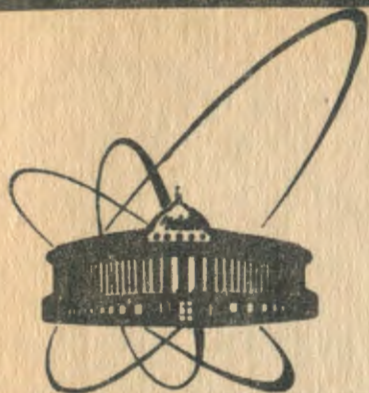


89-19



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E4-89-19

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TWO NEW TYPES OF SOLVABILITY
OF THE ONE-DIMENSIONAL
ANHARMONIC OSCILLATORS

1989

A. SCHROEDINGER PICTURE

Schroedinger equations of the type

$$-\frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x), \quad (1)$$

$$V(x) = ax + bx^2 + cx^3 + dx^4, \quad \psi(x) \in L_2(-\infty, \infty)$$

appear in the models of quantum chemistry as well as in the methodical considerations concerning the quantum field theory^{/1/}. Recently, Estrin et al.^{/2/} proposed a solution by means of a simple ansatz

$$\psi(x) = \exp(-\sigma x^2)(C_0 + C_1 x + C_2 x^2 + \dots). \quad (2)$$

After an insertion in eq. (1), the resulting recurrences for coefficients C were truncated and solved as a matrix Schroedinger equation

$$G^{(N)} \begin{pmatrix} C_0 \\ C_1 \\ \dots \\ C_N \end{pmatrix} = E \begin{pmatrix} C_0 \\ C_1 \\ \dots \\ C_N \end{pmatrix}, \quad N \gg 1, \quad (3)$$

A decisive support of such a "generalized method of Hill determinants" has been given numerically. Indeed, an outline of the rigorous proof (paralleling Ref.^{/3/}) seems insufficient: It is marred not only by imprecisions (e.g., the saddle-point estimates cease to be valid in the physical case — see a more careful discussion in the Appendix of Ref.^{/3/}; also, we have to notice that the $x \gg 1$ asymptotes $\psi(x, a, c)$ and $\psi(-x, -a, -c)$ coincide) but also by the very serious misprints: the leading-order asymptotics of coefficient should read

$$C_n^{(k)} \sim \frac{1}{\Gamma(n)^{1/3}} (d \exp 2\pi i k)^{n/6}, \quad k = 0, 1, \dots, 5; \quad n \gg 1. \quad (4)$$

This makes the related technicalities more complicated than in the $x \rightarrow -x$ symmetric case of Ref. ^{/3/}.

In a way, the difficulties of Ref. ^{/2/} with the proof of eq. (3) are closely related to the $x \rightarrow -x$ asymmetry of eq. (1), and to a rather arbitrary choice of the auxiliary exponential factor in eq. (2). This inspired our present contribution: We propose a use of a new, "discontinuous" type of ansatz

$$\begin{aligned} \psi(x) &= \psi^{(-)}(x) = e^{f(x)} (C_0 + C_1 x + C_2 x^2 + \dots), \quad x < 0, \\ \psi(x) &= \psi^{(+)}(x) = e^{g(x)} (D_0 + D_1 x + D_2 x^2 + \dots), \quad x \geq 0. \end{aligned} \quad (5)$$

For the sake of definiteness, we shall restrict our attention to the "natural", fully WKB exponentials,

$$\begin{aligned} f(x) = -g(x) &= \frac{1}{3} \alpha x^3 + \frac{1}{2} \beta x^2 + \gamma x, \\ \alpha &= |\sqrt{d}|, \quad \beta = v/2 \alpha, \quad \gamma = (b - \beta^2)/2\alpha \end{aligned} \quad (6)$$

representing the physical asymptotics of the bound states $\psi(x)$.

The main motivation of our choice of eq. (6) may be seen in a maximal simplification of the resulting recurrences

$$\tilde{Q}(\alpha, \beta, \gamma) \begin{pmatrix} C_0 \\ C_1 \\ \dots \end{pmatrix} = 0, \quad \tilde{Q}(-\alpha, -\beta, -\gamma) \begin{pmatrix} D_0 \\ D_1 \\ \dots \end{pmatrix} = 0 \quad (7)$$

obtained after an insertion of eq. (5) into eq. (1). Indeed, in contrast to the seven-term formulas of Ref. ^{/2/}, we arrive here at a four-term case,

$$\tilde{Q} = \begin{pmatrix} Q_{10} & Q_{11} & Q_{12} & & \\ Q_{20} & Q_{21} & Q_{22} & Q_{23} & \\ & Q_{31} & Q_{32} & Q_{33} & Q_{34} \\ & & & & \dots \end{pmatrix} \quad (8)$$

with the elementary matrix elements

This enables us to re-write the recurrences (7) and their matching (11) as a single, doubly infinite set of linear relations

$$Q^{(\infty, \infty)} \begin{pmatrix} \dots \\ C_{-1} \\ \\ C_0 \\ \\ C_1 \\ \dots \end{pmatrix} = 0. \quad (14)$$

Finally, we may conjecture its truncation. This leads directly to the condition

$$\det Q^{(M, N)} = 0, \quad M, N \gg 1 \quad (15)$$

as a new "Hill-determinant" specification of the binding energies. Its rigorous proof will be given elsewhere ^{/4/}.

In the conclusion, let us emphasize the following aspects of our present proposal.

(a) A formal analogy with the symmetric case and "Hill-determinant conditions" of the type (3) is preserved — the two independent $|x| \rightarrow \infty$ asymptotics in $\psi(x)$ are simply related to the two independent $M, N \rightarrow \infty$ asymptotics in eq. (15).

(b) There are no "terminating" exact solutions here. In this respect, the symmetric examples (e.g., the sextic oscillator of Singh et al. ^{/5/}) are "exceptional".

(c) Equation (15) fixes the energies. In this setting, the similar equations appearing in the Floquet theory of the so-called Hill differential equations ^{/6/} have an entirely different interpretation.

(d) Our basic idea of matching power series (5) and recurrences (7) does not seem exhausted by its present use. At least, it may be expected to work also in the straightforward polynomial-potential generalizations ^{/4/}.

B. HEISSENBERG PICTURE

Our understanding of the various quantum phenomena is often mediated by the exactly solvable models. A new approach to the simplified Hamiltonians has recently been proposed by Bender ^{/7/} who, in the Heisenberg picture, searches for integration factors of the corresponding operator evolution equations

$$i \frac{d}{dt} A(t) = [A(t), H], \quad t > 0. \quad (1)$$

In particular, a non-numerical construction of the first integrals pertinent to the operator Cauchy problem

$$\dot{q} = \frac{\partial}{\partial p} H, \quad \dot{p} = -\frac{\partial}{\partial q} H, \quad q(0) = Q, \quad p(0) = P, \quad [Q, P] = i \quad (2)$$

proved feasible for the Hamiltonian

$$H = \frac{1}{2} p^2 + \frac{1}{4} q^4 \quad (3)$$

of the quartic oscillators ^{/7/}.

In the present chapter, we intend to treat equations (2) by an alternative technique. For a class of Hamiltonians

$$H = \frac{1}{2} p^2 + \frac{1}{2} q^2 + \sum_{m=2}^M \frac{1}{m+1} \nu_m q^{m+1} \quad (4)$$

we shall consider the operator differential equations (2),

$$\frac{d}{dt} q(t) = p(t) \quad (5)$$

$$\frac{d}{dt} p(t) = -q(t) - \sum_{m=2}^M \nu_m q^m(t)$$

and show that and how the "variation of constants" idea of Peano and Baker ^{/8, 9/} may properly be generalized and employed in such a case.

In the first step, we may easily verify that the formula

$$\begin{pmatrix} q \\ p \end{pmatrix} = e^{Jt} \begin{pmatrix} Q \\ P \end{pmatrix} - \sum_{m=2}^M \nu_m \int_0^t d\tau e^{J(t-\tau)} \begin{pmatrix} 0 \\ q^m(\tau) \end{pmatrix}, \quad (6)$$

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

represents a formal solution to eq. (5). In fact, since

$$e^{Jt} = I \cos t + J \sin t$$

the latter prescription may be interpreted as a definition

$$p(t) = -Q \sin t + P \cos t - \sum_{m=2}^M \nu_m \int_0^t d\tau \cos(t-\tau) q^m(\tau) \quad (7)$$

accompanied by the ordinary (nonlinear) integral equation

$$q(t) = Q \cos t + P \sin t - \sum_{m=2}^M \nu_m \int_0^t d\tau \sin(t-\tau) q^m(\tau) \quad (8)$$

which is solvable by iterations, at least in the perturbative spirit^{/10/}.

In what follows, we may restrict our attention to the $M = 2$ case without any significant loss of the relevant details. In such a specification, our integral equation (8) reads

$$q(t) = Q \cos t + P \sin t - \nu \sin t \int_0^t \cos \tau q^2(\tau) d\tau + \\ + \nu \cos t \int_0^t \sin \tau q^2(\tau) d\tau. \quad (9)$$

Its solutions will have a structure

$$q(t) = q_0(t) + \nu q_1(t) + \nu^2 q_2(t) + \dots \quad (10)$$

with $q_0(t) = Q \cos t + P \sin t$ and

$$q_1 = \Theta(q_0^2),$$

$$q_2 = \Theta(q_0 q_1 + q_1 q_0), \quad (11)$$

$$q_3 = \Theta(q_0 q_2 + q_1^2 + q_2 q_0),$$

...

Here, the symbol Θ denotes an integral transformation $f \rightarrow \hat{f} = \Theta(f)$ where

$$\hat{f}(t) = \cos t \int_0^t \sin \tau f(\tau) d\tau - \sin t \int_0^t \cos \tau f(\tau) d\tau. \quad (12)$$

Now, our main result may be formulated as an observation of a non-numerical feasibility of the sequence of integral transformations (11).

A constructive proof of our statement is tedious but straightforward. It relies upon integrations "per partes" /11/,

$$\begin{aligned}
 & \int_0^t \tau^r \sin^m \tau \cos^n \tau d\tau \quad (= I_{rnm} = \int_0^t V_{rnm}(\tau) d\tau) = \\
 & = \frac{n-1}{m+n} I_{rnm-2} - \frac{r(r-1)}{(m+n)^2} I_{r-2mn} - \frac{rm}{(m+n)^2} I_{r-1m-1n-1} + \\
 & + \frac{1}{m+n} V_{r+1n-1}(t) + \frac{r}{(m+n)^2} [V_{r-1mn}(t) - \delta_{r1} \delta_{m0}], \quad n > 0,
 \end{aligned} \tag{13a}$$

(with Kronecker deltas δ_{ij}) and

$$\begin{aligned}
 I_{rnm} & = \frac{m-1}{m+n} I_{r-2n} - \frac{r(r-1)}{(m+n)^2} I_{r-2mn} + \\
 & + \frac{rm}{(m+n)^2} I_{r-1m-1n-1} + \frac{1}{m+n} [\delta_{r0} \delta_{m1} - V_{r-1n+1}] + \frac{r}{(m+n)^2} V_{r-1mn}, \\
 & \qquad \qquad \qquad m > 0,
 \end{aligned} \tag{13b}$$

which may be treated as recurrences with the initial values

$$I_{r00} = \frac{1}{r+1} t^{r+1}, \quad r \geq 0. \tag{14}$$

These recurrences may also be simplified: it is possible to denote $\Theta_{rnm} = \Theta(V_{rnm})$ and notice that the subtraction of integrals in eq. (12) induces a cancellation of the two inhomogeneous terms in (13a) and (13b). As a consequence, it is easy to see that we may write $\Theta_{rnm}(t)$ as a finite sum

$$\Theta_{rpq}(t) = \sum_{\substack{s,m,n \geq 0 \\ s+m+n \leq M_{rpq}}} V_{smn}(t) d_{smn}^{(rpq)} \tag{15}$$

with $M_{rpq} = r+p+q$ for $r+p+q \geq 1$. The remaining three "exceptional" cases

$$\Theta_{000}(t) = \cos t - 1, \quad \Theta_{010}(t) = \frac{1}{2}(t \cos t - \sin t), \quad \Theta_{001} = -\frac{1}{2}t \sin t \quad (16)$$

violate only slightly such a restriction. The proof is completed.

We may employ eq. (15) as an ansatz. Its insertion would convert equations of the type (13) into recurrences for the unknown coefficients d in (15). With the initial values

$$\begin{aligned} d_{000}^{(000)} &= -1, & d_{001}^{(000)} &= 1, \\ d_{010}^{(010)} &= -\frac{1}{2}, & d_{101}^{(010)} &= \frac{1}{2}, & d_{110}^{(001)} &= -\frac{1}{2} \end{aligned} \quad (17)$$

(cf. eq. (16)), these recurrences give the final solution (10), with

$$\begin{aligned} q_1(t) &= \frac{1}{3}Q^2(-1 + \cos t - \sin^2 t) + \frac{1}{3}(QP + PQ) \sin t(\cos t - 1) - \\ &- \frac{1}{3}P^2(\cos t - 1)^2, \end{aligned} \quad (18)$$

etc. Mutatis mutandis, we might study also the $M > 2$ cases — in particular, a special attention should in principle be paid to the $\nu_3 \rightarrow \infty$ limit of the $M = 3$ case where our Hamiltonian becomes just the Bender oscillator (3).

We may notice that our operator basis (products of Q 's and P 's) is similar to basis used by Bender^{/7/} or Skorobogatko^{/9/}. In the latter comparison, we may also modify our ansatz (10) and convert it into a power series in the time variable t . In the light of formulas of the type (18), we have to denote

$$U_a(t) = W_b(t) = Q^{k_1} (Pt)^{1-k_1} Q^{k_2} (Pt)^{1-k_2} \dots Q^{k_\ell} (Pt)^{1-k_\ell}, \quad (19)$$

$$a = a_\ell = k_1 2^{\ell-1} + k_2 2^{\ell-2} + \dots + k_\ell 2^0, \quad b = b_\ell = k_\ell 2^{\ell-1} + \dots + k_1 2^0, \quad \ell \geq 1$$

and introduce a new ansatz

$$\begin{aligned} q(t) &= q_0(t) + \sum_{\ell=1}^{\infty} (\nu t^2)^\ell \sum_{a=0}^{2^{\ell-1}} \sum_{b=a}^{2^{\ell-1}} [(U_a W_b + U_b W_a) c_{ab}^{(0,\ell)} + \\ &+ \nu t^2 (U_a Q W_b + U_b Q W_a) c_{ab}^{(2,\ell)} + \\ &+ \nu t^3 (U_a P W_b + U_b P W_a) c_{ab}^{(3,\ell)}]. \end{aligned} \quad (20)$$

An appropriate insertion of this series in our integral equation (9) would lead

us very close to the formulas (and, in particular, generalized continued fraction expansions) of the type studied by Skorobogatko ⁹. We may even put

$$c_{ab}^{(n, \ell)} = \sum_{m=0}^{\infty} c_{abm}^{(n, \ell)} t^{2m}, \quad n = 0, 2, 3, \quad \ell \geq 1 \quad (21)$$

and evaluate directly the Taylor coefficients $c_{abm}^{(n, \ell)}$, but this already lies beyond the scope of the present letter.

In the conclusion, let us briefly notice that the $M > 2$, $\nu=1$ recurrence relations of the type (11)

$$\begin{aligned} q_1 &= \Theta(\nu_2 q_0^2 + \nu_3 q_0^3 + \dots + \nu_M q_0^M), \\ q_2 &= \Theta(\nu_2 (q_0 q_1 + q_1 q_0) + \dots + \nu_M (q_0^{M-1} q_1 + \dots + q_1 q_0^{M-1})) \\ &\dots \end{aligned} \quad (22)$$

still remain non-numerical. In a perturbation-theory context, the possibilities of studying the $M \rightarrow \infty$ limit (nonlinear equations with, say, q^2 replaced by $\sin q$ in eq. (9)) or the systems of equations (2) (e.g., coupled oscillators) are under current investigation at present.

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Received by Publishing Department
on January 13, 1989.