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ANHARMONIC OSCILLATOR IN THE NEW PERTURBATIVE PICTURE

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Recently, Bender[1] succeeded in constructing the first integrals of the quantum quartic oscillator in the closed form. In the Heisenberg picture, it is even possible to consider a general polynomial interaction and to show that the integration of the quantum Cauchy problem remains feasible in an iterative Peano - Baker-type manner[2]. Here, we intend to restrict our attention to the one-body Hamiltonians

$$H = -\frac{1}{2m}\Delta + b|\bar{r}|^2 + d|\bar{r}|^4 , \qquad b > 0, \quad d > 0 \tag{1}$$

and, within the framework of the more traditional time-independent approach, describe a new type of construction of the corresponding bound states.

We feel inspired by the enormous popularity of the example (1) and, in particular, by the recent re-interpretation of the concept of perturbation in this context[3]. In fact, we have in mind a long-lasting challenge of interpretation of (1) as a perturbed quasi-exactly solvable system[4]. In the forthcoming text, we shall show that, although the radial form of (1), viz.,

$$H = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + br^2 + dr^4 \tag{2}$$

cannot be assigned the quasi-exact solutions itself, it may easily be interpreted as a perturbation of the slightly more complicated radial Hamiltonian[5]

$$H = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{f}{r} + ar + br^2 + cr^3 + dr^4, \tag{3}$$

where, of course, $\ell = 0,1,\ldots$ (in three dimensions) or, alternatively (in one dimension), $\ell = -1$ or 0.

In the first part of the text, we shall analyse the exact exceptional solutions - bound states of the Hamiltonian (3) -

in more detail. In the second half of our considerations, a perturbative transition from (3) to (2) will be described. A slight generalization of the standard Rayleigh - Schrődinger formalism will be needed - a core of the new Rayleigh - Schroedinger (NRS) technique will lie in the use of the so-called extended continued fractions (ECF, [6]).

A. THE CONSTRUCTION OF THE QUASI-EXACT STATES

Let us consider the Schroedinger equation

$$H\psi(r) = e\psi(r) \tag{4}$$

with the Hamiltonian operator (3) and postulate an Ansatz

$$\psi(r) = \sum_{n=0}^{\infty} p_n r^{n+\ell+1} \exp\left(-\frac{\alpha}{3}r^3 - \frac{\beta}{2}r^2 - \gamma\right) \tag{5}$$

for its bound-state solutions [5]. Obviously, the coefficients p_n must satisfy the recurrences

$$B_n p_{n+1} = D_n p_n + \sum_{j=1}^{5} C_n^{(j)} p_{n-j}, \qquad n = 0, 1, \ldots \tag{6}$$

where

$$p_{-1} = p_{-2} = \ldots = 0, \qquad p_0 \neq 0 \tag{7}$$

in such a case. Here, we shall choose the parameters $\alpha (>0)$, β and γ in (5) in such a manner that

$$\begin{aligned} C_n^{(5)} &= d - \alpha^2 = 0, \\ C_n^{(4)} &= v - 2\alpha\beta = 0, \\ C_n^{(3)} &= b - 2\alpha\gamma - \beta^2 = 0. \end{aligned} \tag{8}$$

The remaining coefficients in (6), viz.,

$$\begin{aligned} C_n^{(2)} &= 2\alpha(n+\ell) - 2\beta\gamma + a, \\ C_n^{(1)} &= 2\beta(n+\ell+\tfrac{1}{2}) - \gamma^2 - e = \bar{C}_n^{(1)} - e, \\ D_n &= 2\gamma(n+\ell+1) + f = \bar{D}_n + f, \\ B_n &= (n+1)(n+2\ell+2) \end{aligned} \tag{9}$$

will be nonzero in general.

In accord with the conclusions of ref. [7], the difference equation (6) admits a truncated-matrix re-interpretation precisely in the following two cases

(i) in the limit of an infinitely large dimension (i.e., in the framework of the so-called Hill-determinant method [8]), and

(ii) in the case of the quasi-exact state [9].

In the former context, our bound-state problem will be considered in the next Section. Now, let us consider the latter possibility, equivalent to the requirement

$$p_{N+1} = p_{N+2} = \ldots = 0, \qquad p_N \neq 0 \tag{10}$$

complementary to equation (7) above.

In the first step, we may notice easily that equation (6) becomes a trivial identity for $n > N+2$. At $n = N+2$, equation (10) implies that we must have $C_{N+2}^{(2)}$ equal to zero, i.e.,

$$a = a(N) = 2\beta\gamma - 2\alpha(N+\ell+2) \tag{11}$$

and

$$C_n^{(2)} = \bar{C}_n^{(2)} = 2\alpha(n-N-2). \tag{9a}$$

The remaining $N+2$ items (6) have to define the N independent components of the (unnormalized) eigenvector p. Hence, two algebraic relations between the independent couplings must be satisfied [9].

For the sake of brevity, let us denote

$$\mathcal{H}_U = \begin{pmatrix} \bar{D}_0 & -B_0 & & & \\ C_1^{(1)} & \bar{D}_1 & -B_1 & & \\ & \ddots & & & \\ & \bar{C}_{N-1}^{(2)} & C_{N-1}^{(1)} & \bar{D}_{N-1} & -B_{N-1} \\ & & \bar{C}_N^{(2)} & C_N^{(1)} & \bar{D}_N \end{pmatrix} \tag{12}$$

and

$$\mathcal{H}_L = \begin{pmatrix} \bar{C}_1^{(1)} & D_1 & -B_1 & \\ \bar{C}_2^{(2)} & \bar{D}_2^{(1)} & D_2 & -B_2 \\ & & \ddots & \\ & \bar{C}_N^{(2)} & \bar{C}_N^{(1)} & D_N \\ & & \bar{C}_{N+1}^{(2)} & \bar{C}_{N+1}^{(1)} \end{pmatrix} \tag{13}$$

with the bars introduced in (9) and (9a). Then, the latter two quasisolvability conditions may be written as a coupled pair of the determinantal equations

$$\det[\mathcal{H}_U - (-f)I] = 0, \qquad (14a)$$

$$\det[\mathcal{H}_L - eI) = 0 \qquad (14b)$$

which define the couplings f and energies e as functions of the dimension cut-off N again. In principle, they may happen to be complex - their reality is not a too relevant property in the present setting.

An important consequence of the vanishing determinants (14) lies in an existence of the pair of the related left eigenvectors or kets,

$$\begin{aligned} &\langle\chi_U | \mathcal{H}_U = -f \langle\chi_U | , \\ &\langle\chi_L | \mathcal{H}_L = e \langle\chi_L | . \end{aligned} \qquad (15)$$

They may be understood as $N+2$ - dimensional vectors χ with the last and first component equal to zero, respectively. They must be constructed numerically in general. Their use will simplify some of our forthcoming considerations.

B. THE NEW FORM OF PERTURBATION THEORY

In the paper [3] mentioned in the introduction of our text, the system (2) + (4) was considered in a "whacko" perturbative interpretation with the number "4" in the exponent of the anharmonicity replaced by the sum $2 + \lambda$, where λ was contemplated as a measure of a small perturbation. In such a context, it is almost boring to take (2) as a perturbed form of (3). Nevertheless, the use of the quasi-exact solvability of the latter Hamiltonian seems quite new and exciting in the anharmonic-oscillator context (see, e.g., the review of literature in [10]).

A "slightly whacko" aspect of our forthcoming construction will lie in our use of the same power-series Ansatz (5) for both the unperturbed and perturbed wavefunctions, with the capital energy E and coefficients P_n in the latter case. For the sake of definitness, let us assume that the respective Hamiltonians (3) and (2) contain the same couplings b, c (=0) and d, so that also the parameters γ, $\beta (=0)$ and $\alpha (>0)$ remain the same. The difference will be given by $a = a(N)$ and $f = f(N)$ with the fixed dimension N.

In the unperturbed case, we may denote $p_i = \langle i | q\rangle$ and rewrite (4) in the finite-dimensional, non-square-matrix form

$$T | q\rangle = eJ | q\rangle \qquad (16)$$

of the set of equations (6) with $J_{ij} = \delta_{i,j+1}$ (Kronecker). Similarly, the perturbed version of (4) (with the "capitalicized" energy

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots \qquad (17)$$

and $E_0 = e = e(N)$) will imply the "capitalicized" modification of (16),

$$(T + \lambda V) | Q\rangle = EJ | Q\rangle , \qquad (18)$$

where the column

$$|Q\rangle = |q\rangle + \lambda |Q_1\rangle + \lambda^2 |Q_2\rangle + \dots \qquad (19)$$

defines the desired or final anharmonic-oscillator coefficients $P_i = \langle i | Q\rangle$ in the Taylor series (5).

The insertion of (19) and (17) in (18) reproduces the equations (16) or (6) of the preceding Section in the zero-order approximation $\lambda = 0$. In the higher orders, we get the standard Rayleigh - Schroedinger hierarchy

$$\begin{aligned} &(T - eJ) | Q_1\rangle + (V - E_1 J) | Q_0\rangle = 0, \\ &(T - eJ) | Q_2\rangle + (V - E_1 J) | Q_1\rangle - E_2 J | Q_0\rangle = 0, \\ &\dots \end{aligned} \qquad (20)$$

where

$$\lambda V_{ij} = -a(N)\delta_{i,j+2} - f(N)\delta_{ij} , \quad i,j = 0,1,\dots \qquad (21)$$

in accord with our preceding specifications.

B1. THE First-Order Corrections

The renormalization ambiguity

$$|Q_n\rangle \to |Q_n\rangle + Z|Q_0\rangle \tag{22}$$

with arbitrary $Z \neq 0$ is an obvious consequence of (16) and of an overall recurrent structure

$$\begin{aligned}(T - eJ)|\phi\rangle + |\tau\rangle &= E_m J|q\rangle \\ |\phi\rangle &= |Q_m\rangle\end{aligned} \tag{23}$$

of each (m-th) row in (20). At $m = 1$, with the $N+3$ - dimensional vector

$$|\tau\rangle = V|q\rangle \tag{24}$$

this ambiguity does not concern the n-th row of (23) with $n \geq N+2$ only.

The matrix interpretation of the latter subset of (23) reads

$$\begin{pmatrix} D_{N+2} & -B_{N+2} & \\ C^{(1)}_{N+3} & D_{N+3} & -B_{N+3} \\ & \cdots & \end{pmatrix}\begin{pmatrix}\phi_{N+2} \\ \phi_{N+3} \\ \cdots\end{pmatrix} = \begin{pmatrix} C^{(1)}_{N+2} \\ C^{(2)}_{N+3} \\ 0 \\ \cdots \end{pmatrix}\phi_{N+1} + \begin{pmatrix}\tau_{N+2} \\ 0 \\ \cdots\end{pmatrix} \tag{25}$$

and does not contain any explicit reference to Z of (22) at all. We may also recommend the ECF matrix inversion solution of this set of equations - its convergence may easily be proved /6/.

In full extent, the explicit Z-dependence concerns the i-th row of (23) with $i = 0, 1, \ldots, N-1$. These rows define ϕ_{i+1} as a determinant (subdeterminant of $T - e\,j$) multiplied by $\phi_0 \neq 0$ /5/.

By means of the auxiliary vectors χ (15), the remaining N-th and N + 1-st rows of (23) may also be given a Z-independent form

$$\begin{aligned}\langle\chi_U|T - eJ|\phi\rangle + \langle\chi_U|\tau\rangle &= E_m\langle\chi_U|J|q\rangle, \\ \langle\chi_L|T - eJ|\phi\rangle + \langle\chi_L|\tau\rangle &= E_m\langle\chi_L|J|q\rangle .\end{aligned} \tag{26}$$

As long as our construction implies that

$$\begin{aligned}\langle\chi_U|T - eJ|\phi\rangle &= -B_N(\chi_U)_N\phi_{N+1}, \\ \langle\chi_L|T - eJ|\phi\rangle &= -B_{N+1}(\chi_L)_{N+1}\phi_{N+2} + \\ &+ [-B_N(\chi_L)_N + D_{N+1}(\chi_L)_{N+1}]\phi_{N+1}\end{aligned} \tag{27}$$

we may insert here the relation $\phi_{N+2} = \mu\phi_{N+1} + \nu$ (obtainable from (25)) and re-interpret equation (27) as a 2x2 - dimensional non-homogeneous set of equations for the quantities E_m and $\phi_{N+1} = (Q_m)_{N+1}$.

B.2. The Higher-Order Corrections

At $m > 1$, the vector $|\tau\rangle$ becomes infinite-dimensional,

$$|\tau\rangle = V|Q_{m-1}\rangle - \sum_{n=1}^{m-1} E_n|Q_{m-n}\rangle . \tag{28}$$

As a consequence, the solution of the equations of the type (25) becomes much more complicated. Fortunately, this does not influence still the solution of the $m = 2$ analogue of the system (27) too much. Moreover, the use of the auxiliary ECF quantities may simplify the infinite-dimensional limiting transitions considerably /5,6/. These technicalities already lie beyond the scope of the present paper.

C. NUMERICAL TESTS

Our construction of the new representation of anharmonic oscillators may lead to the complex representation of real numbers - the simplest example of such a spuriosity is the well-known "cassus irreducibilis" of Cardano. Of course, such a phenomenon would make our prescription less attractive - numerically, we shall therefore show that the zero-order approximants remain real. We shall pay our attention to a few examples only - after all, a complete classification of the real zero-order solutions is not our present aim.

First, we test our numerical algorithms in Tables 1 and 2. In the first Table, the $N = 0$ analytic solvability of our problem is employed. We choose $d = b = 1$, $c = 0$ and let only the angular momentum ℓ vary. In accord with the second Table, the comparison with the analytic $\ell \to \infty$ asymptotics also works very well for the different sets of couplings.

Table 1. Comparison of the numerical and analytic roots e(0) and f(0) of our coupled secular zero-order equations

l	e(0)	f(0)
	computed values	
10000	-2.50000000D-01	-1.00010000D+04
100	-2.50000000D-01	-1.01000000D+02
1	-2.50000000D-01	-2.00000000D+00
0	-2.50000000D-01	-1.00000000D+00
	exact results	
10000	-2.50000000d-01	-1.00010000d+04
100	-2.50000000D-01	-1.01000000D+02
1	-2.50000000D-01	-2.00000000D+00
0	-2.50000000D-01	-1.00000000D+00

Table 2. Similar test with $N = 1 = b$ and with the variable couplings c and d. The second row always displays the respective power - series second - order $\ell \gg 1$ asymptotic approximant

l	d	c	e(1)	f(1)
10000	1	.000	4.28246 E+01 4.28386 E+01	-1.09297 E+04 -1.09283 E+04
100	1	.000	9.99244 9.03317	-1.44711 E+02 -1.43088 E+02

Table 2 (cont.)

l	d	c	e(1)	f(1)
10000	0.01	.000	-1.57883 E+01 -1.57168 E+01	-1.00444 E+05 -1.00430 E+05
100	0.01	.000	-2.49862 E+01 -2.30000 E+01	-1.02002 E+03 -1.02000 E+03
10000	0.01	.100	9.99734 E+03 9.99071 E+03	-7.54564 E+04 -7.54308 E+04
100	0.01	.100	8.74375 E+01 9.80000 E+01	-7.64999 E+02 -7.70000 E+02

Table 3. A sample of results for $\ell = -1$ (one-dimensional ground state)

N	c	d	a(N)	e(N)	f(N)
2	.000	1.000	-6.000	-2.45288	4.89483 E-1
3	.000	1.000	-8.000	-2.97741 E-1	-1.60271
4	.000	1.000	-10.000	-5.57279	2.41352
5	.000	1.000	-12.000	-2.75759	2.52863 E-1
6	.000	1.000	-14.000	-3.49798 E-1	-2.09139
7	.000	1.000	-16.000	-6.04365	2.40505
8	.000	1.000	-18.000	-2.99766	2.41923 E-2
9	.000	1.000	-20.000	-4.02270 E-1	-2.52012
10	.000	1.000	-22.000	-6.43044	2.36283
2	.200	0.01	-.600	3.01968	3.99917 E-1
3	.200	0.01	-.800	2.99913	5.94009 E-1
4	.200	0.01	-1.000	2.95989	7.84695 E-1
5	.200	0.01	-1.200	2.90293	9.72279 E-1
6	.200	0.01	-1.400	2.82908	1.15700
7	.200	0.01	-1.600	2.73908	1.33909
8	.200	0.01	-1.800	2.63359	1.51873
9	.200	0.01	-2.000	2.51320	1.69600
10	.200	0.01	-2.200	2.37845	1.87126

In accord with Table 3, the general features of the present solutions need not be trivial in general - the Table displays certain oscillations of e(N) or f(N) with the period $\Delta N = 3$, and it also exemplifies their suppression at the different parameters, with an extreme choice of $\ell = -1$. These results are complemented by the $\ell = 0$ and $\ell = 1$ examples in Tables 4 and 5.

Table 4. A sample of results for $\ell = 0$ (the three-dimensional ground state)

N	c	d	a(N)	e(N)	f(N)
0	.000	1.000	-4.000	-2.5000 E-1	-1.0000
1	.000	1.000	-6.000	1.4202	-3.3948
2	.000	1.000	-8.000	-2.4528	4.8948 E-1
3	.000	1.000	-10.000	-2.9774 E-1	-1.6027
4	.000	1.000	-12.000	-5.5727	2.4135
5	.000	1.000	-14.000	-2.7575	2.5286 E-1
6	.000	1.000	-16.000	-3.4979 E-1	-2.0913
7	.000	1.000	-18.000	-6.0436	2.4050
8	.000	1.000	-20.000	-2.9976	2.4192 E-2
9	.000	1.000	-22.000	-4.0227 E-1	-2.5201
10	.000	1.000	-24.000	-6.4304	2.3628
0	.100	0.01	3.350	-1.2562 E+1	-7.5000
1	.100	0.01	3.150	-1.3487 E+1	-7.5184
2	.100	0.01	2.950	-1.1644 E+1	-7.2246
3	.100	0.01	2.750	2.3623 E+1	2.8582
4	.100	0.01	2.550	-1.0759 E+1	-6.9461
5	.100	0.01	2.350	-9.8154	-6.6615
6	.100	0.01	2.150	-9.9075	-6.6639
7	.100	0.01	1.950	-8.2585	-2.9955
8	.100	0.01	1.750	-9.0892	-6.3775
9	.100	0.01	1.550	-1.3357 E+1	-1.4232 E+1
10	.100	0.01	1.350	-8.3052	-6.0863

Table 5. A sample of results for $\ell = 1$ (the first excited three-dimensional bound state)

N	c	d	a(N)	e(N)	f(N)
1	.000	1.000	-8.000	-0.2500	-3.00000
2	.000	1.000	-10.000	-2.8715	0.60733
3	.000	1.000	-12.000	-0.2675	-2.75069
4	.000	1.000	-14.000	2.2429	-6.56468
5	.000	1.000	-16.000	-3.1310	0.25339
6	.000	1.000	-18.000	-0.2891	-3.38848
7	.000	1.000	-20.000	-6.5841	3.56905
8	.000	1.000	-22.000	-3.3442	-0.08139
1	.200	0.01	-.800	5.04172	0.40852
2	.200	0.01	-1.000	5.06064	0.80792
3	.200	0.01	-1.200	5.05838	1.19926
4	.200	0.01	-1.400	5.03630	1.58338
5	.200	0.01	-1.600	4.99552	1.96095
6	.200	0.01	-1.800	4.93701	2.33253
7	.200	0.01	-2.000	9.24884	2.49129
8	.200	0.01	-2.200	9.23996	3.04414

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Ангармонический осциллятор в новом построении теории возмущений

Предлагается простой новый метод построения решений уравнения Шредингера с полиномиальным потенциалом. Показывается возможность построения рядов теории возмущений, начиная с квазиточных решений. Для простоты берется только полиномиальное взаимодействие четвертой степени (плюс взаимодействие Кулона). Детально описывается конструкция квазиточного состояния нулевого порядка так же, как и его возмущений высших порядков. Новое представление решений не только чрезвычайно просто, но и полезно (например, дополняет так называемую технику определителей Хилла) и открывает новую возможность преодоления проблем с расходимостью рядов теории возмущений.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Anharmonic Oscillator in the New Perturbative Picture

A new method suitable for solving Schroedinger equations with polynomial potentials is proposed. It is based on a perturbative improvement of the quasi-exact solutions. The simple Coulomb + anharmonic oscillator is analysed in full detail, and a feasibility of the whole scheme is documented. The preliminary numerical tests are encouraging — the method may become a valuable complement and extension of the so-called Hill-determinant approach.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1989