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Symmetrically anharmonic oscillators

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We propose a new nonrelativistic Pauli-type equation where some specific small relativistic terms are retained. With the confining potentials $V_\infty(x)$ approximated by the polynomials $V_m(x)=g_0x^2+\cdots+g_mx^{2m+2}$, $g_m>0$, the nonzero kinematical corrections T_m-T_0, where $T_m=h_0p^2+\cdots+h_mp^{2m+2}\simeq T_\infty=(\mu^2c^4+p^2c^2)^{1/2}-\mu c^2$, are added to the anharmonic-oscillator Schrödinger equation, so that the p-x symmetry typical for a harmonic-oscillator Hamiltonian is restored. As a consequence of this semirelativistic regularization, the analytic diagonalization of an entirely anharmonic Hamiltonian $H_{mm}=T_m+V_m$ in terms of the $m\times m$-matrix continued fractions is obtained. Both the auxiliary fractions and the eigenstates converge very quickly. In the cases of the bounded spectrum of H_{mm} ($m=2q$), it is proved exactly for $q=1$, 2, and 3 and conjectured for $q\geq 4$.

I. INTRODUCTION

Let us recall an introduction of the simplest anharmonic-oscillator potential $V_1=h_0x^2+h_1x^4$. The first term corresponds to the universal shape of any force V near its minimum while the second component represents the phenomenological correction of the simplest mathematical form. In the same spirit, we are permitted to complement the kinetic-energy operator $T_0=g_0p^2$, $g_0=1/2\mu$ by the first relativistic correction g_1p^4, $g_1=-1/8\mu^3c^2$. We get the simplified Pauli equation

$$H_{11}\psi=E\psi\,,\qquad H_{11}=T_1+V_1,\quad T_1=g_0p^2+g_1p^4 \tag{1.1}$$

for the "symmetrically anharmonic" oscillator which is covariant under the Fourier transformation $p\rightarrow x$.

It is rather surprising that an introduction of the physical semirelativistic correction g_1p^4 in Eq. (1.1) may be dictated also by purely formal (numerical) reasons.[1] Moreover, the use of the symmetrically anharmonic unperturbed system may simplify significantly the perturbative diagonalization of the anharmonic Hamiltonian $H_{01}=T_0+V_1$. This follows from the paper by Halliday and Suranyi[2] who have used the squared harmonic-oscillator Hamiltonian $(H_{00})^2$ in lieu of H_{11} in Eq. (1.1) to guarantee its exact solvability. In light of the results of Bender and Wu or Simon[3] concerning the divergence and asymptotic nature of the Rayleigh-Schrödinger perturbation series for the anharmonic oscillator, the symmetrization of the anharmonic Hamiltonians circumvents probably the influence of the essential singularities in the complex coupling-constant plane, so that the generalization of this technique to higher anharmonicities seems to be promising.

The solvable operators $(H_{00})^m$ contain the mixed terms x^2p^2 so that the semirelativistic interpretation of the unperturbed symmetrically anharmonic system is hindered for higher m's. At the same time, the Pauli-type analog of Eq. (1.1),

$$H_{mm}\psi=E\psi\,,\quad H_{mm}=T_m+V_m\,,\qquad T_m=\sum_{j=0}^{m}h_jp^{2j+2}\,,\quad V_m=\sum_{j=0}^{m}g_jx^{2j+2}\,, \tag{1.2}$$

seems to be difficult to solve. In fact, it is not true. The aim of the present paper is to show that Eq. (1.2) may be solved exactly by means of the Hill-determinant methods.[4-6]

The algebraic (nonperturbative) character of the formal solution of Eq. (1.2) is achieved by means of introducing the auxiliary matrix continued fractions (MCF).[5,6] We shall show in Sec. II that (1) the effective Hamiltonian $\mathcal{H}$ is defined by MCF in the finite $m\times m$-dimensional model space, (2) the exact energies are equal to the roots of the relatively simple transcendental equation, and (3) in the full Hilbert space the exact eigenstates are represented by the closed form of the Taylor-type infinite series.

The results (1)–(3) are independent of the specific interpretation of the entirely anharmonic operator H_{mm}. To provide their strict mathematical foundation, we are obliged to prove (A) the convergence of the auxiliary MCF and (B) the convergence of the infinite Taylor-type series. Of course, it must be done for each specific choice of degree m and the type of the coupling sets h_j, g_j, $j=0,1,\ldots,m$ separately.

We shall consider the operator T_m as an approximation of the relativistic prescription $T_\infty=(\mu^2c^4+p^2c^2)^{1/2}-\mu c^2$. Then we have

$$h_j=\frac{(-1)^j\rho_j}{(2\mu)^{2j+1}c^{2j}}\,,\quad \rho_j=\frac{1}{j+1}\begin{pmatrix}2j\\ j\end{pmatrix}\,,\quad j=0,1,\ldots \tag{1.3}$$

in (1.2), ρ_j are positive integers. For the odd values of m, the p-dominant term h_mp^{2m+2} has a ne-

gative sign and the continuous spectrum of the operator H_{mm} is probably not bounded from below. The nonapplicability of the unmodified formalism is illustrated in Sec. III by the simplest $m=1$ case (quartic-quartic oscillator). Although the MCF's degenerate into the classical continued fractions,[7] they are shown to diverge by oscillation. The possibility of modifying and extending the formalism is briefly discussed. The complex poles of the Green's function and the corresponding resonant states may be recovered when using the stationary-point initialization of the MCF sequence in the spirit of Ref. 8.

In Secs. IV, V, and VI, the applicability of the MCF formalism is analyzed rigorously for the semibounded operators H_{mm} with $m=2q$ and $g_m>0$. The easy proof of the convergence properties (A) and (B) for the sextic-sextic oscillator ($q=1$) is shown to be of nonmatrix, one-dimensional character (Sec. IV A). It is complemented by a thorough investigation and illustration of the numerical properties of the solution (Sec. IV B). For general q (Sec. V), the sufficient conditions (A′) and (B′) are formulated for the two convergences (A) and (B), respectively. In the single-precision computer-arithmetic, their universal numerical verification is shown to work and to give an affirmative answer for $q=1$, 2, and 3. In Sec. VI, the performance of the less straightforward but fully non-numerical exact proof is exemplified by the $q=2$ decadic-decadic solution.

II. THE SOLUTION

The linear equations of the type (1.2) may always be solved by the numerical diagonalization techniques[9] provided that the matrix elements of the operator H_{mm} are known in some basis. The distinctive features of this class of methods are the following:

(N1) The necessity to work simultaneously with the $N\times N$-dimensional arrays of the interrelated elements, $N\gg 1$.

(N2) The approximate character of the solution because the limit $N\to\infty$ cannot be properly defined.

On the opposite side of the methodical scale, we may find the closed solutions of some specific equations, usually in terms of the special functions. Their characteristic features are the following:

(C1) The possibility of reducing the original equation to the two-term recurrences.

(C2) Exact proofs of convergence.

(C3) The existence of different equivalent forms (power series, integral representations, etc.) of the solution displaying its different properties.

In between these two extremes lies a broad variety of further (perturbation, variational, etc.) methods. Whenever we succeed in suppressing the drawbacks (N1) and (N2) and satisfy the requirement (C2), the characteristics such as (C3) become less relevant and the obtained solution is virtually exact. In what follows, we shall present a solution of this kind.

A. Matrix representation

In the standard harmonic-oscillator basis

$$\varphi_n(x)=c_n e^{-\lambda x^2/2}H_n(x\sqrt{\lambda}),\quad n=0,1,\ldots$$
$$c_n=(2^n n!\sqrt{\pi}/\sqrt{\lambda})^{-1/2},\quad H_n(z)=(-1)^n e^{z^2}\frac{d^n}{dz^n}e^{-z^2}, \tag{2.1}$$

the matrix elements of H_{mm} are known. The explicit formulas may be easily obtained from the identity ($\sigma=\pm 1$)

$$\hat{O}_\sigma\varphi_n=b_{n-2}\varphi_{n-2}+\sigma a_n\varphi_n+b_n\varphi_{n+2},$$
$$\hat{O}_+=\lambda x^2,\quad \hat{O}_-=\frac{1}{\lambda}\frac{d^2}{dx^2}, \tag{2.2}$$
$$a_n=n+\tfrac{1}{2},\quad b_n=\tfrac{1}{2}[n(n-1)]^{1/2}.$$

In general, the matrix form of H_{mm} will thus be a band matrix with $2m+3$ diagonals since

$$H_{mm}=-\rho'\hat{O}_-^{m+1}-\cdots+\rho\hat{O}_+^{m+1} \tag{2.3}$$

(cf. the simplest example with $m=0$).

The proper choice of the "spring constant" λ in the basis (2.1) enables us to achieve $\rho'=\rho$ in (2.3). Owing to the opposite signs in (2.3) [$p^2=-(\lambda\hbar^2/2\mu)\hat{O}_-$], the two outermost diagonals become identically zero. Hence, the number of diagonals changes to $2m+1$. When the basis is divided into subgroups of $M=m$ states

$$\langle x|X_k^i\rangle=\varphi_\nu(x),\quad \nu=2M(k-1)+2(i-1)+t,$$
$$t=0,1,\quad i=1,2,\ldots,M,\quad k=1,2,\ldots \tag{2.4}$$

the even and odd indices ν become uncoupled and we arrive at the recurrent relation

$$H_{mm}|X_k^i\rangle=\sum_{j=1}^{M}(|X_{k-1}^j\rangle C_k^{ij}+|X_k^j\rangle A_k^{ij}+|X_{k+1}^j\rangle B_k^{ij}), \tag{2.5}$$
$$i=1,2,\ldots,M,\quad M=m,\quad C_{k+1}^{ij}=B_k^{ji}=(B_k^T)^{ij},\quad C_1=0$$

valid for the operator H_{mm} with the $m\times m$-dimensional matrices A, B, and C. For the sake of brevity we shall consider the even states $t=0$ only.

B. The model-space formulation

The band structure of the matrix representation of H_{mm} is very similar to that of H_{0m} obtained by

Graffi and Grecchi in Ref. 5. The same formal representation of the Green's function matrix

$$P_1 \frac{1}{E - H_{mm}} P_1 = F_1(E), \quad P_1 = \sum_{j=1}^{M} |X_1^j\rangle\langle X_1^j| \tag{2.6}$$

may be used. It is a matter of simple algebra[6] to show that the $m\times m$ matrix $F_1(E)$ is defined by the recurrent relations

$$F_k(E) = [EI - A_k - B_k F_{k+1}(E) C_{k+1}]^{-1}, \quad k = N, N-1, \ldots, 1 \tag{2.7}$$

in the limit $N \to \infty$. The trivial initialization $F_{N+1} = 0$ corresponds to the truncation of the basis (2.1) at the cutoff $N \gg 1$, in the spirit of the numerical methods. Then, by analogy with the $M = 1$ case,[7] we may call the quantities $F_k(E)$ the generalized (matrix) continued fractions (MCF).

The existence of the MCF sequence $F_k(E)$ in the vicinity of the Green's function pole $E = E_0$ (eigenvalue of H_{mm}) is a nontrivial assumption. Considering the projected operators

$$(1 - P_K) H_{mm} (1 - P_K), \quad P_K = \sum_{k=1}^{K} \sum_{j=1}^{M} |X_k^j\rangle\langle X_k^j|, \quad K \geq 1, \tag{2.8}$$

we cannot *a priori* exclude, for some "exceptional" operators H_{mm}, the random coincidence of the poles E_0 of the two Green's functions $\det F_1(E)$ and $\det F_{K+1}(E)$. This would mean that $F_{K+1}(E)$, $F_K(E)$, ... are not defined by relations (2.7) for $E = E_0$. Graffi and Grecchi restrict the class of H's to exclude the exceptional operators. In the present context, we prefer to treat the exceptional H_{mm}'s by the inessentially modified MCF method described in Ref. 10. It will not be introduced here because of its rather formal character. We may summarize this discussion in the form of the following:

Lemma 1. The discrete spectrum $\{E_0\}$ of H_{mm} is defined by the roots of the model-space secular determinant $\det 1/F_1(E)$, i.e.,

$$\det(EI - \mathcal{H}) = 0, \quad \mathcal{H} = A_1 + B_1 F_2(E) C_2, \tag{2.9}$$

provided that the MCF expansion of $F_2(E)$ converges [assumption (A) of Sec. I] and the operator H_{mm} is not exceptional, $\det 1/F_k(E_0) \neq 0$, $k > 1$.

Of course, the effective Hamiltonian $\mathcal{H}$ entering Eq. (2.9) may also be used to define the model-space projections $\langle X_1^i|\psi\rangle = \mathcal{X}^i$ of the exact eigenstates $|\psi\rangle$ of H_{mm}. According to Ref. 6, we shall write the corresponding model-space Schrödinger equation in the form

$$\sum_{i=1}^{M} \mathcal{X}^i (E\delta_{ij} - \mathcal{H}_{ij}) = 0, \quad j = 1, 2, \ldots, M \tag{2.10}$$

and have

Lemma 2. The eigenstates $|\psi\rangle$ of H_{mm} corresponding to the eigenvalue E_0 are defined by the infinite Taylor-type series

$$|\psi\rangle = \sum_{i=1}^{M} \mathcal{X}^i \sum_{k=1}^{\infty} \sum_{j=1}^{M} |X_k^j\rangle D_k^{ij},$$

$$D_1^{ij} = \delta_{ij}, \quad D_k^{ij} = (L_2 L_3 \cdots L_k)^{ij}, \tag{2.11}$$

$$L_k = B_{k-1} F_k(E_0)$$

provided that it is well defined (cf. lemma 1) and convergent [assumption (B) of Sec. I]. This assertion may be verified in a straightforward way, employing only Eq. (1.2) and the recurrences (2.5) and (2.7).

III. THE QUARTIC-QUARTIC OSCILLATORS

The simplest special case of the symmetrically anharmonic operator H_{mm} reads ($a \neq 0$)

$$H_{11} = -\frac{\hbar^4}{8\mu^3 c^2}\frac{d^4}{dx^4} - \frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 + \frac{2}{c^2}\mu a^4 x^4. \tag{3.1}$$

Formally, we may illustrate by it the detailed structure of Eq. (2.3):

$$H_{11} = -\eta\hat{O}_-^2 - \beta\hat{O}_- + \gamma\hat{O}_+ + \eta\hat{O}_+^2,$$

$$\eta = \frac{\hbar^2 a^2}{2\mu c^2}, \quad \beta = \hbar a, \quad \gamma = \frac{\hbar\omega^2}{4a}, \quad \lambda = \frac{2\mu a}{\hbar}, \tag{3.2}$$

and of the matrix elements of H_{mm}, $m = 1 = M$,

$$\langle X_k|H_{11}|X_k\rangle = (\gamma + \beta)(2k - \tfrac{3}{2}) = A_k,$$

$$\langle X_k|H_{11}|X_{k+1}\rangle = \langle X_{k+1}|H_{11}|X_k\rangle = B_k = C_{k+1} \tag{3.3}$$

$$= [2k(2k-1)]^{1/2}[(4k-1)\eta + (\gamma - \beta)/2].$$

Since $m = 1$, the corresponding auxiliary MCF's $F_k(E)$ degenerate into the classical continued fractions and their well-established theory[7] may be applied. As already mentioned in Sec. I, we must stop at this point, the method of Ref. 6 is not applicable to the odd-m operators $H_{2q+1,2q+1}$. Really, performing the Fourier transform $x \to p$, we get "potential" $V(p)$ decreasing quickly for large p so that the spectrum of the operator (3.1) is not bounded from below.

From the physical point of view, the possible discrete resonant states of H_{11} are still of interest. In fact, the "spurious" negative-energy eigenstates of H_{11} originate from the "wrong" truncation of the expansion T_∞ and may be ignored. At the same time, the small imaginary part of the energy E_0 is irrelevant. It is part of the overall uncertainty caused by those relativistic corrections which are neglected.

We devote this separate section to H_{11} to outline

briefly the interesting and quite natural extension of the MCF method, which could enable us to cover the full class of the symmetrically anharmonic oscillators in the future. Here, we shall not go into details because the strict foundation of this extension represents a subtle problem of mathematical rather than physical character.

First, we realize that the very formulation of the problem must be modified. Owing to the presence of the perturbation $H_{11}-H_{01}\sim -d^4/dx^4$, any discrete state may decay and must therefore correspond to the complex energy E_0. The simple-minded finite truncation N of the basis and *a fortiori* any real initialization F_{N+1} of the sequence F_k may lead to oscillations and it need not even define uniquely the Green's function $\det F_1(E)$.

Being inspired by the papers employing the many-term recurrences[11] we contemplate weakening the assumption (A) of Sec. I. In the asymptotic region, we transform the MCF $F_k(E)$, $k\gg 1$ into the convergent series expansion, e.g. in the powers of $1/k$. This expansion is employed to initialize the recurrence (2.7).

In accordance with Ref. 8, the first-order approximation to $F_{N+1}(E)$ will be represented by the stationary ("fixed") point $F_{k(\mathrm{st})}(E)$ of the mapping $F_{k+1}\to F_k$ at $k=N+1$. For the convergent MCF, a stable root of the corresponding quadratic equation $F_{K+1}=F_k=F_{k(\mathrm{st})}$ is to be chosen.[8] In the present application, none of the two roots $F_{k(\mathrm{st})\pm}(E)=-\pm i/B_{k-1}$ is stable. As expected, this implies the oscillatory divergence of MCF $F_1(E)$.

The next term of the asymptotic expansion of $F_k(E)$ may be obtained in the same way. Considering the asymptotically k-independent quantities $L_k=B_{k-1}F_k(E)$, we have the first-order terms specified exactly by the formula

$$L_{k(\mathrm{st})\pm}=L^{(1)}_{k(\mathrm{st})\pm}=\frac{A_k-E}{2B_k}(\pm i\sinh\tau_k-1)\,,\qquad \cosh^2\tau_k=\frac{4B_{k-1}B_k}{(A_k-E)^2}\,. \tag{3.4}$$

It is easy to demonstrate that the subtraction of this dominant term does not define the stationary MCF $L^{(2)}_{k\pm}=L_k-L^{(1)}_{k(\mathrm{st})\pm}$ since

$$L^{(2)}_{k\pm}=L^{(2)}_{k+2\pm}\left[1\pm i\frac{\beta+\gamma}{2k\eta}+O(k^{-2})\right]. \tag{3.5}$$

This means that the $O(1/k)$ component of $L^{(2)}_{k\pm}$ does not decrease and the verification of the assumption (A) remains open. Hence, the same subtraction procedure must be iterated. Of course, the higher-order stationary roots $L^{(2)}_{k(\mathrm{st})\pm}$, $L^{(3)}_{k(\mathrm{st})\pm},\ldots$, are determined uniquely by the requirement of their smallness.

The expansion $L_{k\pm}=L^{(1)}_{k(\mathrm{st})\pm}+L^{(2)}_{k(\mathrm{st})\pm}+\cdots$ defines the two possible initializations of MCF sequence L_n, $n<k$, and leads presumably to the two complex energies E_0 and E_0^*. They may of course lie on different (physical or unphysical) sheets in the energy plane. It is important to note that the interpretation of the corresponding states $|\psi\rangle$ as resonances is not contradictory because their norm

$$\langle\psi|\psi\rangle=\mathrm{const}\sum_{k=1}^{\infty}|D_k|^2 \tag{3.6}$$

is a finite number. The proof of the convergence of the infinite series (3.6) follows from the estimate

$$|L^{(1)}_{k\pm}|=1-\frac{\mathrm{Re}[E/(\beta+\gamma)]+\frac{17}{8}}{k}+O\left(\frac{1}{k^2}\right), \tag{3.7}$$

which satisfies Raabe's criterion for $E/(\beta+\gamma)>-\frac{9}{8}$.

IV. THE SEXTIC-SEXTIC OSCILLATORS

A. Convergence of the solution

The solution of the symmetrically anharmonic oscillator Eq. (1.2) of the order $4q+2$ with an integer $q=m/2=1,2,\ldots$ is formally represented by Eqs. (2.9) and (2.11), in accord with lemmas 1 and 2 of Sec. II. It becomes exact when we prove the assumptions (A) and (B) concerning the convergence of MCF and ψ, respectively. In the remaining parts of the paper, we shall present the separate proofs for the first few q's. Let us start with $q=1$. From the form ($b\neq 0$)

$$\begin{aligned}H_{22}&=-\frac{\hbar^6}{16\mu^5c^4}\frac{d^6}{dx^6}+H_{11}+\frac{4\mu b^6}{c^4}x^6\\&=-\rho\hat{O}_-^3-\eta\hat{O}_-^2-\beta\hat{O}_-+\gamma\hat{O}_++\nu\hat{O}_+^2+\rho\hat{O}_+^3\,,\\ \rho&=\frac{\hbar^3b^3}{2\mu^2c^4}=\frac{2\eta^2}{\beta}\,,\quad \eta=\frac{\hbar^2b^2}{2\mu c^2}\,,\quad \beta=\hbar b\,,\\ \gamma&=\frac{\hbar\omega^2}{4b}\,,\quad \upsilon=\frac{\hbar^2a^4}{2\mu c^2b^2}\,,\quad \lambda=\frac{2\mu b}{\hbar}\end{aligned} \tag{4.1}$$

of the sextic-sextic operator we obtain the two-dimensional model space and the MCF representation of the effective Hamiltonian $\mathcal{H}$ with the parameters

$$\begin{aligned}A_k^{ii}&=10\rho(4J^3+3J^2+2J+\tfrac{3}{8})\\&\quad+3(\nu-\eta)(2J^2+J+\tfrac{1}{4})+(\beta+\gamma)(2J+\tfrac{1}{2})\,,\\ B_k^{ii}&=\tfrac{1}{4}[(2J+1)(2J+2)(2J+3)(2J+4)]^{1/2}\\&\quad\times[3\rho(4J+5)+\nu-\eta]\,,\\ J&=2k+i-3\,,\quad i=1,2\\ A_k^{12}&=A_k^{21}=\tfrac{1}{2}[(4k-3)(4k-2)]^{1/2}[(\nu+\eta)(8k-5)+\gamma-\beta]\,,\\ B_k^{21}&=\tfrac{1}{2}[4k(4k-1)]^{1/2}[(\nu+\eta)(8k-1)+\gamma-\beta]\,,\quad B_k^{12}=0\,.\end{aligned} \tag{4.2}$$

In the $k \gg 1$ asymptotic region we get

$$A_k^{ij} = 5\rho(4k)^3\delta_{ij} + O(k^2)\,,$$
$$B_k^{ij} = \tfrac{3}{2}\rho(4k)^3\delta_{ij} + O(k^2)\,, \quad i,j = 1,2\,. \tag{4.3}$$

Owing to the presence of the Kronecker delta δ_{ij}, the mapping $L_{k+1}^{ij} \to L_k^{ij}$ may be decomposed into the pair of the two independent and identical scalar mappings numbered by the upper indices $i = j = 1,2$. The classical continued fraction methods[7] may be used. In the leading order in $1/k$, the stationary point has a simple geometric interpretation as an intersection of the two curves $L_k(L_{k+1})$ and $L_k = L_{k+1}$. Algebraically, the stable one is therefore obtained as the plus-sign root[8]

$$L_{k(\mathrm{st})}^{ij} = \frac{-5 + (25-9)^{1/2}}{3}\delta_{ij} = -\frac{\delta_{ij}}{3} = L_{k(\mathrm{st})+}^{(1)} \tag{4.4}$$

of the pair of the identical and uncoupled quadratic equations $L_{k+1}^{ij} = L_k^{ij} = L_{k(\mathrm{st})}^{ij}$. In this way, the assumptions (A) and (B) are proved since $L_{k+}^{(2)} = O(1/k)$ and $|L_{k+}^{(1)}| < 1$, respectively.

The formal discussion of the $q = 1$ case is finished. Nevertheless, since H_{22} is the simplest representative of the entirely anharmonic oscillators, we feel that it is necessary to complement the formal proof by a numerical example. Actually, this is somewhat related to the requirement (C3) of Sec. II since the properties of the computational algorithms specify the real range of applicability of the abstract solution.

B. The numerical example

The MCF-based algorithms are extremely compact and may be implemented even on the programmable pocket calculators. In this respect they are able to compete even with the special function solutions. Owing to the extremely favorable convergence rates of both the MCF representation of the exact effective Hamiltonian $\mathcal{H}$ and the Taylor-type expansions (2.11) of ψ, the precise calculations are also very quick. Hence, the only important problem is the choice of the root-searching procedure solving the transcendental Eq. (2.9). In what follows, we use $\beta = \gamma = 1$, $\nu = 0$ and change η and test the cutoff $N = 50$ at the value $N = 650$.

TABLE I. Sample of the sextic-sextic ground-state energies.

η	E_0
0	1.000 000 0
4	92.698 380 15
8	373.395 369 5
12	843.087 188 2
16	1501.773 892
20	2349.455 494
24	3386.131 996
28	4611.803 402
32	6026.469 712
36	7630.130 926

The almost linear shape of the function $\det 1/F_1(E)$ for E lying below the ground-state energy E_{00} makes it easy to determine the η dependence $E_{00}(\eta)$, e.g., by the Newton method (Table I). Moreover, this dependence is very well reproduced by the empirical extrapolation formula

$$E_{on} = a_n + b_n\eta + c_n\eta^2\,,$$
$$a_0 = 0.996\,544, \quad b_0 = -0.698\,867\,5\,, \tag{4.5}$$
$$c_0 = 5.906\,0.0\,75\,.$$

At $\eta = 4$, Eq. (4.5) overestimates the correct value at the sixth digit. Only for $\eta < 4$ and especially for $\eta < 0.6$, the significant deviations from (4.5) may be detected and reach 1–2 % for $\eta \simeq 0.15$–0.10. The same holds for the excited states $n = 1,2,\ldots$ (Table II). The minima of $E_{on}(\eta)$ (Table III) occurring at $\eta_{\min} = 0.0593,\ 0.0321,\ 0.019,\ 0.014,\ldots$, deepen and shrink with the increasing level number $n = 0,1,2,3,\ldots$, respectively, and represent the boundary of the approximate validity of Eq. (4.5).

From the physical interpretation of the operator

TABLE II. The parabolic shape of the spectrum $E_{0n}(\eta)$.

Fitting points[a] η					Level	Parameters		In (4.5)
0.100	0.120	0.125	0.140	0.145	n	a_n	b_n	c_n
	×	×	×		0	0.998 77	−0.694 5	5.828 97
×	×	×			0	0.998 08	−0.683 3	5.783 2
×	×		×		1	5.015 55	−10.744 76	163.799 7
		×	×	×	2	8.875 2	−27.194	826.865
×		×		×	2	8.843 4	−26.720	825.110
		×	×	×	3	12.782 27	−62.642 7	2445.742
×	×		×		3	12.897 95	−64.247 6	2452.588 9

[a] In the remaining points, the deviations $E - E_{\mathrm{fit}}$ are of the order of 10^{-4}.

TABLE III. Low-lying spectrum of the sextic-sextic oscillator for small η's, $\nu=0$ and $\beta=\gamma=1$.

η	E_{00}-1	E_{01}-5	E_{02}-9	E_{03}-13
0.000[a]	−0.000 005[a]	−0.000 05[a]	−0.001 70[a]	0.029 94[a]
0.005	−0.003 59	−0.045 01	−0.134 68	−0.254 26[a]
0.010	−0.006 88	−0.082 52	−0.230 88	−0.413 24[a]
0.015	−0.009 84	−0.112 48	−0.286 90	−0.447 00[a]
0.020	−0.012 48	−0.134 85	−0.300 37	−0.355 54[a]
0.025	−0.014 80	−0.149 60	−0.269 23	−0.138 86
0.030	−0.016 80	−0.156 71	−0.192 46	0.203 04
0.035	−0.018 48	−0.156 14	−0.070 01	0.670 16
0.040	−0.019 83	−0.147 85	0.097 59	1.261 80
0.045	−0.020 87	−0.131 77	0.309 58	1.977 51
0.050	−0.021 60	−0.107 83	0.565 17	2.817 04
0.055	−0.022 01	−0.075 93	0.863 67	3.780 24
0.060	−0.022 13	−0.036 01	1.204 50	4.867 00
0.065	−0.021 94	0.012 03	1.587 23	6.077 19
0.120	−0.000 64	1.084 90	8.518 68	27.505 52
0.125	0.003 02	1.231 87	9.395 73	30.189 15

[a] Parabolic extrapolation.

H_{mm} it follows that the most interesting part of the spectrum is the region of the small η's ($H_{mm} \simeq H_{om-1}$ for $c \to \infty$, cf. Sec. I). Unfortunately, in this domain the tangentlike structure of the function $\det 1/F_1(E)$ changes in such a way that the Newton method becomes less effective. The peaks of $\det 1/F_1(E)$ shrink and move closer to its zeros. The grid of the test points E must be refined to detect any deviation of $\det 1/F_1(E)$ from the almost constant function. Although the second derivatives are of considerable help and the increasing slope of the peak improves the final precision, the approximate location of E_{on} becomes quite time consuming and represents the limitation of applicability of the method for $\eta \to 0$.

In practice, the fairly good results may still be obtained for $\eta=0$ and the low-lying states (cf. the harmonic-oscillator limit in Table I–III). As an independent illustration we evaluate in Table IV Green's functions for two E's and three η's. The exact value of the $\nu=0.1$ quartic-oscillator ground-state energy E_0 given by Biswas *et al.*[4] is quite well reproduced by the parabolic extrapolation of the type (4.5). It is even improved when $\sqrt{\eta}$ is used in lieu of η. In conclusion, we note that the precision of $\det 1/F_1(E)$ given in Table IV is fully reproduced by the cutoff $N=4$.

V. THE OSCILLATORS OF THE ORDER $4q+2$ AND THE CONVERGENCE PROOFS

Although the analytic theory of the MCF's is not yet worked out, their properties may be derived very easily from analogy with the scalar case.[7,8] The convergence of $\mathfrak{C}$ and ψ should be proved in the two respective steps, showing the following:

(A′) In the asymptotic region, $N \gg n \gg 1$, the values of the MCF sequence $L_{N+1}(=0), L_N, L_{N-1}, \ldots, L_n, \ldots$ accumulate near some stationary "fixed" point $L^{(1)}_{n(\mathrm{st})}$ of the mapping $L_{n+1} \to L_n$. In other words, the deviations $L^{(2)}_n = L_n - L^{(1)}_{n(\mathrm{st})}$ of the true sequence L_n from the stationary-point approximation become negligible with the increasing cutoff, $\|L^{(2)}_n\| \ll \|L^{(1)}_{n(\mathrm{st})}\|$.

(B′) The infinite series

$$Q(L) = 1 + LQ(L)L^T = 1 + LL^T + LLL^TL^T + \cdots \tag{5.1}$$

converges. This is practically equivalent to the old formulation of (B) in Sec. I since

$$\begin{aligned} \langle\psi|\psi\rangle &= \sum_{i,j=1}^{M} \mathfrak{N}^i \left(\sum_{k=1}^{\infty} D_k D_k^T\right)^{ij} \mathfrak{N}^j \\ &= \text{const} + \sum_{i,j=1}^{M} \bar{\mathfrak{N}}^i Q^{ij}(L) \bar{\mathfrak{N}}^j , \\ \bar{\mathfrak{N}}^j &= \sum_{i=1}^{M} \mathfrak{N}^i D_N^{ij} \left(1 + O\left(\frac{1}{N}\right)\right), \\ D_{N+1} &= D_N L_{N+1}, \quad L_{N+1} \sim L_N, \quad M = 2q . \end{aligned} \tag{5.2}$$

We intend now to describe the sufficient conditions for (A′) and (B′) and the general method of their verification. Hence, let us consider the dominant terms of the matrix elements of H_{2q2q} (2.3) with $\rho' = \rho$:

$$\begin{aligned} A_k^{ij} &= 2\rho(kM)^{M+1} \begin{pmatrix} 2M+2 \\ M+1-|i-j| \end{pmatrix} \pi_{ij} + O(k^M) , \\ B_k^{ij} &= 2\rho(kM)^{M+1} \begin{pmatrix} 2M+2 \\ 1+i-j \end{pmatrix} \pi_{ij} + O(k^M) . \end{aligned} \tag{5.3}$$

Owing to the parity decoupling ($\pi_{ij}=0$ for $|i-j|$

TABLE IV. Numerical deviation of the nonrelativistic limit $E_{00}(\eta)$, $\eta \to 0$ from the exact (Ref. 4) anharmonic-oscillator energy $E_0 = 1.065\,285\,5$ ($\nu=0.1$).

η	0.05	0.0005	0.000 005	0
$\det 1/F_1(E_0)$	−0.138 07	−0.002 30	−0.000 13	
$\det 1/F_1(E_0+0.002)$	−0.147 15	−0.011 82	−0.009 67	
$E_{00}(\eta) - E_0$	−0.030 41	−0.000 48	−0.000 027	
$E_{00}(0) - E_0$, parabolic extrapolation in η				−0.000 022
$E_{00}(0) - E_0$, parabolic extrapolation in $\sqrt{\eta}$				−0.000 005 2

$=$odd, $\pi_{ij}=1$ otherwise), the resulting k-independent mapping $L_{k+1}\to L_k$ may be decomposed into the two identical mappings $l\to l'$, where $l=bf$,

$$l'=-b\frac{1}{a+lb^T} \tag{5.4}$$

and, with arbitrary $y\neq 0$ (e.g., $y=1$), the quantities

$$a^{ij}=\frac{1}{y}\begin{pmatrix} & 2M+2 & \\ M+1-2|i-j| & & \end{pmatrix}, \quad b^{it}=\frac{1}{y}\begin{pmatrix} 2M+2 & \\ 1+2i-2t & \end{pmatrix},$$

$$b^{t\,i+1}=0$$

$$f^{ij}=2\rho y(kM)^{M+1}F^{pr}+O(k^{-1}), \tag{5.5}$$

$$p,r=2i,2j \text{ or } 2i-1,\quad 2j-1,\quad 1\leq t\leq i,\quad 1\leq i,j\leq q$$

are the half-dimensional matrices $q\times q$ (cf. the $q=1$ case in Sec. IV). We point out that (A′) and (B′) concern practically the Eq. (5.4) only, which is independent of any dynamical details in H_{2q2q} except for the value of the dimension q. Thus, each proof of (A′) will be entirely universal and we may examine directly the numerical iteration of (5.4). In the convergent case we get the value $l=l'=l_{(\mathrm{st})}$ of the stable stationary point. The first few results obtainable in the single-precision computer-arithmetic are presented in Table V. For higher q's, due care must be paid to the sufficiency of the computer precision because of the quick growth of a and b.

As a by-product of the above procedure, the N- and E-independent initialization $L^{(1)}_{(\mathrm{st})}[=l_{(\mathrm{st})}\oplus l_{(\mathrm{st})}$, cf. (5.5)] for the MCF recurrence (2.7) is at our disposal. Its use may not only significantly shorten the energy determination, but also render possible the convergence proof of the Taylor-type series (5.1). Namely, using the identity

$$Q(L)=Q(L^n)+LQ(L^n)L^T+\cdots+L^{n-1}Q(L^n)L^{Tn-1} \tag{5.6}$$

it is sufficient to prove the smallness of the product $L^n\times L^{Tn}$ for some fixed n. More exactly, the comparison with the geometric series provides the criterion

$$\max_{\beta}\frac{\sum_{i,j=1}^{M}\beta_i(L_k^nL_k^{Tn})^{ij}\beta_j}{\sum_{r=1}^{M}\beta_r^{\,2}}=\zeta<1 \tag{5.7}$$

for the convergence of $Q(L)$. We observe that Eq. (5.7) defines the squared norm $\zeta=\|L_k^n\|^2$ of the matrix L_k^n, the value of which coincides with the maximal eigenvalue of $L_k^nL_k^{nT}$ or, equivalently, $L_k^{nT}L_k^n$. Using the stationary-point approximation $L_k\sim L_{(\mathrm{st})}$ the relevant numerical results are presented in Table VI and demonstrate the validity of the sufficient condition $\|L^n\|^2<1$ for $\langle\psi|\psi\rangle<\infty$.

The purely numerical treatment of Eq. (5.4) was chosen just because of its simplicity. Alternatively, the more rigorous approach to the matrix form of the quadratic stationary-point equation $L_{k+}=L_k$, i.e., to Eq. (5.4), $l=l'=l_{(\mathrm{st})}$, may be based on its purely algebraical solution. In the form

$$\left(l+a\frac{1}{g}\right)g\left(l^T+\frac{1}{g}a\right)=a\frac{1}{g}a-g,\quad g=b+b^T, \tag{5.8}$$

this equation is solvable and may be treated in close analogy with the scalar $q=1$ case. Introducing the $q\times q$ orthogonal matrices U and W such that

$$g=U^TSU,\quad a\frac{1}{g}a-g=WRW^T,$$

$$S^{ij}=\delta_{ij}s_i^{\,2}\sigma_i,\quad R^{ij}=\delta_{ij}r_i^{\,2}\rho_i, \tag{5.9}$$

$$\sigma_i=\pm1=\rho_j,\quad i,j=1,2,\ldots,q$$

we get the general solution of Eq. (5.8) in the form

$$l=-a\frac{1}{g}+WrZ\frac{1}{s}U \tag{5.10}$$

with the diagonal matrices $r^{ij}=\delta_{ij}r_i$ and $s^{ij}=\delta_{ij}s_i$ and with the arbitrary pseudo-orthogonal matrix Z:

$$Z\sigma Z^T=\rho,\quad \sigma^{ij}=\delta_{ij}\sigma_i,\quad \rho^{ij}=\delta_{ij}\rho_i. \tag{5.11}$$

The $q(q+1)/2$ continuous parameters in the pseudo-orthogonal matrix Z are to be fixed by the $q(q+1)/2$ restrictions guaranteeing the symmetry of the

TABLE V. Fixed points of the mapping $f_{k+1}\to f_k$, $k\gg1$.

	$q=1$	$q=2$	$q=3$
f^{11}	−0.055 56	−0.055 73	−0.007 683
f^{12}		0.035 30	0.007 069
f^{13}			−0.005 022
f^{22}		−0.078 09	−0.014 186
f^{23}			0.011 689
f^{33}			−0.017 469

TABLE VI. Eigenvalues of the matrices L^nL^{Tn}.

q	n	ζ		
1	1	0.111 111 111		
2	1	0.524 955 634	0.000 018 372	
2	2	0.043 582 891	0.000 000 002	
3	2	2 166 35	0.000 000 2	0.000 000 02
3	3	1.125 637	0.000 000 0	0.000 000 00
3	4	0.584 150	0.000 000 0	0.000 000 00

$q \times q$ matrix $f = b^{-1}l$. The first few metrics σ and ρ are given in Table VII. Its reliability was checked by the precision test $\mathrm{tr}S = 4q(2q+1)$.

In conclusion, we conjecture that for each q, the sign freedom which remains present in the resulting stationary solutions $l_{(\mathrm{st})}$ will be completely removed by the stability (i.e, convergence) requirement (A′) and that this unique solution defines also the convergent eigenstate ψ in accordance with the assumption (B′). A detailed proof of this conjecture for the first nontrivial $q = 2$ case is presented in the next section. The validity for $q = 3$ is strongly supported by the preceding numerical proof. The necessity to increase the computer precision for $q \geq 4$ cases is compatible with the rough estimate $(l + a/g)_{jj'} = O(r_j/s_{j'})$ [cf. Eq. (5.10) and Table VII].

VI. THE DECADIC-DECADIC OSCILLATORS

Besides the sextic-sextic oscillator, also the decadic-decadic solution may be defined by wholly non-numerical means since the algebraic diagonalization of the 4×4-dimensional effective Hamiltonian $\mathcal{H}$ can be performed in radicals. In principle, it is not difficult to derive also the asymptotic expansion of the type $L_N = L^{(1)}_{(\mathrm{st})} + L^{(2)}_{N(\mathrm{st})} + \cdots$, which initializes efficiently the Green's function MCF. Finally, the algebraic proof of convergences (A′) and (B′) is still rather straightforward. This will be present in detail to illustrate and support the numerical conclusions and conjectures of the preceding section.

According to the general formalism, we may put $y = 2M + 2$ in (5.5) and get

$$U = U^T = W = W^T = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \tag{6.1}$$

so that

$$s_1^2 = 14, \quad s_2^2 = 10, \quad r_1^2 = s_1^2 \sinh^2\gamma, \quad r_2^2 = s_2^2 \sinh^2\delta,$$
$$\cosh\gamma = \tfrac{12}{14}(3 + \tfrac{1}{10}) > \cosh\delta = \tfrac{12}{10}(1 + \tfrac{1}{10}), \tag{6.2}$$
$$\sigma_1 = \rho_1 = 1, \quad \sigma_2 = \rho_2 = -1.$$

From (5.10) and with the $\pm$ sign freedom in s_1, s_2, γ, and δ we get

$$l = U \begin{bmatrix} \sinh\gamma \cosh\alpha - \cosh\gamma & \frac{s_1}{s_2}\sinh\gamma \sinh\alpha \\ \frac{s_2}{s_1}\sinh\delta \sinh\alpha & \sinh\delta \cosh\alpha + \cosh\delta \end{bmatrix} U. \tag{6.3}$$

The symmetry of $f = b^{-1}l$ implies that

$$\cosh\alpha + \frac{2s_1 s_2}{s_1^2 + s_2^2}\sinh\alpha = \tanh\frac{\gamma - \delta}{2}. \tag{6.4}$$

This is the quadratic equation for e^{α} with the pair of solutions $\alpha(\epsilon)$, $\epsilon = \pm 1$,

$$\cosh\alpha = 36\left[\tanh\frac{\gamma-\delta}{1} - \frac{\epsilon s_1 s_2}{12}\left(\tanh^2\frac{\gamma-\delta}{2} - \frac{1}{36}\right)^{1/2}\right],$$
$$\sinh\alpha = 36\left[-\frac{s_1 s_2}{12}\tanh\frac{\gamma-\delta}{2} + \epsilon\left(\tanh^2\frac{\gamma-\delta}{2} - \frac{1}{36}\right)^{1/2}\right]. \tag{6.5}$$

Of course, not all of the free $\pm$ signs in s_1, s_2, γ, δ, ϵ, and α are independent. Firstly, s_1, s_2, and

TABLE VII. Structure of the auxiliary matrices S and R.

q	σ_i	ρ_i	$\sigma_i \max s_i^2$	$\sigma_i \min s_i^2$	$\rho_i \max r_i^2$	$\rho_i \min r_i^2$
1	+	+	12		$\frac{64}{3}$	
2	+−	+−	140	−100	$\frac{14848}{175}$	∼−74.24
3	+−−	+−−	$\sim 2\times10^3$	∼−96.61	$\sim -10^6$	$\sim 3\times10^3$
4	++−−	+−−−	$\sim 3\times10^4$	1050	$\sim -2\times10^6$	$\sim -10^4$
5	+++−−	++−−−	$\sim 5\times10^5$	$\sim 6\times10^2$	$\sim 5\times10^8$	$\sim -10^5$
6	+++−−−	++++−−	$\sim 8\times10^6$	$\sim -8\times10^3$	$\sim 10^{10}$	$\sim 10^6$
7	+++−−−−		$\sim 10^8$	$\sim -4\times10^3$	$\sim -3\times10^{12}$	$0(10^7)$
8	++++−−−−		$\sim 2\times10^9$	$\sim 5\times10^4$		
9	+++++−−−−		$\sim 3\times10^{10}$	$\sim 2\times10^2$		
10	+++++−−−−−		$\sim 5\times10^{10}$	$\sim -3\times10^5$		

α enter Eq. (6.3) in the form of product, and we may put $s_1>0$, $s_2>0$. Secondly, $\cosh\alpha \geq 1$ in (6.5) implies that $\gamma>\delta$, i.e., $\gamma>0$. Thirdly, the solution of (6.4) has the property $\alpha(\epsilon, s_1 s_2) = -\alpha(-\epsilon, -s_1 s_2)$ and $\epsilon = \mathrm{sign}\alpha$. Finally, the two eigenvalues of $l^n l^{nT}$ or, equivalently,

$$l^{nT} l^n \left[= 2 \begin{pmatrix} u & v \\ v & w \end{pmatrix} \right]$$

are $\epsilon_{1n}, \epsilon_{2n}$,

$$\epsilon_{1n} = u + w + [(u-w)^2 + 4v^2]^{1/2} > \epsilon_{2n}$$
$$= u + w - [(u-w)^2 + 4v^2]^{1/2} > 0 \qquad (6.6)$$

[cf. (6.3)]. It is rather tedious but straightforward to show that ϵ_{1n} is greater than one and increases with the increasing power n except when $\delta<0$ and $\epsilon>0$. Hence, the sign freedom is eliminated completely and $l_{(\mathrm{st})}$ is uniquely defined by (6.3). The numerical value (6.6) of $\epsilon_{11}(\delta<0,\ \epsilon>0)$ $=0.524\,955\,634$ strictly confirms the convergence (B′) of ψ and the corresponding numerical results of Tables V and VI.

An elegant non-numerical proof of (A′) is closely related to the preceding discussion. When we put $l_k = l_{(\mathrm{st})} + \Delta_k / b^T$, the insertion into (2.7) gives the exact MCF recurrent definition of the subtracted quantities $\Delta_k = b f_k^{(2)} b^T$, which implies $\Delta_k = l_{(\mathrm{st})} \Delta_{k+1} l_{(\mathrm{st})}^T + O(\Delta^2) + O((1/k)\Delta)$. Hence, $\|\Delta_k\| \leq \|L\| \, \|\Delta_{k+1}\| \, \|L^T\| \, [1 + O(1/k)]$ and the smallness (5.7) of the eigenvalues [i.e., (B′)] is sufficient to guarantee also the MCF convergence (A′).

VII. SUMMARY

We have presented a new phenomenological model designed to describe the particle confinement in a way closely related to the standard Schrödinger equation with the potentials of the polynomial type. It differs from the original anaharmonic-oscillator equation in the additional p-anharmonic corrections. This specific restoration of the p- and x-representation symmetry incorporates the exclusive linear harmonic oscillator into the broader class of the solvable Hamiltonians.

For definiteness, the new p-dependent terms are interpreted as the appropriately chosen subclass of the usually neglected relativistic kinematical corrections. Their influence may, among other things, represent the efficient validity test of the nonrelativistic methods in the domains which lie on the boundary between the nonrelativistic and relativistic kinematical regions (cf. quarkonium). The practical aspects of our symmetrically anharmonic oscillators may of course be complemented in the future, for example, by incorporating the mixed terms such as x^2p^2 and/or the different physical interpretations (p-dependent or nonlocal forces, dispersive influence of the medium, etc.).

The main contribution of the paper lies in the description of the nonperturbative solution method adequate to symmetrically anharmonic oscillator of the arbitrary order $4q+2$. The model-space MCF techniques of Graffi and Grecchi complemented by our recently suggested construction of the complete wave functions are strictly proved to be convergent for $q=1$, 2, and 3. We have shown that the matrix continued fractions work extremely well in the practical determination of energies, at least for the sextic-sextic oscillators.

The quick convergence and a close relation to the standard harmonic-oscillator functions are among the practical merits of introducing the small anharmonic terms $\sim p^4, p^6, \ldots$ into the Schrödinger equation. In this respect, our approach may be favorably compared with the other analytic Hill-determinant solutions such as that found recently by Singh *et al.*[12] for the sextic anharmonic oscillators in terms of the classical continued fractions.

[1] J. Killingbeck, J. Phys. A 13, 49 (1980).
[2] I. G. Halliday and P. Suranyi, Phys. Rev. D 21, 1529 (1980).
[3] B. Simon, Ann. Phys. (N. Y.) 58, 76 (1969); C. M. Bender and T. T. Wu, Phys. Rev. 184, 1231 (1969).
[4] S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, Phys. Rev. D 4, 3617 (1971); J. Math. Phys. 14, 1190 (1973).
[5] S. Graffi and V. Grecchi, Lett. Nuovo Cimento 12, 425 (1975).
[6] M. Znojil, J. Math. Phys. 18, 717 (1977); 20, 2330 (1979); 21, 1629 (1980).
[7] H. S. Wall, *Analytic Theory of Continued Fractions* (Van Nostrand, New York, 1948).
[8] M. Znojil, J. Phys. A 13, 2375 (1980).
[9] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Clarendon, Oxford, 1965).
[10] M. Znojil, J. Phys. A 11, 1501 (1978).
[11] R. Blankenbecler and R. L. Sugar, Phys. Rev. D 19, 3139 (1979); B. Ram and R. Halasa, Lett. Nuovo Cimento 26, 551 (1979).
[12] V. Singh, S. N. Biswas, and K. Datta, Phys. Rev. D 18, 1901 (1978).