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An algebraic procedure is proposed for the analytical solution of Schrödinger equations that can be viewed as a factorizable equation with an adequately chosen perturbation. This procedure relies on the solution of the Riccati equation associated with the given eigenequation and the use of power series of suitable functions which are specific to each factorization type. As illustrative examples, analytical solution of the symmetric anharmonic oscillator, perturbed Morse oscillator and singular anharmonic oscillator equations are carried out. Further applications are pointed out. © *1995 American Institute of Physics.*

I. INTRODUCTION

In many problems of current interest in quantum mechanics, particularly in atomic and molecular physics, one requires analytical solutions of wave equations which, in most cases, are not exactly solvable equations. Nevertheless, very often, at many stages of the physical modelization, after exact or approximate separation of variables, it is possible to manage in order to deal with the solution of equations which are, or are amenable to be exactly solvable eigenequations with an additional perturbation. After appropriate transformations of variable and function, these equations can be written in the standard form

$$\left\{ \frac{d^2}{dx^2} + U^{(0)}(x,m) + V(x) + \Lambda \right\} \Psi(x) = 0, \tag{1}$$

where $V(x)$ is a perturbation and $m = m_0,\ m_0+1, m_0+2,...$ is a quantum number which takes successive discrete values labeling the eigenfunctions.

Actually, the potential functions $U^{(0)}(x,m)$ leading to an exactly solvable eigenequation are comparatively few and, mostly, can be related to a Infeld and Hull[1] factorizable equation (see Table I). If we restrict ourselves to bound states, analytical expressions of the unperturbed eigenvalues are readily obtained from the knowledge of the factorization function, i.e.,

$$\Lambda^{(0)} = L^{(0)}(\tilde{j}), \tag{2}$$

where $\tilde{j} = m + v + 1$ (or $\tilde{j} = m - v$) according to the class of factorization, i.e., according to whether $L^{(0)}(m)$ is an increasing (or a decreasing) function of m; $v = 0,1,2,...$ is a non negative integer.

Closed-form expressions of the eigenfunctions have been obtained[2] and involve classical orthogonal polynomials (see Table I). The whole set of unperturbed eigenvalues and eigenfunctions being known, one can resort to the usual perturbation theories such as the traditional Rayleigh–Schrödinger framework. One can also use the logarithmic perturbation method,[3] or the perturbed ladder operator method,[4] and obtain analytical expressions of the perturbed eigenvalues and perturbed eigenfunctions showing their dependence in the quantum numbers m and v.

In the present paper, a straightforward procedure is proposed which is based on the solution of the perturbed Riccati equation associated with the given Eq. (1) and the use of power series of suitable functions which are specific to each factorizable type of Table I. For any given state, this procedure provides the analytical solution of eigenequation (1) without having either to get analytical expressions of the required matrix elements between unperturbed functions and manage with the many summations of the Rayleigh–Schrödinger method, or to perform the successive integrations of the logarithmic method, or to solve the finite-difference equations of the perturbed ladder operator method.

After giving the main features of the method, it is shown that, provided the perturbation $V(x)$ is conveniently chosen, the present procedure works well for all the unperturbed potential $U^{(0)}(x,m)$ belonging to Table I and, for any given state, one can obtain analytical expressions of the perturbed eigenfunctions and eigenvalues by merely using algebraic operations (Sec. II). As illustrative examples, analytical expressions of the symmetric anharmonic-oscillator, perturbed Morse-oscillator, and singular anharmonic-oscillator energies and eigenfunctions are carried out (Sec. III). Further applications of the method are pointed out (Sec. IV).

II. METHOD

When setting $d\Psi/dx = F(x)\Psi(x)$, the given eigenequation (1) is readily transformed into the following Riccati equation

$$\frac{dF}{dx} + [F(x)]^2 + U^{(0)}(x,m) + V(x) + \Lambda = 0. \tag{3}$$

Let us assume that $V(x)$ as well as Λ can be expanded in a perturbation series of a parameter η and let us set

$$\begin{aligned} V(x) &= \eta V^{(1)}(x) + \eta^2 V^{(2)}(x) + \cdots\ , \\ \Lambda &= \Lambda^{(0)} + \eta\Lambda^{(1)} + \eta^2\Lambda^{(2)} + \cdots\ , \\ F_v(x) &= \frac{R_v^{(0)}(x) + \eta R_v^{(1)}(x) + \eta^2 R_v^{(2)}(x) + \cdots}{S_v^{(0)}(x) + \eta S_v^{(1)}(x) + \eta^2 S_v^{(2)}(x) + \cdots}, \end{aligned} \tag{4}$$

where the $R_v^{(N)}(x)$ and $S_v^{(N)}(x)$ functions have to be found for each state v.

Since the unperturbed function $F_v^{(0)}(x) = R_v^{(0)}(x)/S_v^{(0)}(x) = [1/\Psi_v^{(0)}(x)](d\Psi_v^{(0)}/dx)$ is solution of the zeroth-order Riccati equation, when substituting for $V(x)$, $F_v(x)$, and Λ from Eq. (4) into Eq. (3), at each order N of the

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TABLE I. Infeld–Hull exact factorizable eigenequations. $\epsilon=+1$ *and* $\tilde{j}=m+v+1$ (or $\epsilon=-1$ *and* $\tilde{j}=m-v$) according to whether the factorization function $L^{(0)}(m)$ is an increasing (or a decreasing) function of m. $P_v^{(\alpha,\beta)}$ ( ), L_v^{α} ( ) and H_v ( ) are, respectively, a Jacobi, Laguerre and Hermite polynomial of degree v.

Type	$U^{(0)}(x,m)$	$\Psi_v^{(0)}(x)$	Parameters	$L^{(0)}(m)$
A	$-\dfrac{a^2[m(m+1)+d^2+(2m+1)d\cos ax]}{\sin^2 ax}$	$\approx\left(\sin\dfrac{ax}{2}\right)^{\alpha+1/2}\left(\cos\dfrac{ax}{2}\right)^{\beta+1/2}P_v^{(\alpha,\beta)}(\cos ax)$	$\alpha=\epsilon(m+d+1/2)$ $\beta=\epsilon(m-d+1/2)$	a^2m^2
B	$-a^2d^2e^{2ax}+a^2(2m+1)de^{ax}$	$\approx\exp[\frac{1}{2}(\alpha ax-\beta e^{ax})]L_v^{\alpha}(\beta e^{ax})$	$\alpha=-2\epsilon\tilde{j}$ $\beta=-2\epsilon d$	$-a^2m^2$
C	$-\dfrac{m(m+1)}{x^2}-b^2x^2+b(2m+1)$	$\approx x^{\alpha+1/2}\exp\left(-\dfrac{\beta x^2}{2}\right)L_v^{\alpha}(\beta x^2)$	$\alpha=\epsilon(m+1/2)$ $\beta=-\epsilon b$	$-4bm$
D	$-b^2x^2+b(2m+1)$	$\approx\exp\left(-\dfrac{\beta^2x^2}{2}\right)H_v[\beta x]$	$\beta=(-\epsilon b)^{1/2}$	$-2bm$
E	$-\dfrac{a^2m(m+1)}{\sin^2 ax}-2aq\cot ax$	$\approx(\sin ax)^{-\alpha}\exp(-\epsilon\beta x)P_v^{(\alpha+i\beta,\alpha-i\beta)}(-i\cot ax)$	$\alpha=-\epsilon\tilde{j}$ $\beta=-q/\tilde{j}$	$a^2m^2-\dfrac{q^2}{m^2}$
F	$-\dfrac{m(m+1)}{x^2}-\dfrac{2q}{x}$	$\approx x^{m+1}\exp\left(-\dfrac{\beta x}{2}\right)L_v^{\alpha}(\beta x)$	$\alpha=2m+1$ $\beta=-2q/\tilde{j}$	$-\dfrac{q^2}{m^2}$

perturbation, the quadratic character of the original Riccati equation is blown off and the resulting equations to be solved are linear equations. At the successive orders ($N=1,2,...$) of the perturbation, we get

$$S_v^{(0)}\frac{dR_v^{(1)}}{dx}-R_v^{(1)}\frac{dS_v^{(0)}}{dx}+2R_v^{(0)}R_v^{(1)}+2S_v^{(0)}S_v^{(1)}[U^{(0)}+\Lambda^{(0)}]+(S_v^{(0)})^2[V^{(1)}+\Lambda^{(1)}]=0, \tag{5}$$

$$\begin{aligned}S_v^{(0)}\frac{dR_v^{(2)}}{dx}&+S_v^{(1)}\frac{dR_v^{(1)}}{dx}-R_v^{(0)}\frac{dS_v^{(2)}}{dx}-R_v^{(1)}\frac{dS_v^{(1)}}{dx}+2R_v^{(0)}R_v^{(2)}\\&+(R_v^{(1)})^2+[2S_v^{(0)}S_v^{(2)}+(S_v^{(1)})^2][U^{(0)}+\Lambda^{(0)}]\\&+2S_v^{(0)}S_v^{(1)}[V^{(1)}+\Lambda^{(1)}]+(S_v^{(0)})^2[V^{(2)}+\Lambda^{(2)}]\\&=0\ldots\text{and so on}\end{aligned} \tag{6}$$

where, at each order N under consideration, the $R_v^{(n)}(x)$ and $S_v^{(n)}(x)$ functions of the preceding orders ($n=0,1,\ldots N-1$) are known.

For each factorization type, the unperturbed function $F_v^{(0)}(x)=R_v^{(0)}(x)/S_v^{(0)}(x)$ is easily obtained in closed form from the knowledge of its counterpart $\Psi_v^{(0)}(x)$ which is solution of a factorizable equation. We get

$$F_v^{(0)}(x)=F^{(0)}(x)+\frac{1}{\Phi_v}\frac{d\Phi_v}{dx}, \tag{7}$$

where $F^{(0)}(x)=F_{v=0}^{(0)}(x)$ is the ground state ($v=0$) function and $\Phi_v=\Phi_v(x)$ is the polynomial which is involved in the expression of the unperturbed function $\Psi_v^{(0)}(x)$ of Table I.

Since these polynomials $\Phi_v(x)$ are either Jacobi, associated Laguerre or Hermite polynomials, the second term in the expression (7) of the unperturbed functions $F_v^{(0)}(x)$ is easily obtained, for any value of v, by using, together with the already known expressions of the polynomials, the following relations[5]

$$\frac{d}{dy}P_v^{(\alpha,\beta)}(y)=\tfrac{1}{2}(v+\alpha+\beta+1)P_{v-1}^{(\alpha+1,\beta+1)}(y),$$

$$\frac{d}{dy}L_v^{\alpha}(y)=-L_{v-1}^{\alpha+1}(y),\quad \frac{d}{dy}H_v(y)=2vH_{v-1}(y).$$

We get

$$\frac{1}{\phi_v}\frac{d\phi_v}{dx}=\frac{a(v+\alpha+\beta+1)\Sigma_{t=0}^{v-1}(-1)^{t+1}\binom{v+\alpha}{v-t-1}\binom{v+\beta}{t}u^{2t+1}}{\Sigma_{t=0}^{v}(-1)^t\binom{v+\alpha}{v-t}\binom{v+\beta}{t}u^{2t}}\quad\text{(type A)}; \tag{8}$$

$$\frac{1}{\phi_v}\frac{d\phi_v}{dx}=\frac{\beta\Sigma_{t=0}^{v-1}(-1)^{t+1}\binom{v+\alpha}{v-t-1}[(\beta u)^t/t!]}{\Sigma_{t=0}^{v}(-1)^t\binom{v+\alpha}{v-t}[(\beta u)^t/t!]}\quad\text{(types B, C, and F)}; \tag{9}$$

$$\frac{1}{\phi_v}\frac{d\phi_v}{dx}=\frac{\beta\Sigma_{t=0}^{[(v-1)/2]}(-1)^t[(\beta u)^{v-2t-1}/t!(v-2t-1)!]}{\Sigma_{t=0}^{[(v)/2]}(-1)^t[(\beta u)^{v-2t}/t!(v-2t)!]}\quad\text{(type D)}; \tag{10}$$

where $u=\tan(ax/2)$ for type A, $u=e^{ax}$ for type B, $u=x$ for types C, D, F and $u=\cot ax$ for type E. The expression (9) has to be multiplied by a factor (au) for type B and a factor $(2u)$ for type C. $[v/2]$ denotes the integer part of $v/2$.

Briefly stated, as a consequence of the expression (7) of $F_v^{(0)}(x)=R_v^{(0)}(x)/S_v^{(0)}(x)$, the unperturbed functions $R_v^{(0)}(x)$ and $S_v^{(0)}(x)$ are both already known polynomials of $u=u(x)$

TABLE II. The unperturbed functions $F_v^{(0)}(x)=R_v^{(0)}(x)/S_v^{(0)}(x)$ in terms of $u=u(x)$.

Type	$u(x)$	$v=0$	$v=1$
A	$\tan\frac{ax}{2}$	$\frac{a[(\alpha+\frac{1}{2})-(\beta+\frac{1}{2})u^2]}{2u}$	$\frac{a[(2\alpha+1)(\alpha+1)-(4\alpha\beta+7(\alpha+\beta)+10)u^2+(2\beta+1)(\beta+1)u^4]}{4[(\alpha+1)u-(\beta+1)u^3]}$
B	e^{ax}	$\frac{a}{2}(\alpha-\beta u)$	$\frac{a[\alpha(\alpha+1)-(2\alpha+3)\beta u+\beta^2u^2]}{2(\alpha+1-\beta u)}$
C	x	$\frac{(\alpha+\frac{1}{2})-\beta u^2}{u}$	$\frac{(2\alpha+1)(\alpha+1)-(4\alpha+7)\beta u^2+2\beta^2u^4}{2u(\alpha+1-\beta u^2)}$
D	x	$-\beta^2u$	$\frac{1-\beta^2u^2}{u}$
E	$\cot ax$	$-a\alpha u-\beta$	$\frac{a(\alpha+1)-\beta^2+\beta(1+\alpha-\alpha a)u+a(\alpha+1)^2u^2}{\beta-(\alpha+1)u}$
F	x	$\frac{\alpha+1-\beta u}{2u}$	$\frac{(\alpha+1)^2-2(\alpha+2)\beta u+\beta^2u^2}{2u(\alpha+1-\beta u)}$

(see Table II, for $v=0,1$). Moreover, we remark that, for each of the six factorization types, the unperturbed potential $U^{(0)}(x,m)$ involves only powers of the same $u=u(x)$ as the unperturbed function $F_v^{(0)}(x)$ (see Tables I and II). This is obvious for factorization types B, C, D, and F. For types A and E, it is easily checked that the unperturbed potentials $U^{(0)}(x,m)$ can be conveniently written again.

For type A,

$$U^{(0)}(x,m)=-\frac{a^2[(m+d+1)(m+d)+2(d^2+m(m+1))u^2+(m-d+1)(m-d)u^4]}{4u^2},\quad \text{where}\quad u=\tan(ax/2). \tag{11}$$

For type E

$$U^{(0)}(x,m)=-a^2m(m+1)(1+u^2)-2aqu;$$
$$u=\cot ax. \tag{12}$$

Now, let us assume that, at each order N of the perturbation, the given perturbation can be expanded in power series of $u=u(x)$, i.e., that the perturbation terms $V^{(N)}(x)$ can be written

$$V^{(N)}(x)=\sum_{s=1}^{S_N} b_s^{(N)}u^s \tag{13}$$

and let us set

$$R_v^{(N)}(x)=\sum_s c_s^{(N)}u^s;\quad S_v^{(N)}(x)=\sum_s d_s^{(N)}u^s, \tag{14}$$

then, at each order N of the perturbation, the solution of the original Eq. (3), i.e., the determination of the perturbed eigenvalue $\Lambda_v^{(N)}$ and of the expansion coefficients $c_s^{(N)}$ and $d_s^{(N)}$ of the $R_v^{(N)}(u)$, and $S_v^{(N)}(u)$ functions to be found, amounts to the solution of a linear system of equations.

III. ILLUSTRATIVE EXAMPLES

Since the main purpose of this paper is to illustrate the simplicity of the procedure rather than to give new results or extensive tables, we limit ourselves to some test examples.

A. Symmetric anharmonic-oscillator eigenvalues and eigenfunctions

As a first example, let us consider the anharmonic-oscillator eigenequation, that is the perturbed type D eigenequation $(-\infty<x<+\infty)$

$$\left\{\frac{d^2}{dx^2}-b^2x^2+b(2m+1)+V(x)+\Lambda\right\}\Psi(x)=0, \tag{15}$$

where $V(x)$ is a symmetric perturbation with perturbation terms

$$V^{(N)}(x)=b_1^{(N)}x^2+b_2^{(N)}x^4+b_3^{(N)}x^6+\cdots .$$

When $V(x)=0$, this eigenequation (15) reduces to an exact type D factorizable equation (see Table I). Let us assume $b>0$:[6] The factorization function $L^{(0)}(m)=-2bm$ is a decreasing function of m so that $\epsilon=-1$ and $\tilde{j}=m-v$. The unperturbed eigenvalue is $\Lambda^{(0)}=L^{(0)}(m-v)=-2b(m-v)$ and we find again the expected expression of the unperturbed harmonic-oscillator energies $E^{(0)}$, i.e., $2E^{(0)}=b(2m+1)+\Lambda^{(0)}=2b(v+\frac{1}{2})$.

Let us now consider the perturbed eigenequation (15) and, in order to avoid writing down too much extensive expressions, let us consider the x^4 anharmonic-oscillator eigenequation

$$\left\{\frac{d^2}{dx^2}-b^2x^2-2gx^4+2E\right\}\Psi(x)=0, \tag{16}$$

where the perturbation reduces to

$$V(x)=\eta V^{(1)}(x)=-2\,\eta g x^4. \tag{17}$$

When dealing with the ground state ($v=0$), since the unperturbed type D function is $F_0^{(0)}=R_0^{(0)}=-2\beta^2 u$; $S_0^{(0)}=1$ (see Table II), we set

$$F_0(x)=-2\beta^2 u+\eta R_0^{(1)}+\eta^2 R_0^{(2)}+\eta^3 R_0^{(3)}+\eta^4 R_0^{(4)}, \tag{18}$$

where

$$R_0^{(N)}=c_1^{(N)}u+c_2^{(N)}u^3+c_3^{(N)}u^5+\cdots\ .$$

When substituting for $F_0(x)$ from Eq. (18) and for $V(x)$, Λ from Eqs. (17) and (4) into Eq. (3), and then equating to zero the coefficients of η^N successively for $N=1$ *to* $N=4$, we get four linear systems of equations allowing the determination of the expansion coefficients $c_k^{(N)}$ of $R_0^{(N)}$ and of the perturbed eigenvalues $\Lambda^{(N)}$. Solving successively these systems and setting $u=x$, $\beta^2=-\epsilon b=b$, we get

$$E_0=\frac{1}{2}\,\Lambda_0=\frac{b}{2}+\eta g\,\frac{3}{4b^2}-\eta^2 g^2\,\frac{21}{8b^5}+\eta^3 g^3\,\frac{333}{16b^8}-\eta^4 g^4\,\frac{30885}{128b^{11}}, \tag{19}$$

$$\begin{aligned}F_0(x)={}&-bx-\eta g\left(\frac{x^3}{b}+\frac{3x}{2b^2}\right)+\eta^2 g^2\left(\frac{x^5}{2b^3}+\frac{11x^3}{4b^4}+\frac{21x}{4b^5}\right)\\&-\eta^3 g^3\left(\frac{x^7}{2b^5}+\frac{21x^5}{4b^6}+\frac{45x^3}{2b^7}+\frac{333x}{8b^8}\right)+\eta^4 g^4\left(\frac{5x^9}{8b^7}\right.\\&\left.+\frac{163x^7}{16b^8}+\frac{1159x^5}{16b^9}+\frac{8669x^3}{32b^{10}}+\frac{30885x}{64b^{11}}\right).\end{aligned} \tag{20}$$

When dealing with the first excited state ($v=1$), owing to the expression of the unperturbed function (see type D in Table II), we set

$$F_1(x)=\frac{1-bu^2+\eta R_1^{(1)}+\eta^2 R_1^{(2)}+\cdots}{u+\eta S_1^{(1)}+\eta^2 S_1^{(2)}+\cdots},$$

where the $R_v^{(N)}$ and $S_v^{(N)}$ are polynomials in $u=x$

When substituting this expression into Eq. (3) and multiplying both sides by $(u+\eta S_1^{(1)}+...)^2$, we obtain relations leading to the following solution

$$E_1=\frac{1}{2}\,\Lambda_1=\frac{3b}{2}+\eta g\,\frac{15}{4b^2}-\eta^2 g^2\,\frac{165}{8b^5}+\eta^3 g^3\,\frac{3915}{16b^8}-\eta^4 g^4\,\frac{520485}{128b^{11}}, \tag{21}$$

$$F_1(x)=R_1/S_1,$$

$$R_1=1-bx^2-\eta g\,\frac{7x^2}{2b^2}+\eta^2 g^2\,\frac{22x^2}{b^5}-\eta^3 g^3\,\frac{551x^2}{2b^8}+\eta^4 g^4\,\frac{298229x^2}{64b^{11}}, \tag{22}$$

$$\begin{aligned}S_1={}&x-\eta g\,\frac{x^3}{b^2}+\eta^2 g^2\left(\frac{3x^5}{2b^4}+\frac{33x^3}{4b^5}\right)-\eta^3 g^3\left(\frac{5x^7}{2b^6}+\frac{53x^5}{2b^7}+\frac{899x^3}{8b^8}\right)\\&+\eta^4 g^4\left(\frac{35x^9}{8b^8}+\frac{1119x^7}{16b^9}+\frac{8129x^5}{16b^{10}}+\frac{62367x^3}{32b^{11}}\right).\end{aligned}$$

When dealing with the second excited state ($v=2$), we set

$$F_2(x)=\frac{2b^2u^3-5bu+\eta R_2^{(1)}+\eta^2 R_2^{(2)}+\cdots}{1-2bu^2+\eta S_2^{(1)}+\eta^2 S_2^{(2)}+\cdots}$$

and we get

$$E_2=\frac{5b}{2}+\eta g\,\frac{39}{4b^2}-\eta^2 g^2\,\frac{615}{8b^5}+\eta^3 g^3\,\frac{20079}{16b^8}-\eta^4 g^4\,\frac{3576255}{128b^{11}}+\eta^5 g^5\,\frac{191998593}{256b^{14}}, \tag{23}$$

$$F_2(x)=R_2/S_2,$$

where

$$R_2=2b^2x^3-5bx+\eta g\,\frac{28x^2}{b^2}-\eta^2 g^2\,\frac{1699x}{4b^5}+\eta^3 g^3\,\frac{70\,117x}{8b^8}-\eta^4 g^4\,\frac{1375\,411x}{64b^{11}}+\eta^5 g^5\,\frac{760\,529\,019x}{128b^{14}},$$

$$\begin{aligned}S_2={}&1-2bx^2+\eta g\left(\frac{2x^4}{b}+\frac{10x^2}{b^2}-\frac{19}{2b^3}\right)-\eta^2 g^2\left(-\frac{3x^6}{b^3}-\frac{34x^4}{b^4}-\frac{577x^2}{4b^5}+\frac{611}{4b^6}\right)+\eta^3 g^3\left(\frac{5x^8}{b^5}+\frac{91x^6}{b^6}+\frac{2933x^4}{4b^7}\right.\\&\left.+\frac{11641x^2}{4b^8}-\frac{12\,571}{4b^9}\right)-\eta^4 g^4\left(\frac{35x^{10}}{4b^7}+\frac{223x^8}{b^8}+\frac{42\,373x^6}{16b^9}+\frac{293\,943x^4}{16b^{10}}+\frac{282\,701x^2}{4b^{11}}+\frac{2428\,159}{32b^{12}}\right)\\&+\eta^5 g^5\left(\frac{63x^{12}}{4b^9}+\frac{2087x^{10}}{4b^{10}}+\frac{132\,051x^8}{16b^{11}}+\frac{1287\,363x^6}{16b^{12}}+\frac{16\,439\,691x^4}{32b^{13}}+\frac{62\,324\,979x^2}{32b^{14}}-\frac{264\,159\,051}{128b^{15}}\right).\end{aligned} \tag{24}$$

It is easily checked that the expressions (19), (21), and (23) of E_0, E_1, and E_2 give again already known results.[7]

With the help of a general software system, such as *Mathematica*,[8] the computation can be performed up to higher orders N of the perturbation, higher excited states and, if required, with a more extensive perturbation $V(x)$ than expression (17), without any other special difficulty than dealing with more and more extensive expressions. Moreover, the procedure provides simultaneously the energies and the perturbed eigenfunctions $\Psi_v(x)\approx\exp\int F_v(x)dx$, which are solutions of the original eigenequation (15).

Let us remark that, when comparing the above expressions of the first-order energies with their counterparts within the traditional Rayleigh–Schrödinger framework, we get, as a byproduct, the expressions of the diagonal matrix elements $\langle x^4\rangle$ between the unperturbed harmonic oscillator functions $\Psi_v^{(0)}(x)$ of Table I

$$\langle v=0|x^4|v=0\rangle=\frac{3}{4b^2};\quad \langle v=1|x^4|v=1\rangle=\frac{15}{4b^2};$$

$$\langle v=2|x^4|v=2\rangle=\frac{39}{4b^2}.$$

This is in accordance with the known expression $\langle v|x^4|v\rangle=(3/2b^2)[\,(v+\tfrac{1}{2})^2+\tfrac{1}{4}]$.

B. Perturbed Morse-oscillator eigenvalues and eigenfunctions

We consider the perturbed type B equation

$$\left\{\frac{d^2}{dx^2}-a^2d^2e^{2ax}+a^2d(2m+1)e^{ax}+V(x)+\Lambda\right\}\Psi(x)=0 \tag{25}$$

and assume that the given perturbation is, with $u=e^{ax}$ (see type B in Table II)

$$V(x)=\eta V^{(1)}(x)=\eta a^2(g_1u+g_2u^2+g_3u^3+g_4u^4). \tag{26}$$

Since $du/dx=au$, the Riccati equation to be solved is

$$au\,\frac{dF}{du}+[F(u)]^2+U^{(0)}+V+\Lambda=0. \tag{27}$$

When dealing with the ground state ($v=0$) eigenvalues and eigenfunctions, after picking up the expression of the unperturbed function from Table II, we set

$$F_0(u)=\frac{a}{2}\,(\alpha-\beta u)+\eta R_0^{(1)}+\eta^2R_0^{(2)}+\cdots\;.$$

After substituting this expression into Eq. (27), we readily obtain the following results:

$$\begin{aligned}\Lambda_0=&-a^2m^2-a^2\eta\left\{\frac{g_1}{2d}\,(2m)+\frac{g_2}{(2d)^2}\,(2m+1)_2+\frac{g_3}{(2d)^3}\,(2m+2)_3+\frac{g_4}{(2d)^4}\,(2m+3)_4\right\}\\&-2\eta^2a^2\left\{\frac{g_1^2}{(2d)^2}+\frac{2g_1g_2}{(2d)^3}\,(4m+1)+\frac{4g_1g_3}{(2d)^4}\,(6m^2+6m+1)+\frac{4g_1g_4}{(2d)^5}\,(16m^3+36m^2+22m+3)\right.\\&+\frac{g_2^2}{(2d)^4}\,(16m^2+10m+1)+\frac{4g_2g_3}{(2d)^5}\,(24m^3+36m^2+14m+1)+\frac{4g_2g_4}{(2d)^6}\,(64m^4+184m^3+168m^2+52m+3)\\&\left.+\frac{g_3^2}{(2d)^6}\,(36m^4+90m^3+74m^2+21m+1)+\frac{8g_3g_4}{(2d)^7}\,(96m^5+384m^4+560m^3+354m^2+85m+3)\right\}+\cdots,\end{aligned} \tag{28}$$

$$\begin{aligned}F_0(u)=&a(m-du)+a\eta\left\{\frac{g_1}{2d}+\frac{g_2}{(2d)^2}\,(2m+1)+\frac{g_3}{(2d)^3}\,(2m+2)_2+\frac{g_4}{(2d)^4}\,(2m+3)_3\right.\\&\left.+\left[\frac{g_2}{2d}+\frac{g_3}{(2d)^2}\,(2m+2)+\frac{g_4}{(2d)^3}\,(2m+3)_2\right]u+\left[\frac{g_3}{2d}+\frac{g_4}{(2d)^2}\,(2m+1)\right]u^2+\frac{g_4}{2d}\,u^3\right\}+\cdots\;.\end{aligned} \tag{29}$$

For the sake of brevity, but only the expression of the first-order perturbed eigenfunction is reproduced. It has been assumed that "a" is a real constant so that we have $\alpha=2(m-v)=2m$, $\beta=2d$. $(n)_k=n(n-1)\ldots(n-k+1)$ is a generalized factorial.

When dealing with the first excited state ($v=1$), we set

$$F_1(u)=\frac{a[\alpha(\alpha+1)-(2\alpha+3)\beta u+\beta u^2+\eta R_1^{(1)}+\eta R_1^{(1)}+\cdots]}{2(\alpha+1-\beta u+\eta S_1^{(1)}+\eta S_1^{(1)}+\cdots)}$$

After substituting this expression into Eq. (27) and setting $\alpha=2m-2$, $\beta=2d$, we readily obtain the $c_k^{(N)}$ and $d_k^{(N)}$ coefficients of the $R_1^{(N)}$ and $S_1^{(N)}$ functions and the perturbed eigenvalue

$$\begin{aligned}\Lambda_1=&-a^2(m-1)^2+\eta\left\{\frac{g_1}{2d}\,(2m-2)+\frac{g_2}{(2d)^2}\,(2m+1)\right.\\&\times(2m-2)+\frac{g_3}{(2d)^3}\,4m(m-1)(2m+5)\\&\left.+\frac{g_4}{(2d)^4}\,4m(2m+1)(10m^2-22m+3)\right\}+\cdots\;.\end{aligned} \tag{30}$$

With the help of *Mathematica*, the computation can be carried out up to higher orders and higher excited states without any other difficulty than dealing, of course, with more and more cumbersome expressions.

Then, these type B results can be used in order to obtain analytical expressions of the perturbed Morse-oscillator energies and eigenfunctions. When introducing the dimensionless coordinate $x=(\mu\omega_e/\hbar)^{1/2}(r-r_e)$, the vibrational constant $\omega_e=(2D_e/\mu)^{1/2}\beta$ and the harmonicity constants $\zeta_e=\hbar\omega_e/4D_e$, the perturbed Morse-oscillator eigenequation $(0\leqslant r<\infty)$

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

$$U(r)=D_e\sum_t b_t(1-e^{-\beta(r-r_e)})^t$$

becomes $(-r_e\leqslant x<\infty)$

$$\left\{\frac{d^2}{dx^2}-\frac{1}{2\zeta_e}e^{-2(2\zeta_e)^{1/2}x}+\frac{1}{\zeta_e}e^{-(2\zeta_e)^{1/2}x}+\frac{1}{2\zeta_e}+V(x)+\frac{2}{\hbar\omega_e}E\right\}\times\Psi(x)=0, \tag{31}$$

$$V(x)=\frac{1}{2\zeta_e}\sum_t b_t(1-e^{-(2\zeta_e)^{1/2}x})^t. \tag{32}$$

When $V(x)=0$, the eigenequation (31) reduces to an exact type B factorizable equation where

$$a=-(2\zeta_e)^{1/2};\quad d=\frac{1}{2\zeta_e};$$
$$m=-\frac{1}{2}+\frac{1}{2\zeta_e};\quad \Lambda^{(0)}=\frac{2E^{(0)}}{\hbar w_e}+\frac{1}{2\zeta_e}. \tag{33}$$

Since $a=-(2\zeta_e)^{1/2}$ is a real constant, $L^{(0)}(m)=-a^2m^2$ (see Table I) is a decreasing function of m and $\Lambda^{(0)}=-a^2(m-v)^2$. Setting $m=-1/2+1/2\zeta_e$, we get the expected expression of the unperturbed Morse energy $E_v^{(0)}=\hbar w_e[v+\frac{1}{2}-\zeta_e(v+\frac{1}{2})^2]$. Note that, as usually done, it is implicitly assumed that the Ter Haar approximation[9] holds, i.e., that a sufficiently close approximation of the solution of eigenequation (31) is obtained when taking the range of x to be $)-\infty,+\infty($.

When giving to the type B parameters their actual values (33), setting $\alpha=2(m-v)$; $\beta=2d$ and introducing suitable expressions for the g_k expansion coefficients of the given perturbation (32) in a series of $e^{-x\sqrt{2\zeta_e}}$, one can use the present perturbed type B results in order to obtain analytical expressions of the perturbed Morse-oscillator energies and eigenfunctions. Particularly, one can introduce for the rotational term $(r_e/r)^2$ a rather extensive expansion and obtain elaborate expressions of the diatomic rotation–vibration energies, or one can extract the internuclear distance dependence of diatomic structure constants (fine structure, Λ-doubling, spin-rotation constants,...) from the experimental centrifugal data.[10]

C. Singular anharmonic-oscillator energies and eigenfunctions

In order to test the capabilities of the procedure when dealing with a singular potential and as a last example, let us consider the solution of the spiked anharmonic-oscillator eigenequation

$$\left\{\frac{d^2}{dx^2}-b^2x^2-\frac{\lambda}{x^4}+E\right\}\Phi(x)=0. \tag{34}$$

As already pointed out,[11] the solution of Eq. (34) can be obtained via the solution of a perturbed type C eigenequation $(0\leqslant x<\infty)$

$$\left\{\frac{d^2}{dx^2}-\frac{m(m+1)}{x^2}-b^2x^2+b(2m+1)+V(x)+\Lambda\right\}\Psi(x)=0, \tag{35}$$

where

$$V(x)=\eta V^{(1)}(x)=\eta(g_1x^{-2}+g_2x^{-4}). \tag{36}$$

When $V(x)=0$, this eigenequation reduces to an exact type C factorizable equation of Table I. Assuming $b<0$, the factorization function $L^{(0)}(m)=-4bm$ is an increasing function of m, the unperturbed eigenvalue is $\Lambda^{(0)}=-4b(m+v+1)$ and we get the expression of the unperturbed energy, i.e., $E^{(0)}(m)=b(2m+1)+\Lambda^{(0)}=-b(4v+2m+3)$.

Let us now consider, for instance, the ground state $(v=0)$ of the perturbed eigenequation (35). We set (see Table II)

$$F_0(x)=\frac{(\alpha+\frac{1}{2})-\beta x^2+\eta R_0^{(1)}+\eta^2R_0^{(2)}+\cdots}{x+\eta S_0^{(1)}+\eta^2S_0^{(2)}+\cdots}.$$

When substituting this expression into Eq. (3), multiplying both sides by $(x+\eta S_0^{(1)}+\cdots)^2$ and setting $\alpha=m+\frac{1}{2};\beta=-b$, we obtain relations leading to the following solution

$$
\begin{aligned}
E_0(m)=&-b(2m+3)+\eta\left\{\frac{2g_1b}{2m+1}-\frac{4g_2b^2}{(2m+1)(2m-1)}\right\}-\eta^2\left\{\frac{2g_1^2b}{(2m+1)^3}+\frac{16g_1g_2b^2}{(2m+1)^3(2m-1)^2}\right.\\
&\left.-\frac{16g_2^2b^3(8m^2-6m-1)}{(2m+1)^3(2m-1)^3(2m-3)}\right\}+4\,\eta^3\left\{\frac{g_1^3b}{(2m+1)^5}-\frac{4g_1^2g_2b^2(16m^2-2m+1)}{(2m+1)^5(2m-1)^3}\right.\\
&+\frac{16g_1g_2^2b^3(80m^4-168m^3-80m^2+6m+5)}{(2m+1)^5(2m-1)^4(2m-3)^2}\\
&\left.-\frac{g_2^4b^4(4096m^5-14\,080m^4+13\,312m^3-2176m^2-1024m-368)}{(2m+1)^5(2m-1)^5(2m-3)^2(2m-5)}\right\}+\cdots\,,
\end{aligned}
\tag{37}
$$

$$
\begin{aligned}
F_0(x)=&\frac{m+1}{x}+bx-\eta\left\{\left(\frac{g_2}{2m-1}\right)\frac{1}{x^3}+\left(\frac{g_1}{2m+1}+\frac{2g_2b}{(2m+1)(2m-1)}\right)\frac{1}{x}\right\}-\eta^2\left\{\left(\frac{g_2^2}{(2m-1)^2(2m-3)}\right)\frac{1}{x^5}\right.\\
&+\left(\frac{2g_1g_2}{(2m+1)(2m-1)^2}-\frac{2g_2^2b(6m-5)}{(2m+1)(2m-1)^3(2m-3)}\right)\frac{1}{x^3}+\left(\frac{g_1^2}{(2m+1)^3}+\frac{16g_1g_2bm}{(2m+1)^3(2m-1)^2}\right.\\
&\left.\left.+\frac{8g_2^2b^2(8m^2-6m-1)}{(2m+1)^3(2m-1)^3}\,(2m-3)\right)\frac{1}{x}\right\}+\cdots\,.
\end{aligned}
\tag{38}
$$

These expressions (37) and (38) can be used in order to obtain an analytical solution of the spiked anharmonic-oscillator equation (34) when setting $g_1=m(m+1)$, $g_2=-\lambda$. Moreover, in order to deal with a core potential conveniently adapted to the perturbation, that is an unperturbed potential virtually induced by the singular potential (Klauder effect[12]), the values of m can be chosen so that they contain, in addition, a dependence upon the coupling constant λ.[11]

IV. CONCLUSION

Finally, the present procedure allows an analytical solution of perturbed eigenequations by means of very simple algebraic operations, provided these eigenequations can be conveniently described by a factorizable equation with an adequately chosen perturbation. Moreover, when using a software system such as *Mathematica* or else, for any required state, analytical expressions of the perturbed eigenvalues and perturbed eigenfunctions can be obtained up to rather high orders N of the perturbation. Nevertheless, the given perturbation $V(x)$ has to be expanded in power series of the functions $u(x)$ which are specific to each factorization type. This necessary condition is not at all fortituous or surprising. Within the perturbed ladder operator framework,[4] this is a necessary condition for building up perturbed ladder operators associated with $V(x)$ and allowing the perturbed factorization of the given eigenequation. Briefly stated, the present procedure provides, in a simple way, the results that should be obtained from more elaborate v-dependent results when giving to v its actual value. This way of doing may be very useful since, in many cases, such v-dependent results may be at disposal but only for low orders of the perturbation, or, even, are not at all available. Furthermore, the expressions of the perturbed eigenfunctions are obtained in the same batch.

Although only three illustrative examples have been worked out, the range of application of the method is rather large. Indeed, the use of perturbed model equations enables one to tackle many real problems encountered in quantum physics. Among unperturbed functions of current interest in atomic and molecular calculations, let us briefly mention that the Wigner $D^{(i)}_{m,m'}(\varphi,\theta,\phi)$ or the symmetric top functions, the associated spherical harmonic functions $Y_l^m(\theta,\varphi)$, the Pöschl–Teller functions, and more generally, the Gauss hypergeometric functions can be directly related to type A eigenfunctions while the Morse-oscillator functions and confluent hypergeometric functions belong to the family of type B functions.[1] Type C and type D factorization play a central role for harmonic-oscillator problems while type F (or type E) factorizations serve for problems involving Coulomb interactions in the usual Euclidean Space (or in a curved three space with constant curvature), either within the Schrödinger or within the Dirac framework.[1] Moreover, the use of an exactly solvable equation together with an adequate perturbation may also be of interest in order to obtain approximate analytical solutions of equations involving several other model potentials such as the Hulthén potential, the screened Coulombic potential,[13] the $\lambda x^2/(1+gx^2)$ potential[14] or the Gaussian potential.[15] Hence, in many cases, the present procedure can be used as a preliminary approach to an analytical expression of the eigenvalues and eigenfunctions which are involved in the physical modelization, before tackling a more elaborate and sophistical solution of the actual equations to be considered.

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