanishing condition $j\leq k\leq j+\sigma$. This formula allows the determination of any $d_j(\sigma,k,s)$. Particularly, we get

$$d_j(\sigma,j,s)=(2\mu+s-2j)_\sigma\,,$$
$$d_j(\sigma,j+1,s)=(2\mu+s-2j)_{\sigma-1}(2s-2j-2\sigma)+(2\mu+s-2j-\sigma-1)d_j(\sigma-1,j+1,s)\cdots\,.$$
$$d_j(\sigma,j+\sigma-1,s)=(2\mu+s-2j-3\sigma+3)(2s-2j-2)_{\sigma-1,4}+(2s-2j-4\sigma+4)d_j(\sigma-1,j+\sigma-2,s)\,,$$
$$d_j(\sigma,j+\sigma,s)=(2s-2j-2)_{\sigma,4}\,,$$

where $(n)_{\sigma,h}=n(n-h)(n-2h)\cdots(n-h\sigma+h)$ is a generalized factorial of step h.

Hence, we get the following expression of the perturbed ladder function in terms of the data coefficients $b_u^{(N)}(i)$ by means of Eqs. (31), (35), and (41),

$$K^{(N)}(x,m;\mu)=\sum_{i=0}^{S_N}\sum_{u=1}^{S_N+1}b_u^{(N)}(i)\chi_{ui}(x,m;\mu)\,, \tag{43}$$

where

$$\chi_{ui}(x,m;\mu)=-a\sum_{s=0}^{u-1}\left[\frac{1}{2d}\right]^{u-s}e^{sax}\sum_{t=i}^{u+i-s-1}\begin{bmatrix}\mu-m\\t\end{bmatrix}d_i(u-s-1,t,u-1)\,. \tag{44}$$

Let us emphasize that, since the expressions of the $d_j(\sigma,k,s)$ depend neither on the order N of the perturbation nor on the expansion coefficients of $V^{(N)}(x)$, the determination of these "ladder basis" functions $\chi_{ui}(x,m;\mu)$ can be performed once and for all.

We get

$$\chi_{10}=-a\left[\frac{1}{2d}\right],\quad \chi_{11}=-a\left[\frac{1}{2d}\right]\begin{bmatrix}\mu-m\\1\end{bmatrix},\quad \chi_{12}=-a\left[\frac{1}{2d}\right]\begin{bmatrix}\mu-m\\2\end{bmatrix},$$

$$\chi_{20}=-a\left[\frac{1}{2d}\right]^2\{(2\mu+1)+2de^{ax}\},$$

$$\chi_{30}=-a\left[\frac{1}{2d}\right]^3\left[(2\mu+2)(2\mu+1)+2(2\mu-1)\begin{bmatrix}\mu-m\\1\end{bmatrix}-4\begin{bmatrix}\mu-m\\2\end{bmatrix}\right]$$
$$-a\left[\frac{1}{2d}\right]^2e^{ax}\left[2\mu+2+2\begin{bmatrix}\mu-m\\1\end{bmatrix}\right]-a\left[\frac{1}{2d}\right]e^{2ax},\tag{45}$$

$$\chi_{21}=-a\left[\frac{1}{2d}\right]^2\left\{(2\mu-1)\begin{bmatrix}\mu-m\\1\end{bmatrix}-2\begin{bmatrix}\mu-m\\2\end{bmatrix}+2de^{ax}\begin{bmatrix}\mu-m\\1\end{bmatrix}\right\},$$

$$\chi_{40}=-a\left[\frac{1}{2d}\right]^4\left[(2\mu+3)_3+6(2\mu+1)(2\mu-1)\begin{bmatrix}\mu-m\\1\end{bmatrix}-12(2\mu+1)\begin{bmatrix}\mu-m\\2\end{bmatrix}\right]$$
$$-a\left[\frac{1}{2d}\right]^3e^{ax}\left[(2\mu+3)_2+6(2\mu+1)\begin{bmatrix}\mu-m\\1\end{bmatrix}\right]-a\left[\frac{1}{2d}\right]^2e^{2ax}\left[2\mu+3+4\begin{bmatrix}\mu-m\\1\end{bmatrix}\right]-a\left[\frac{1}{2d}\right]e^{3ax},$$

and so on.

Then, as soon as the particular problem under consideration is relevant to perturbed type-B factorization, the expression (43) allows a straightforward determination of the perturbed ladder functions $K^{(N)}(x,m;\mu)$ in terms of the data coefficients $b_u^{(N)}(i)$, which are specific to the particular problem under consideration.

B. Determination of the perturbed eigenvalues

Using (17) together with the expression (29) of $A_s(m)$ and α_s, we get the following expression of the perturbed factorization function:

$$L^{(N)}(m;\mu)=-W_0^{(N)}(m;\mu)+2m[k_0^{(N)}+F_0^{(N)}(m;\mu)].\tag{46}$$

When comparing this expression with the expression (32) of $F_{s-1}^{(N)}(m)$, it is seen that, formally, and within an arbitrary summation constant, we have $L^{(N)}(m;\mu)=2dF_{-1}^{(N)}(m)$ and that, consequently, we can write

$$L^{(N)}(m;\mu)=2d\sum_{t=0}^{S_N+1}C_{-1}^{(N)}(t)\begin{bmatrix}\mu-m\\t\end{bmatrix}.\tag{47}$$

Indeed, the arbitrary summation constant, which has to be chosen so that the condition (18) is fulfilled, is $L^{(N)}(m=\mu;\mu)=-w_0^{(N)}(0)+2\mu k_0^{(N)}=2dk_{-1}^{(N)}=2dC_{-1}^{(N)}(0)$ [use Eqs. (46) and (38)]. Then, substituting for $C_{-1}^{(N)}(t)$ from Eq. (41) into Eq. (47), we obtain the following expression of the perturbed factorization function in terms of the data coefficients:

$$L^{(N)}(m;\mu)=\sum_{i=0}^{S_N}\sum_{u=0}^{S_N+1-i}I_u(i;m,\mu)b_u^{(N)}(i),\tag{48}$$

where

$$I_u(i;m,\mu)=-\left[\frac{1}{2d}\right]^u\sum_{t=i}^{u+i}d_i(u,t,u-1)\begin{bmatrix}\mu-m\\t\end{bmatrix}.\tag{49}$$

Consequently, when substituting m with $\tilde{j}$ and μ with m into this expression, we obtain the required expression of the perturbed eigenvalue associated with the perturbation $V^{(N)}(x)$,

$$\Lambda_v^{(N)}(m)=\sum_{i=0}^{S_N}\sum_{u=0}^{S_N+1-i}I_u(i)b_u^{(N)}(i),\tag{50}$$

where $I_u(i)=I_u(i;\tilde{j},m)$.

For class-II problems ($\tilde{j}=j$, $m-j=v$), we have

$$I_u(i)=-\left[\frac{1}{2d}\right]^u\sum_{t=i}^{u+i}d_i(u,t,u-1)\begin{bmatrix}v\\t\end{bmatrix},\tag{51}$$

where μ has to be substituted with m in the expressions of the $d_i(u,t,u-1)$. Closed-form expressions of the $I_u(i)$ are given in Appendix A and can serve for the analytical solution of any eigenequation relevant to (class-II) perturbed type-B factorization.

At any order N of the perturbation and for any given problem involving a perturbation that can be expanded in a series of the $y_t(x)$ functions, the determination of the perturbed value $\Lambda_v^{(N)}(m)$ amounts to the determination of the data coefficients $b_t^{(N)}(i)$ in terms of the expansion coefficients of the perturbation. Note that, in the same way as at the first order, the v dependence of $\Lambda_v^{(N)}(m)$ is entirely contained in the expressions of the "pseudointegrals" $I_u(i)$.

Finally, the total eigenvalue of eigenequation (28), up to the Nth order of the perturbation, is

$$\Lambda_v(m)=\Lambda_v^{(0)}(m)+\sum_{\nu=1}^{N}\Lambda_v^{(\nu)}(m),\tag{52}$$

where $\Lambda_j^{(\nu)}(m)$ is given by Eq. (50).

Let us remark that, at the first order $N=1$ of the perturbation, since $W^{(1)}(m)=0$, we have $w_u^{(1)}(i)=0$ for any i, and the data coefficients $b_u^{(1)}(i)$ reduce to the expansion coefficients $b_u^{(1)}$ of the perturbation $V^{(1)}(x)$ in a series of the basis functions $y_u(x)=a^2e^{uax}$ [see Eq. (40)]. Hence, the expression of the first-order perturbed eigenvalue reduces to

$$\Lambda_v^{(1)}(m)=\sum_{t=0}^{S_1} I_t(0)b_t^{(1)} . \tag{53}$$

When comparing this expression of $\Lambda_v^{(1)}(m)$, with its alternative expression within the classical Rayleigh-Schrödinger framework, we obtain, as a by-product, the expression of the diagonal matrix elements $\langle y_t(x)\rangle$ between the (unperturbed) type-B eigenfunctions $\Psi_{jm}^{(0)}(x)$ [see Eq. (26)],

$$\langle y_t(x)\rangle=a^2\langle e^{atx}\rangle=-I_t(0) . \tag{54}$$

C. Recursive determination of the data coefficients

At each order N of the perturbation, the data coefficients $b_t^{(N)}(i)$ are defined by Eq. (40) and involve, in addition to the expansion coefficients $b_t^{(N)}$ of the given perturbation $V^{(N)}(x)$ in a series of the $y_t(x)$, the expansion coefficients $w_t^{(N)}(i)$ of

$$\Theta^{(N)}(x,m;\mu)=\sum_{\nu=1}^{N-1} K^{(\nu)}(x,m;\mu)K^{(N-\nu)}(x,m;\mu)$$

in a series of $a^2e^{atx}(\mu_i^{-}m)$ [see Eqs. (33) and (36)].

Using the definition (33) of $W_s^{(N)}(m)$ together with the expressions (31) and (35) of $K^{(N)}(x,m)$ and $F_s^{(N)}(m)$, we get $(0\le s\le S_N)$

$$W_s^{(N)}(m)=\sum_{\nu=1}^{N-1}\sum_{r=0}^{s}\sum_{t=0}^{S_\nu-s+r}\sum_{u=0}^{S_{N-\nu}-r} C_{s-r}^{(\nu)}(t)C_r^{(N-\nu)}(u)\begin{bmatrix}\mu-m\\ t\end{bmatrix}\begin{bmatrix}\mu-m\\ u\end{bmatrix} . \tag{55}$$

Since we can write [14]

$$\begin{bmatrix}\mu-m\\ t\end{bmatrix}\begin{bmatrix}\mu-m\\ u\end{bmatrix}=\sum_{k=t}^{u+t}\begin{bmatrix}k\\ t\end{bmatrix}\begin{bmatrix}t\\ k-u\end{bmatrix}\begin{bmatrix}\mu-m\\ k\end{bmatrix} ,$$

we obtain, after some rearrangements, the expression (36) of $W_s^{(N)}(m)$, where

$$w_s^{(N)}(k)=\sum_{\nu=1}^{N-1}\sum_{r=0}^{s}\sum_{t=0}^{k}\sum_{u=k-t}^{k}\begin{bmatrix}k\\ t\end{bmatrix}\begin{bmatrix}t\\ k-u\end{bmatrix}C_{s-r}^{(\nu)}(t)C_r^{(N-\nu)}(u) . \tag{56}$$

Then, using the expression (41) of the $C_s^{(N)}(t)$, making again some rearrangements and keeping in mind the definition (40) of the data coefficients, we obtain

$$\begin{aligned} b_s^{(N)}(0)&=b_s^{(N)}+\sum_{\nu=1}^{N-1}\sum_{p=1}^{S_\nu+1}\sum_{q=1}^{S_{N-\nu}+1} X(s,0|p,0;q,0)b_p^{(\nu)}(0)b_q^{(N-\nu)}(0) ,\\ b_s^{(N)}(k)&=\sum_{\nu=1}^{N-1}\sum_{l=0}^{k}\sum_{n=0}^{k}\sum_{p=1}^{S_\nu+1}\sum_{q=1}^{S_{N-\nu}+1} X(s,k|p,l;q,n)b_p^{(\nu)}(l)b_q^{(N-\nu)}(n) , \end{aligned} \tag{57}$$

where the $b_s^{(N)}$ are the expansion coefficients of the given perturbation $V^{(N)}(x)$ in a series of $y_s(x)$, and

$$X(s,k|p,l;q,n)=\left[\frac{1}{2d}\right]^{p+q+s}\sum_{r=0}^{s}\sum_{t=l}^{k}\sum_{u=n}^{k}\begin{bmatrix}k\\ t\end{bmatrix}\begin{bmatrix}t\\ k-u\end{bmatrix}d_l(p-s+r-1,t,p-1)d_n(q-r-1,u,q-1) . \tag{58}$$

Since, at the first order $(\nu=1)$, the data coefficients reduce to $b_u^{(1)}(0)=b_u^{(1)}$ and $b_u^{(1)}(p)=0$ for any $p\neq0$, relations (57) allow a recursive determination of the $b_s^{(N)}(k)$ up to any order N of the perturbation.

The expressions of the "data coupling coefficients" $X(s,k|p,l;q,n)$ depend neither on the order of the perturbation nor on the particular problem under consideration. Tables and/or subroutines giving these expressions can be made available once and for all, and can serve for the solution of any perturbed type-B eigenequation. Particularly, when dealing with extensive perturbations and/or high orders of the perturbation, this recursive formulation of the data coefficients may be well adapted for microcomputer programming.

From a practical point of view, let us add that the bounds of u and of i in the expressions (50) of the perturbed eigenvalue $\Lambda_v^{(N)}(m)$, as well as in the expression (43) of the perturbed ladder function $K^{(N)}(x,m;\mu)$, are enlarged ones, as a matter of fact, the actual bounds are narrower and will follow from the vanishing conditions of the data coefficients $b_u^{(N)}(i)$ that are specific to the particular problem under consideration.

D. Illustrative example

Since the main purpose of this paper is to present the method and to test its capabilities rather than to give new results or extensive tables, we limit ourselves to a short example of perturbed type-*B* factorization. Let us consider the solution of the perturbed type-*B* eigenequation (28) up to the third order ($N=3$) of the perturbation, and in order to avoid writing down too many expressions, let us assume that the perturbation corresponds to the choice $S_1=1$ and, therefore, $S_2=2$ and $S_3=3$ [see Eq. (34)]. This choice corresponds to perturbation terms that are

$$V^{(1)}(x)=a^2\{g_1e^{ax}+g_2e^{2ax}\}\ ,$$
$$V^{(2)}(x)=a^2\{h_1e^{ax}+h_2e^{2ax}+h_3e^{3ax}\}\ , \tag{59}$$
$$V^{(3)}(x)=a^2\{p_1e^{ax}+p_2e^{2ax}+p_3e^{3ax}+p_4e^{4ax}\}\ .$$

1. First order ($N=1$) of the perturbation ($S_1=1$)

The first-order (nonvanishing) data coefficients are $b_1^{(1)}(0)=g_1$ and $b_2^{(1)}(0)=g_2$ and, consequently, the perturbed eigenvalue is [use Eq. (53) and Appendix B]

$$\Lambda_v^{(1)}(m)=\left[g_1\left[\frac{1}{2d}\right]+g_2\left[\frac{1}{2d}\right]^2(2m+1)\right]\times\left[2m-2\begin{bmatrix}v\\1\end{bmatrix}\right]\ . \tag{60}$$

The perturbed ladder function is given by Eq. (43). Using the expressions (45) of χ_{10} and χ_{20}, we get

$$K^{(1)}(x,m;\mu)=-ag_1\left[\frac{1}{2d}\right]-ag_2\left[\frac{1}{2d}\right]^2[2\mu+1+2de^{ax}]\ . \tag{61}$$

2. Second order ($N=2$) of the perturbation ($S_2=2$)

One has to first determine the nonvanishing second-order data coefficients $b_u^{(2)}(i)$. One can use either their expression (57) together with the required coupling coefficients $X(s,k|p,l;q,n)$ or the expression (61) of $K^{(1)}(x,m;\mu)$ and keep in mind that the required $w^{(2)}(i)$ are the expansion coefficients of $\Theta^{(2)}=(K^{(1)})^2$ in a series of $a^2e^{uax}\binom{\mu-m}{i}$. Since $b_1^{(2)}=h_1$, $b_2^{(2)}=h_2$, and $b_3^{(2)}=h_3$, we get

$$b_0^{(2)}(0)=\left[\frac{1}{2d}\right]^4\{4d^2g_1^2+4d(2\mu+1)g_1g_2+(2\mu+1)^2g_2^2\}\ ,$$
$$b_1^{(2)}(0)=h_1+2\left[\frac{1}{2d}\right]^3[2dg_1g_2+(2\mu+1)g_2^2]\ , \tag{62}$$
$$b_2^{(2)}(0)=h_2+\left[\frac{1}{2d}\right]^2g_2^2\ ,$$
$$b_3^{(2)}(0)=h_3\ .$$

The perturbed eigenvalue is

$$\Lambda_v^{(2)}(m)=\sum_{u=0}^{3}I_u(0)b_u^{(2)}(0)\ , \tag{63}$$

where, for class-II problems, the required closed-form expressions of the $I_u(0)$ have already been written down (see Appendix A). We get

$$\Lambda_v^{(2)}(m)=\left[\frac{1}{2d}\right]^3[2m(2m+1)(2m+2)b_3^{(2)}(0)+4md(2m+1)b_2^{(2)}(0)+8md^2b_1^{(2)}(0)+b_0^{(2)}(0)]-\left[\frac{1}{2d}\right]^3[24b_3^{(2)}(0)+4d(2m+1)b_2^{(2)}(0)+8d^2b_1^{(2)}(0)]\begin{bmatrix}v\\1\end{bmatrix}-\left[\frac{1}{2d}\right]^3\left[-24(m-1)b_3^{(2)}(0)\begin{bmatrix}v\\2\end{bmatrix}+24b_3^{(2)}(0)\begin{bmatrix}v\\3\end{bmatrix}\right]\ . \tag{64}$$

The perturbed ladder function is

$$K^{(2)}(x,m;\mu)=-a\left[\frac{1}{2d}\right]^3\left\{4d^2b_1^{(2)}(0)+2d(2\mu+1)b_2^{(2)}(0)+\left[(2\mu+2)(2\mu+1)+2(2\mu-1)\begin{bmatrix}\mu-m\\1\end{bmatrix}-4\begin{bmatrix}\mu-m\\2\end{bmatrix}\right]b_3^{(2)}(0)\right\}-ae^{ax}\left[\frac{1}{2d}\right]^2\left\{2db_2^{(2)}(0)+\left[2\mu+2+2\begin{bmatrix}\mu-m\\1\end{bmatrix}\right]b_3^{(2)}(0)\right\}-ae^{2ax}\left[\frac{1}{2d}\right]b_3^{(2)}(0)\ . \tag{65}$$

3. *Third order* ($N=3$) *of the perturbation* ($S_3=3$)

Using Eqs. (57) or picking up the expansion coefficients of $\Theta^{(3)}=2K^{(1)}K^{(2)}$ in a series of $a^2e^{uax}\binom{\mu-m}{i}$, we get the following expressions of the (nonvanishing) third-order data coefficients:

$$b_0^{(3)}(0)=2\left[\frac{1}{2d}\right]^5(2\mu+2)(2\mu+1)[2dg_1+(2\mu+1+2d)g_2]b_3^{(2)}(0)+2\left[\frac{1}{2d}\right]^4(2\mu+1)[2dg_1+(2\mu+1)g_2]b_2^{(2)}(0)$$
$$+2\left[\frac{1}{2d}\right]^3[2dg_1+(2\mu+1)g_2]b_1^{(2)}(0)\ ,$$
$$b_1^{(3)}(0)=p_1+2(2\mu+2)\left[\frac{1}{2d}\right]^4[2dg_1+(4\mu+2)g_2]b_3^{(2)}(0)+2\left[\frac{1}{2d}\right]^3(2dg_1+(4\mu+2)g_2)b_2^{(2)}(0)+2\left[\frac{1}{2d}\right]^2g_2b_1^{(2)}(0)\ ,$$
$$b_2^{(3)}(0)=p_2+2\left[\frac{1}{2d}\right]^3(4\mu+3)g_2b_3^{(2)}(0)+2\left[\frac{1}{2d}\right]^2g_2b_2^{(2)}(0)\ ,$$
$$b_3^{(3)}(0)=p_3+2\left[\frac{1}{2d}\right]^2g_2b_3^{(2)}(0)\ ,$$
$$b_4^{(3)}(0)=p_4\ ,$$
$$b_0^{(3)}(1)=4\left[\frac{1}{2d}\right]^5(2\mu-1)[2dg_1+(2\mu+1)g_2]b_3^{(2)}(0)\ ,$$
$$b_1^{(3)}(1)=4\left[\frac{1}{2d}\right]^4[2dg_1+(2\mu+1)g_2](2d+2\mu-1)b_3^{(2)}(0)\ ,$$
$$b_2^{(3)}(1)=4\left[\frac{1}{2d}\right]^3g_2b_3^{(2)}(0)\ ,$$
$$b_0^{(3)}(2)=-8\left[\frac{1}{2d}\right]^5[2dg_1+(2\mu+1)g_2]b_3^{(2)}(0)\ ,$$
$$b_1^{(3)}(2)=-8\left[\frac{1}{2d}\right]^4g_2b_3^{(2)}(0)\ . \tag{66}$$

The perturbed eigenvalue and associated ladder function are

$$\Lambda_v^{(3)}(m)=\sum_{u=0}^{4}I_u(0)b_u^{(3)}(0)+\sum_{u=0}^{2}I_u(1)b_u^{(3)}(1)+\sum_{u=0}^{1}I_u(2)b_u^{(3)}(2)\ ,$$
$$K^{(3)}(x,m;\mu)=\sum_{u=1}^{4}b_u^{(3)}(0)\chi_{u0}+\sum_{u=1}^{2}b_u^{(3)}(1)\chi_{u1}+\sum_{u=1}^{1}b_u^{(3)}(2)\chi_{u2}\ , \tag{67}$$

where the pseudointegrals $I_u(i)$ and the ladder basis functions $\chi_{ui}(x,m;\mu)$ have to be replaced by their closed-form expressions [see Appendix A and Eqs. (45)]. For the sake of brevity, the final analytical expressions of $\Lambda_v^{(3)}(m)$ and of $K^{(3)}(x,m;\mu)$ have not been reproduced.

The computation can be pursued up to any higher order of the perturbation without any special difficulty, at any order N, the same expressions (57), (50), and (43) serve for the determination of the data coefficients $b_u^{(N)}(i)$, of the perturbed eigenvalue $\Lambda_v^{(N)}(m)$ and of the perturbed ladder function $K^{(N)}(x,m;\mu)$, respectively.

V. ANALYTICAL SOLUTION OF THE PERTURBED MORSE-OSCILLATOR EIGENEQUATION

Let us consider now the solution of the perturbed Morse-oscillator eigenequation

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+D_e[1-e^{-\beta(r-r_e)}]^2+U(r)\right\}\phi(r)=E\phi(r)\ , \tag{68}$$

where $U(r)$ is a perturbation that can be displayed into perturbation terms $U^{(N)}(r)$ of the form

$$U^{(N)}(r)=D_e\sum_{t=t_0}^{S_N+1}g_t^{(N)}(1-e^{-\beta(r-r_e)})^t\ ,$$

which can be written again,

$$U^{(N)}(r)=D_e\sum_{s=0}^{S_N+1}c_s^{(N)}e^{-s\beta(r-r_e)} . \tag{69}$$

Then, analytical expressions of the perturbed Morse-oscillator energies and wave functions are readily obtainable when merely setting in the final type-B expressions,

$$a=-(2\zeta_e)^{1/2},\quad d=\frac{1}{2\zeta_e},\quad \mu=m=-\frac{1}{2}+\frac{1}{2\zeta_e} . \tag{70}$$

A. Analytical determination of the Morse-Pekeris energies

As a first example, let us consider the analytical solution of the diatomic rotation-vibration Morse equation when the rotational term is treated as a perturbation by means of a truncated Pekeris expansion [15],

$$\left[\frac{r_e}{r}\right]^2\approx(1-3\alpha+3\alpha^2)+(4\alpha-6\alpha^2)e^{-\beta(r-r_e)} -(\alpha-3\alpha^2)e^{-2\beta(r-r_e)} , \tag{71}$$

where $\alpha=1/\beta r_e$. One has to work out the solution of the perturbed Morse-oscillator eigenequation (68) with a perturbation,

$$U(r)=U^{(1)}(r)=A\{(4\alpha-6\alpha^2)e^{-\beta(r-r_e)} -(\alpha-3\alpha^2)e^{-2\beta(r-r_e)}\} , \tag{72}$$

where $A=B_e[J(J+1)-\Omega^2]$ in the Hund-(a) coupling scheme, or $A=B_e[N(N+1)-\Lambda^2]$ in the Hund-(b) coupling scheme, $\mathbf{J}=\mathbf{N}+\mathbf{S}$, $\mathbf{N}$ is the total orbital momentum of the molecule, $\mathbf{S}$ is the total spin of the electrons, and B_e is the rotational constant.

It is easily checked that $V(x)=V^{(1)}(x)$ is the type-B counterpart of $U(r)$ when setting

$$\begin{aligned} b_1^{(1)}&=g_1=-\tfrac{1}{2}\zeta_e^{-1}AD_e^{-1}(4\alpha-6\alpha^2) ,\\ b_2^{(1)}&=g_2=\tfrac{1}{2}\zeta_e^{-1}AD_e^{-1}(\alpha-3\alpha^2) ,\\ \Lambda^{(1)}&=\frac{2}{\hbar\omega_e}[E^{(1)}-A(1-3\alpha+3\alpha^2)] ,\\ \Lambda^{(N)}&=\frac{2}{\hbar\omega_e}E^{(N)} \end{aligned} \tag{73}$$

At the first order ($N=1$) of the perturbation, the perturbed type-B eigenvalue is [see Eq. (50)]

$$\Lambda_v^{(1)}=g_1I_1(0)+g_2I_2(0) . \tag{74}$$

Picking up the expressions of $I_1(0)$ and $I_2(0)$ in Appendix A and giving the type-B parameters their Morse-oscillator expressions (70), we get

$$\Lambda_v^{(1)}=(g_1+g_2)\left[1-\zeta_e-2\zeta_e\begin{bmatrix}v\\1\end{bmatrix}\right] , \tag{75}$$

and then [see Eq. (73)]

$$E_v^{(1)}=A\{1-2\zeta_e(3\alpha-3\alpha^2)(v+\tfrac{1}{2})\} . \tag{76}$$

The associated perturbed ladder function is given by Eq. (43) and, after setting $2d=2\mu+1=\zeta_e^{-1}$ in the expressions (45) of χ_{10} and χ_{20}, we get

$$K^{(1)}(x,m)=-a\zeta_e\{g_1+g_2+g_2e^{ax}\} . \tag{77}$$

At the second order ($N=2$) of the perturbation, the nonvanishing data coefficients $b_u^{(2)}(i)$ are the expansion coefficients of $\Theta^{(2)}=(K^{(1)})^2$ in a series of $a^2e^{uax}(^{\mu}_{i}{}^{-m})$. We get

$$\begin{aligned} b_0^{(2)}(0)&=(g_1+g_2)^2\zeta_e^2 ,\\ b_1^{(2)}(0)&=2g_2(g_1+g_2)\zeta_e^2 ,\\ b_2^{(2)}(0)&=g_2^2\zeta_e^2 . \end{aligned} \tag{78}$$

The second-order perturbed eigenvalue is [see Eq. (50)]

$$\Lambda_v^{(2)}=-\zeta_e^2\{g_1^2+4g_2(g_1+g_2) -2\zeta_e(2g_1g_2+3g_2^2)(v+\tfrac{1}{2})\} , \tag{79}$$

and we obtain

$$E_v^{(2)}=-A^2D_e^{-1}\{\alpha^2+\tfrac{1}{2}\zeta_e(5\alpha^2-18\alpha^3+9\alpha^4)(v+\tfrac{1}{2})\} . \tag{80}$$

The associated perturbed ladder function is [see Eq. (43)]

$$K^{(2)}(x,m)=-a\zeta_e\{b_1+b_2+b_2e^{ax}\} , \tag{81}$$

where the shortened notation $b_u=b_u^{(2)}(0)$ is used.

At the third order ($N=3$) of the perturbation, the nonvanishing data coefficients $b_u^{(3)}(i)$ are the expansion coefficients of $2K^{(1)}K^{(2)}$ in a series of $a^2e^{uax}(^{\mu}_{i}{}^{-m})$, and we get

$$\begin{aligned} b_0^{(3)}(0)&=2\zeta_e^2(g_1+g_2)(b_1+b_2) ,\\ b_1^{(3)}&=2\zeta_e^2[b_2(g_1+g_2)+g_2(b_1+b_2)] ,\\ b_2^{(2)}(0)&=2\zeta_e^2g_2b_2 . \end{aligned} \tag{82}$$

The third-order perturbed eigenvalue is

$$\Lambda_v^{(3)}=-\{b_0^{(3)}(0)+b_1^{(3)}(0)+b_2^{(3)}(0) -2\zeta_e[b_1^{(3)}(0)+b_2^{(3)}(0)](v+\tfrac{1}{2})\} . \tag{83}$$

Then, after giving the data parameters their Morse-Pekeris expressions (78) and (73), we obtain

$$E_v^{(3)}=-A^3D_e^{-2}\{\alpha^3(1-3\alpha) +\tfrac{1}{2}\zeta_e(v+\tfrac{1}{2})\alpha^3(1-3\alpha)^2(7-3\alpha)\} . \tag{84}$$

The determination of the Morse-Pekeris energies can be pursued, up to any higher order, by computing successively the expansion coefficients of $\Theta^{(4)}=(K^{(2)})^2+2K^{(1)}K^{(3)}$, $\Theta^{(5)}=2K^{(1)}K^{(4)}+2K^{(2)}K^{(3)}, \ldots$, and so on.

Of course, the expressions (76), (80), and (84), of $E_v^{(1)}$, $E_v^{(2)}$, and $E_v^{(3)}$, are directly obtainable as a particular case of Eqs. (60), (64), and (67) by setting $h_i=p_i=0$ and giving the type-B parameters their Morse-Pekeris expressions.

It should be noted that, when introducing the rotational term by means of the Pekeris expansion (71), the

Morse-Pekeris equation is relevant to exact type-B factorization and, in this case, the perturbed factorization process (up to the Nth order) provides only an approximation of the exact result (see, for instance, formula (10) of Ref. [16]), i.e., the expansion of the exact compact expression of the rotation-vibration energy in a series of $A^{v}D_e^{-v+1}$, truncated at the Nth term.

B. $(1-e^{-\alpha(r-re)})^4$-perturbed Morse-oscillator energies

As another illustrative example, let us consider the solution of the perturbed Morse-oscillator equation (68) with a perturbation

$$U(r)=2gD_e(1-e^{-\beta(r-r_e)})^4 . \tag{85}$$

In its present form, the method does not directly apply to the solution of the Morse-oscillator eigenequation with the perturbation

$$V(x)=c_1(1-e^{ax})+c_2(1-e^{ax})^2+c_3(1-e^{ax})^3+\cdots .$$

Indeed, setting $y_s(x)=aY_s(x)=a^2(1-e^{ax})^s$, we get

$$2K^0(x,m;\mu)Y_s(x)=-2(m-d)y_s-2dy_{s+1} ,$$

$$\frac{dY_s}{dx}=-sy_{s-1}+sy_s ,$$

and, therefore, the two-term ladderlike condition (8) is not fulfilled, an extension of the method should be needed. Of course, in that case, one may expand the perturbation in a series of the suitable x basis $y_s=a^2e^{asx}$ and, after an adequate dispatching of the perturbation, one can use the general perturbed type-B results of the present paper.

One has first to work out the solution of the perturbed type-B eigenequation (28) with a perturbation

$$V(x)=V^{(1)}(x)$$
$$=a^2[b_1e^{ax}+b_2e^{2ax}+b_3e^{3ax}+b_4e^{4ax}] . \tag{86}$$

It is easily checked that $V(x)$ is the type-B counterpart of $U(r)$ when setting

$$b_1=g\zeta_e^{-2},\quad b_2=-\tfrac{3}{2}g\zeta_e^{-2},\quad b_3=g\zeta_e^{-2},\quad b_4=-\tfrac{1}{4}g\zeta_e^2 ,$$
$$\Lambda^{(1)}=\frac{2}{\hbar\omega_e}[E^{(1)}-2gD_e],\quad \Lambda^{(N)}=\frac{2}{\hbar\omega_e}E^{(N)} . \tag{87}$$

At the first order ($N=1$) of the perturbation, the perturbed eigenvalue is [see Eq. (50) with $S_1=3$]

$$\Lambda_v^{(1)}(m)=b_1I_1(0)+b_2I_2(0)+b_3I_3(0)+b_4I_4(0) , \tag{88}$$

where the $I_u(0)$ are given in Appendix A. When giving the type-B constants their Morse-oscillator expressions (70) and (87), we obtain the following expression of the first-order perturbed Morse-oscillator energy (in $\hbar\omega_e$ units),

$$E_v^{(1)}=g\left\{(\tfrac{3}{4}-\tfrac{1}{2}\zeta_e)+(3-4\zeta_e)\begin{bmatrix}v\\1\end{bmatrix}+(3-9\zeta_e)\begin{bmatrix}v\\2\end{bmatrix}-6\zeta_e\begin{bmatrix}v\\3\end{bmatrix}\right\} . \tag{89}$$

The first-order perturbed ladder function is

$$K^{(1)}(x,m;\mu)=a\sum_{u=1}^{4}b_u\chi_{u0}(x,m;\mu) , \tag{90}$$

where the $\chi_{u0}(x,m;\mu)$ are given by Eq. (45).

At the second order ($N=2$) of the perturbation ($S_2=6$), the expressions of the data coefficients $b_u^{(2)}(i)$ can be obtained either as the expansion coefficients of $(K^{(1)})^2$ in a series of $a^2e^{uax}(^{\mu}_{i}{}^{-m})$ or by means of Eq. (57), i.e.,

$$b_u^{(2)}(i)=\sum_{p=1}^{4}\sum_{q=1}^{4}X(u,i|p,0;q,0)b_pb_q . \tag{91}$$

After some straightforward algebraic manipulations and after setting $2\mu+1=2d=\zeta_e^{-1}$, we obtain the expressions of the nonvanishing $b_u^{(2)}(i)$, which have been reported in Appendix B. Then, using the expression (50) of $\Lambda_v^{(N)}(m)$ and picking up the required expressions of the $I_u(i)$ in Appendix A, we obtain the following expression of the second-order perturbed Morse-oscillator energy:

$$E_v^{(2)}=-g^2\left\{(\tfrac{21}{8}+\tfrac{3}{2}\zeta_e-\tfrac{21}{3}\zeta_e^2)+(18-\tfrac{233}{4}\zeta_e+\tfrac{99}{2}\zeta_e^2)\begin{bmatrix}v\\1\end{bmatrix}+(\tfrac{153}{4}-\tfrac{1061}{4}\zeta_e+405\zeta_e^2)\begin{bmatrix}v\\2\end{bmatrix}\right.$$
$$\left.+(\tfrac{51}{2}-390\zeta_e-660\zeta_e^2)\begin{bmatrix}v\\3\end{bmatrix}-5\zeta_e(84-495\zeta_e+225\zeta_e^2)\begin{bmatrix}v\\4\end{bmatrix}-10\zeta_e(6+57\zeta_e)\begin{bmatrix}v\\5\end{bmatrix}\right\} . \tag{92}$$

The associated second-order perturbed ladder function is given by the standard expression (43).

The analytical determination of the perturbed Morse-oscillator energies can be pursued up to any higher order of the perturbation without any other special difficulty than, of course, writing down more and more extensive expressions.

As expected, the general expression (51) of the (class-II) type-B pseudointegrals $I_u(i)$ gives again, as a particular case ($i=0$, $2d=2\mu+1=\zeta_e^{-1}$) the analytical expressions of the diagonal matrix elements $\langle e^{-s\beta(r-r_e)}\rangle=-I_s(0)$ between the (unperturbed) Morse-oscillator functions. We get

$$\langle e^{-\beta(r-r_e)}\rangle=\langle e^{-2\beta(r-r_e)}\rangle=1-\zeta_e-2\zeta_e\begin{bmatrix}v\\1\end{bmatrix},$$

$$\langle e^{-3\beta(r-r_e)}\rangle=1-\zeta_e^2-12\zeta_e^2(1-\zeta_e)\begin{bmatrix}v\\1\end{bmatrix}-12\zeta_e^2(1-3\zeta_e)\begin{bmatrix}v\\2\end{bmatrix}+24\zeta_e^3\begin{bmatrix}v\\3\end{bmatrix}, \quad (93)$$

$$\langle e^{-4\beta(r-r_e)}\rangle=(1-\zeta_e^2)(1+2\zeta_e)+4\zeta_e(1-\zeta_e)(1-8\zeta_e)\begin{bmatrix}v\\1\end{bmatrix}-36\zeta_e^2(1-3\zeta_e)\begin{bmatrix}v\\2\end{bmatrix}+72\zeta_e^3\begin{bmatrix}v\\3\end{bmatrix},$$

and so on. These expressions are quite in accordance with previous results (use, for instance, formula (33) of Ref. [17]).

Finally, let us remark that as $\zeta_e\to 0$, the expressions (89) and (92) of the perturbed Morse-oscillator energies $E_v^{(1)}$ and $E_v^{(2)}$ reduce to

$$E_v^{(1)}=3g\left[\frac{1}{4}+\begin{bmatrix}v\\1\end{bmatrix}+\begin{bmatrix}v\\2\end{bmatrix}\right],$$
$$E_v^{(2)}=-g^2\left[\frac{21}{8}+18\begin{bmatrix}v\\1\end{bmatrix}+\frac{153}{4}\begin{bmatrix}v\\2\end{bmatrix}+\frac{51}{2}\begin{bmatrix}v\\3\end{bmatrix}\right]. \quad (94)$$

One finds again the already known expressions [18,5] of the x^4-perturbed harmonic-oscillator energies. This is not surprising since, as already pointed out [19], the Morse-oscillator equation (23) reduces to the harmonic-oscillator equation as the anharmonicity constant ζ_e tends to zero. Finally, let us note that perturbed type-*B* factorization with a perturbation $V(x)$ given by Eq. (86) can also be used for the determination of the rotation-vibration Morse-oscillator energies taking into account a more elaborate expression of the rotational term.

C. Determination of the perturbed eigenfunctions

Let us now consider the determination of the perturbed eigenfunctions up to any order N of the perturbation and apply the usual factorization scheme. The total (type-*B*) ladder function is

$$K(x,m;\mu)=-am+ade^{ax}+K_N(x,m;\mu), \quad (95)$$

where

$$K_N(x,m;\mu)=\eta K^{(1)}(x,m;\mu)+\eta^2K^{(2)}(x,m;\mu)+\cdots+\eta^NK^{(N)}(x,m;\mu).$$

The (class-II) perturbed key function ($v=0$) is the solution of the first-order differential equation [see Eq. (6)]

$$\left\{K(x,j;\mu)+\frac{d}{dx}\right\}\Psi_{jj}(x;\mu)=0. \quad (96)$$

One finds

$$\Psi_{jj}(x;\mu)\approx\Psi_{jj}^{(0)}(x)\exp\left[-\int K_N(x,j;\mu)dx\right], \quad (97)$$

where $\Psi_{jj}^{(0)}(x)=N_{jj}\exp[jax+2de^{ax}]$ is the zeroth-order (type-*B*) key function. Then, the complete set of the perturbed eigenfunctions can be generated stepwise by successive application of the ladder operation,

$$\left\{K(x,m;\mu)-\frac{d}{dx}\right\}\Psi_{jm}(x;\mu)=[L(j;\mu)-L(m;\mu)]^{1/2}\Psi_{jm+1}(x;\mu), \quad (98)$$

where

$$L(m;\mu)=-a^2m^2+\eta L^{(1)}(m;\mu)+\eta^2L^{(2)}(m;\mu)+\cdots+\eta^NL^{(N)}(m;\mu).$$

Starting from the perturbed key function ($v=0$), the ladder process (98) can be pursued until the determination of the required ($v=m-j$) eigenfunction. Once the μ dependent $\Psi_{jm}(x;\mu)$ is obtained, the artificial parameter μ has to be set equal to its actual value $\mu=m$.

The expressions of the perturbed Morse-oscillator functions (within the Ter Haar approximation [12]) are readily obtainable from their (type-*B*) counterpart $\Psi_{jm}(x;m)$ after setting $x=(\mu\omega_e/\hbar)^{1/2}(r-r_e)$, introducing the suitable normalization constant and giving the type-*B* parameters their Morse-oscillator expressions (70). This point is going to be considered elsewhere in more detail, together with the computation of the perturbed Morse-oscillator transition probabilities and intensities.

VI. CONCLUSION

Owing to the fundamental and practical interest of the Morse-oscillator model, many various methods [20] have been made available for the solution of the (unperturbed) Morse-oscillator eigenequation. This is not quite the case when an analytical solution of the Morse equation with an additional perturbation $V(x)$ is required, and it may be useful to resort to perturbed type-*B* factorization. An analytical solution of the perturbed eigenequation is readily obtained without any prior knowledge of the excited spectra and without having to calculate any matrix element. This is an advantageous feature of perturbed factorization with regard to other perturbative methods since off-diagonal matrix elements $\langle v'|e^{-s\beta(r-r_e)}|v\rangle$ between (unperturbed) Morse-oscillator eigenfunctions are nonvanishing for all v'. Moreover, once the perturbed ladder and factorization functions have been obtained, one finds again all the advantages of the exact factorizable (unperturbed) method: determination of any perturbed eigenfunction $\Psi_{jm}(x;\mu)$ from the knowledge of the perturbed key perturbed function $\Psi_{jj}(x;\mu)$ by means of μ-dependent ladder equations (5) and/or determination of recursive formulas [21] for the computation of matrix elements between perturbed eigenfunctions.

Of course, perturbed type-*B* factorization can also be applied to any problem involving the solution of a perturbed confluent hypergeometric eigenequation [3]. Let us emphasize that, since the ladder basis functions

$\chi_{ui}(x,m;\mu)$ as well as the pseudointegrals $I_u(i;m,\mu)$ do not depend on the order N of the perturbation, the Nth order of the perturbation is not significantly more difficult to handle than the first order. At any order N of the perturbation, the perturbed eigenvalue is obtained in the same way as at the first order, i.e., by adding the products $b_u^{(N)}(i)I_u(i;m,\mu)$ of the data coefficients $b_u^{(N)}(i)$, which are specific to the particular problem under consideration, with the required standard (type-B) pseudointegrals $I_u(i;m,\mu)$. For any problem relevant to perturbed type-B factorization and at any order N, once the data coefficients $b_u^{(N)}(i)$ have been obtained in terms of the expansion coefficients of the given perturbation $V^{(N)}(x)$ by means of algebraic manipulations, the determination of the perturbed eigenvalue (and perturbed ladder function merely amounts to picking up the required type-B pseudointegrals (and ladder basis functions).

Being algebraic and recursive, the perturbed ladder-operator method may be easier to use (with the help of computer algebra) than other traditional methods, such as the Rayleigh-Schrödinger one. Nevertheless, the use of perturbed factorization imperatively requires the given perturbation $V(x)$ to be expanded in a series of the specific x basis functions $y_s(x)$, namely, for perturbed type B, $y_s(x)=a^2\exp(asx)$. Fortunately, for the case of the Morse potential, once each perturbation term $V^{(N)}(x)$ of the total perturbation $V(x)$ has been expanded in a series of the natural expansion basis functions $z_t(r)=(1-e^{-\beta(r-r_e)})^t$, it can be identically transformed into a finite series of the required basis functions $y_s(r)=e^{-s\beta(r-r_e)}$. Hence, our working expansion is exactly equivalent to the traditional one. Of course, the convergence of the perturbation expansion can be preliminarily improved by considering $V(x)$ as a polynomial in $z_1(x)=1-e^{-\beta(r-r_e)}$ and using, for instance, a (conveniently shifted) Chebyshev series economization technique [22].

Let us mention that the choice of the suitable perturbed type-B x basis functions $y_s(x)=a^2\exp(asx)$ and $Y_s(x)=a\exp(asx)$, which have been used in the present paper, is not at all exhaustive. The associated basis functions $y_s(x)=a^2\exp(-asx)$ and $Y_s(x)=a\exp(-asx)$ also satisfy the ladderlike properties (8), with associated data $A_s(m)=2d$, $B_s(m)=-2m$, $\alpha_s=0$, and $\beta_s=-(s+1)$. Nevertheless, in this case, the solution of the finite-difference equation (11) is more intricate. One encounters analogous intricacy when dealing with the solution of the spiked or, more generally, the singular anharmonic-oscillator eigenequation involving $(1/x)^k$ perturbations (perturbed type-C factorization, with associated data $y_s(m)=(1/x)^{2s}$, $Y_s(m)=(1/x)^{2s+1}$, $A_s(m)=2b$, $B_s(m)=2m$, $\alpha_s=0$, and $\beta_s=-(2s+1)$. Owing to their particular interest in quantum physics, these two last cases, as well as the solution of the perturbed transformed-Jacobi eigenequation [determination of perturbed Wigner functions $D_{M,Q}^{(J)}(\varphi,\theta,\phi)$ or of perturbed spherical harmonics $Y_l^m(\theta,\varphi)$, analytical solution of the Schrödinger equation with a perturbed Pöschl-Teller potential [23], with a Gaussian potential, etc. are under consideration.

APPENDIX A: EXPRESSIONS OF THE TYPE-B PSEUDOINTEGRALS

Using the standard expression (51), we get

$$I_0(i)=-\begin{bmatrix} v\\ i\end{bmatrix} \quad \text{for any } i\ ,$$

$$I_1(0)=-\frac{1}{2d}\left\{2m-2\begin{bmatrix} v\\ 1\end{bmatrix}\right\},$$

$$I_1(1)=-\frac{1}{2d}\left\{(2m-2)\begin{bmatrix} v\\ 1\end{bmatrix}-4\begin{bmatrix} v\\ 2\end{bmatrix}\right\},$$

$$I_1(2)=-\frac{1}{2d}\left\{(2m-4)\begin{bmatrix} v\\ 2\end{bmatrix}-6\begin{bmatrix} v\\ 3\end{bmatrix}\right\},$$

$$I_1(3)=-\frac{1}{2d}\left\{(2m-6)\begin{bmatrix} v\\ 3\end{bmatrix}-8\begin{bmatrix} v\\ 4\end{bmatrix}\right\},$$

$$I_2(0)=-\left[\frac{1}{2d}\right]^2(2m+1)\left\{2m-2\begin{bmatrix} v\\ 1\end{bmatrix}\right\},$$

$$I_2(1)=-\left[\frac{1}{2d}\right]^2\left\{(2m-1)(2m-2)\begin{bmatrix} v\\ 1\end{bmatrix}-12(m-1)\begin{bmatrix} v\\ 2\end{bmatrix}+12\begin{bmatrix} v\\ 3\end{bmatrix}\right\},$$

$$I_2(2)=-\left[\frac{1}{2d}\right]^2\left\{(2m-3)(2m-4)\begin{bmatrix} v\\ 2\end{bmatrix}-(20m-42)\begin{bmatrix} v\\ 3\end{bmatrix}+32\begin{bmatrix} v\\ 4\end{bmatrix}\right\},$$

$$I_2(3)=-\left[\frac{1}{2d}\right]^2\left\{(2m-5)(2m-6)\begin{bmatrix}v\\3\end{bmatrix}-(28m-88)\begin{bmatrix}v\\4\end{bmatrix}+60\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_3(0)=-\left[\frac{1}{2d}\right]^3\left\{2m(2m+1)(2m+2)-24m\begin{bmatrix}v\\1\end{bmatrix}-24(m-1)\begin{bmatrix}v\\2\end{bmatrix}+24\begin{bmatrix}v\\3\end{bmatrix}\right\},$$

$$I_3(1)=-\left[\frac{1}{2d}\right]^3\left\{2m(2m-1)(2m-2)\begin{bmatrix}v\\1\end{bmatrix}-24m(m-1)\begin{bmatrix}v\\2\end{bmatrix}+24m\begin{bmatrix}v\\3\end{bmatrix}\right\},$$

$$I_3(2)=-\left[\frac{1}{2d}\right]^3\left\{(2m-2)_3\begin{bmatrix}v\\2\end{bmatrix}-12(2m-3)_2\begin{bmatrix}v\\3\end{bmatrix}+(120m-240)\begin{bmatrix}v\\4\end{bmatrix}-120\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_4(0)=-\left[\frac{1}{2d}\right]^4(2m+1)\left\{2m(2m+3)_2+8m(2m-7)\begin{bmatrix}v\\1\end{bmatrix}-72(m-1)\begin{bmatrix}v\\2\end{bmatrix}+72\begin{bmatrix}v\\3\end{bmatrix}\right\},$$

$$I_4(1)=-\left[\frac{1}{2d}\right]^4\left\{(2m+1)_4\begin{bmatrix}v\\1\end{bmatrix}-16(m-1)(m+3)(2m-1)\begin{bmatrix}v\\2\end{bmatrix}\right.$$
$$\left.-24(2m^2-15m+12)\begin{bmatrix}v\\3\end{bmatrix}+240(m-2)\begin{bmatrix}v\\4\end{bmatrix}-240\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_4(2)=-\left[\frac{1}{2d}\right]^4(2m-1)\left\{(2m-2)_3\begin{bmatrix}v\\2\end{bmatrix}-24(2m^2-7m+6)\begin{bmatrix}v\\3\end{bmatrix}+60(2m-4)\begin{bmatrix}v\\4\end{bmatrix}-120\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_5(0)=-\left[\frac{1}{2d}\right]^5\left\{(2m+4)_5+40m(m+1)(2m+1)(2m-5)\begin{bmatrix}v\\1\end{bmatrix}\right.$$
$$\left.-240m(m-1)(2m+5)\begin{bmatrix}v\\2\end{bmatrix}+1440(2m-1)\begin{bmatrix}v\\3\end{bmatrix}+1440(m-2)\begin{bmatrix}v\\4\end{bmatrix}-1440\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_5(1)=-\left[\frac{1}{2d}\right]^5\left\{(2m+2)_5\begin{bmatrix}v\\1\end{bmatrix}-120m(2m-1)(2m-2)\begin{bmatrix}v\\2\end{bmatrix}\right.$$
$$\left.-120m(2m-2)(2m-7)\begin{bmatrix}v\\3\end{bmatrix}+1440m(m-2)\begin{bmatrix}v\\4\end{bmatrix}-1440m\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

$$I_6(0)=-\left[\frac{1}{2d}\right]^6(2m+1)\left\{2m(2m+5)_4+12m(2m+3)_2(6m-13)\begin{bmatrix}v\\1\end{bmatrix}-240m(m-1)(2m+17)\begin{bmatrix}v\\2\end{bmatrix}\right.$$
$$\left.-480(4m^2-26m+15)\begin{bmatrix}v\\3\end{bmatrix}+7200(m-2)\begin{bmatrix}v\\4\end{bmatrix}-7200\begin{bmatrix}v\\5\end{bmatrix}\right\},$$

and so on.

APPENDIX B: PERTURBED MORSE-OSCILLATOR DATA COEFFICIENTS

The second-order data coefficients associated with the perturbation $U(r)=2gD_e(1-e^{-\beta(r-r_e)})^4$ can be obtained by using the expression (90) of the first-order perturbed ladder function $K^{(1)}(x,m;\mu)$. We get (within a factor $g\zeta_e^{-2}$)

$$K^{(1)}(x,m;\mu)=f_0+g_0\begin{bmatrix}\mu-m\\1\end{bmatrix}+h_0\begin{bmatrix}\mu-m\\2\end{bmatrix}$$
$$+e^{ax}\left\{f_1+g_1\begin{bmatrix}\mu-m\\1\end{bmatrix}\right\}$$
$$+e^{2ax}\left\{f_2+g_2\begin{bmatrix}\mu-m\\1\end{bmatrix}\right\}+e^{3ax}f_3,$$

where, after setting $2\mu+1=2d=\zeta_e^{-1}$, we have

$$f_0=\tfrac{1}{4}\zeta_e(1+\zeta_e-2\zeta_e^2),\quad g_0=\tfrac{1}{2}\zeta_e^2(1-2\zeta_e)\ ,$$

$$h_0=-\zeta_e^3,\quad f_1=-\tfrac{3}{4}\zeta_e(1-\tfrac{1}{3}\zeta_e+\tfrac{2}{3}\zeta_e^2),\quad g_1=\tfrac{1}{2}\zeta_e^2\ ,$$

$$f_2=\tfrac{3}{4}\zeta_e(1-\tfrac{2}{3}\zeta_e),\quad g_2=-\zeta_e^2,\quad f_3=-\tfrac{1}{4}\zeta_e\ .$$

Then, $(K^{(1)})^2$ is easily expandable in a series of $a^2e^{uax}\binom{\mu-m}{i}$ by means of the relations

$$\begin{bmatrix}\mu-m\\1\end{bmatrix}\begin{bmatrix}\mu-m\\1\end{bmatrix}=\begin{bmatrix}\mu-m\\1\end{bmatrix}+2\begin{bmatrix}\mu-m\\2\end{bmatrix},$$

$$\begin{bmatrix}\mu-m\\1\end{bmatrix}\begin{bmatrix}\mu-m\\2\end{bmatrix}=2\begin{bmatrix}\mu-m\\2\end{bmatrix}+3\begin{bmatrix}\mu-m\\3\end{bmatrix},$$

$$\begin{bmatrix}\mu-m\\2\end{bmatrix}\begin{bmatrix}\mu-m\\2\end{bmatrix}=\begin{bmatrix}\mu-m\\2\end{bmatrix}+6\begin{bmatrix}\mu-m\\3\end{bmatrix}+6\begin{bmatrix}\mu-m\\4\end{bmatrix},$$

and we get the required expressions of the second-order nonvanishing expansion coefficients $b_u^{(2)}(i)=w_u^{(2)}(i)$ [noted $b_u(i)$],

$$b_0(0)=f_0^2,\quad b_0(1)=g_0^2+2f_0g_0\ ,$$

$$b_0(2)=2g_0^2+h_0^2+2f_0h_0+4g_0h_0\ ,$$

$$b_0(3)=6h_0^2+6g_0h_0,\quad b_0(4)=6h_0^2\ ,$$

$$b_1(0)=2f_0f_1,\quad b_1(1)=2f_1g_0+2g_1g_0+2g_1f_0\ ,$$

$$b_1(2)=2f_1h_0+4g_1g_0+4g_1h_0,\quad b_1(3)=6g_1h_0\ ,$$

$$b_2(0)=2f_0f_2+f_1^2\ ,$$

$$b_2(1)=2f_0g_2+2g_0f_2+2g_0g_2+2f_1g_1+g_1^2\ ,$$

$$b_2(2)=4g_0g_2+4h_0g_2+2g_1^2+2h_0f_2,\quad b_2(3)=6h_0g_2\ ,$$

$$b_3(0)=2f_0f_3+2f_1f_2\ ,$$

$$b_3(1)=2g_0f_3+2f_1g_2+2g_1f_2+2g_1g_2\ ,$$

$$b_3(2)=2h_0f_3+4g_1g_2,\quad b_4(0)=2f_1f_3+f_2^2\ ,$$

$$b_4(1)=2g_1f_3+2f_2g_2+g_2^2,\quad b_4(2)=2g_2^2\ ,$$

$$b_5(0)=2f_2f_3,\quad b_5(1)=2g_2f_3,\quad b_6(0)=f_3^2\ .$$

---

[1] N. Bessis and G. Bessis, Phys. Rev. A **42**, 1096 (1990).
[2] E. Schrödinger, Proc. R. Ir. Acad. Sect. A **46**, 183 (1940); **47**, 53 (1941).
[3] L. Infeld and T. E. Hull, Rev. Mod. Phys. **23**, 21 (1951).
[4] N. Bessis and G. Bessis, Phys. Rev. A **44**, 5503 (1991).
[5] N. Bessis and G. Bessis, Phys. Rev. A **46**, 6824 (1992).
[6] J. N. Huffaker, J. Chem. Phys. **72**, 2601 (1980).
[7] N. Bessis and Y. S. Tergiman, J. Mol. Spectrosc. **93**, 16 (1982).
[8] N. Bessis, G. Hadinger, and Y. S. Tergiman, J. Mol. Spectrosc. **107**, 343 (1984).
[9] G. Hadinger, N. Bessis, and G. Bessis, J. Math. Phys. **15**, 716 (1974).
[10] Note that, since the term $\Theta^{(N)}(x,m)=\sum_{\nu=1}^{N-1}K^{(\nu)}(x,m)K^{(N-\nu)}(x,m)$ is involved within the factorizability condition, at each order N of the perturbation, the value of S_N cannot be chosen arbitrarily, i.e., it depends both on the value of N and of S_1.
[11] P. M. Morse, Phys. Rev. **34**, 67 (1929).
[12] The range for x in the Morse-oscillator equation (23) is $(-r_e,+\infty($, but, in most cases, a sufficiently close approximation is obtained if we take the range to be $)-\infty,+\infty($ [see D. Ter Haar, Phys. Rev. **70**, 222 (1946)].
[13] This choice of the perturbation $V(x)$, which may contain the terms e^{ax} and e^{2ax} homogeneous to the unperturbed potential may be convenient for a more versatile dispatching of the total perturbation.
[14] C. Jordan, *Calculus of Finite Differences* (Chelsea, New York, 1965).
[15] C. L. Pekeris, Phys. Rev. **45**, 98 (1934).
[16] M. Badawi, N. Bessis, G. Bessis, and G. Hadinger, Can. J. Phys. **52**, 110 (1974).
[17] M. Berrondo, A. Palma, and J. L. Lopez-Bonilla, Int. J. Quantum Chem. **31**, 243 (1987).
[18] G. Alvarez, S. Graffi, and H. J. Silverstone, Phys. Rev. A **38**, 1687 (1988).
[19] I. L. Cooper, Chem. Phys. **112**, 67 (1987).
[20] See, for instance, I. L. Copper, J. Phys. A **26**, 1601 (1993), and references therein.
[21] N. Bessis and G. Bessis, J. Phys. A **20**, 5745 (1987).
[22] M. A. Snyder, *Chebyshev Methods in Numerical Approximation* (Prentice Hall, Englewood Cliffs, NJ, 1966).
[23] G. Pöschl and E. Teller, Z. Phys. **83**, 143 (1933).