сообщения
объединенного
института
ядерных
исследований
дубна

E5-87-481

M.Znojil

THE STRUCTURE OF BOUND STATES IN THE POLYNOMIAL POTENTIALS

1987

1. INTRODUCTION

In the atomic, molecular or nuclear physics, Slater determinants represent a transition to the fully correlated picture of bound states. They are usually constructed from the simple one-particle harmonic-oscillator components

$$\phi(r) = \mathcal{N}\exp(-\frac{1}{2}r^2) \sum_{m=0}^{n} \binom{n}{m} \frac{r^{2m+\ell+1}}{(m+\ell+1/2)} . \tag{1.1}$$

For some particular anharmonic Hartree-Fock potentials

$$V(r) = \sum_{m=1}^{2q+1} g_m r^{2m}, \quad g_{2q+1} > 0, \; q > 0 \tag{1.2}$$

the elementary expressions (1.1) may be generalised to the exact anharmonic particular solutions

$$\phi(r) = \exp[-P(r)] \sum_{m=0}^{N} h_m r^{2m+\ell+1} \tag{1.3}$$

with the WKB polynomial $P(r)$ [1,2]. For the general $q > 0$ force and/or more energy levels, we must consider here the $N \to \infty$ limit, of course. Even then, the truncated $N = \infty$ expansions (1.3) remain sufficiently precise in both the threshold and asymptotic regions, and remain one of the most natural descriptions of bound states.

In practice, the solution of the general anharmonic one-body Schrödinger equation

$$[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r)]\,\phi(r) = E\,\phi(r), \quad \ell = 0, 1, \ldots \tag{1.4}$$

by means of the ansatz (1.3) may lead to certain methematical difficulties [3,4]. In particular, for the present class of potentials (1.2) and WKB exponents $P(r)$ we must demand that the fources are "super-confining" [2], i.e.,

$$\lim_{r\to\infty} [V(r) - g_{2q+1} r^{4q+2}]\, r^{-2q} = +\infty . \tag{1.5}$$

Here, we intend to get rid of the puzzling restriction (1.5) by using a broader class of $P(r)$'s, and describe in detail the universal $N=\infty$ solution of the type (1.3) valid for an arbitrary polynomial potential.

The material is arranged with an emphasis put upon the general $q \geq 1$ features of the $N=\infty$ solution. Its more detailed properties may be illustrated on the simplest nontrivial examples [5].

In §2, we start our discussion by a conversion of the differential Schrödinger equation into its difference equation equivalent for coefficients h_n, $n = 0, 1, \ldots$. Their asymptotically correct form is derived as certain discrete analogue of the standard Jost solutions [6] of (1.4).

In §3, we analyse a reduction of the latter equation into a finite-dimensional matrix equation and construct the corresponding "effective Hamiltonian" $Q^{eff(N)}$. Finally, §4 delivers an alternative definition of the approximate binding energies as roots of a N+1 - dimensional determinant.

A detailed illustration of technicalities is referred to the forthcoming paper.

2. THE DIFFERENCE SCHRÖDINGER EQUATION AND ITS BOUNDARY CONDITIONS

In the trivial $q = 0$ special case of (1.2), an insertion of ansatz (1.3) in the differential equation (1.4) leads to the two-term recurrences for h_n's and to their well-known gammafunction solution (cf. (1.1)). With $q \geq 1$, the recurrences acquire a more-term character. Now, we shall show that asymptotically, they degenerate back to the solvable two-term case for all $q \geq 1$.

In the first step, we notice that our special choice of polynomials (1.2) is fully general. Indeed [2], any force regular or weakly singular in the origin may be approximated by a truncated power series, while the latter force may be replaced exactly by (1.2) after a suitable change of variables.

In the second step, we may insert our ansatz (1.3) and potential (1.2) in the radial Schrödinger equation (1.4). After a choice of the polynomial $P(r)$ in accord with the leading-order WKB asymptotic prescription,

$$P(r) = \frac{a}{2q+2} r^{2q+2} + \sum_{j=1}^{q} \beta_j \frac{r^{2j}}{2j}, \quad a = g_{2q+1}^{1/2} > 0 \qquad (2.1)$$

this converts this differential equation into its difference equation equivalent

$$B_n h_{n+1} = \sum_{j=0}^{q} C_n^{(j)} h_{n-j} + \sum_{\ell=1}^{t} D^{(\ell)} h_{n-q-\ell}, \quad n = 0, 1, \ldots , \qquad (2.2)$$

where $t \leq q$ in general.

The original interpretation of h_n's as coefficients in (1.3) introduces the natural boundary conditions "in the origin",

$$h_{-1} = h_{-2} = \ldots = h_{-q-t} = 0 \qquad (2.3)$$

and leads also to the explicit specification of the separate coefficients $B_n, C_n^{(j)}$ and $D^{(k)}$, $j = 0, 1, \ldots, q$ and $k = 1, 2, \ldots, t$. In the $n \gg 1$ asymptotic domain with $n = O(M)$ and $M \gg 1$, we may write

$$B_n = (2n+2)(2n+2\ell+3) = 4M^2 + O(M),$$

$$C_n^{(j)} = 4\beta_{j+1} M + O(1), \quad j = 0, 1, \ldots, q, \qquad (2.4)$$

$$D^{(k)} = O(1), \quad k = 1, 2, \ldots, t, \quad t \leq q,$$

where $\beta_{q+1} = a = g_{2q+1}^{1/2} > 0$, $D^{(t)} \neq 0$ and $D^{(q+1)} = 0$ due to (2.1).

In the light of (2.4), the asymptotic structure of the difference eq. (2.2) is very simple. For the smooth functions h_n, it admits in fact the two alternative possibilities of the mutual cancellation of the dominant contributions in (2.2), with

$$4M^2 h_{n+1} = 2aM h_{n-q} + \text{corrections} \qquad (2.5a)$$

or

$$4Ma h_{n-q} = D^{(t)} h_{n-q-t} + \text{corrections}. \qquad (2.5b)$$

Here, we shall asuume that $t = q$ for $D^{(q)} \neq 0$, $t = q-1$ for $D^{(q)} = 0$, $D^{(q-1)} \neq 0$, etc.

In the case (2.5a), we have $h_{n+1}/h_{n-q} = O(1/M)$ and arrive at an estimate

$$h_{M+m} \sim \left(\frac{a}{M}\right)^{m/(q+1)} + \text{corrections}. \qquad (2.6a)$$

In the complex plane, this represents precisely $q+1$ different possible asymptotics of the corresponding solutions h_n.

A similar analysis of (2.5b) recovers that $h_{n-q}/h_{n-q-t} = O(1/M)$ and leads to the further $t \leq q$ different complex roots

$$h_{M+m} \sim \left(\frac{b}{M}\right)^{m/t} + \text{corrections} \qquad (2.6b)$$

where $b = D^{(t)}/4a \neq 0$. The set may also prove empty ($t = 0$). Obviously, the latter class of solutions in asymptotically suppressed (subdominant),

$$\left| \left(\frac{a}{M}\right)^{m/(q+1)} \Big/ \left(\frac{b}{M}\right)^{m/t} \right| \sim M^{m(q+1-t)/t(q+1)} \gg 1. \qquad (2.7)$$

An algebraic independence of the $q+t+1$ roots (2.6) implies that we may use them as boundary conditions in infinity: In this interpretation, they specify a complete (fundamental) set of $q+t+1$ solutions of the linear difference equation (2.2),

$$h_n^{(d,k)} \sim \left| \left(\frac{a}{n}\right)^{n/(q+1)} \right| \exp \frac{2\pi i k n}{q+1}, \quad n \gg 1, \; k = 1,2,\dots,q+1 \qquad (2.8a)$$

(the superscript means "dominant") and

$$h_n^{(s,k)} \sim \left| \left(\frac{b}{n}\right)^{n/t} \right| \exp \frac{2\pi i k n}{t}, \quad n \gg 1, \; k = 1,2,\dots,t \qquad (2.8b)$$

(with s for "subdominant" in the sense of eq.(2.7)).

In a backward insertion of solutions (2.8) in the wavefunctions $\phi(r)$ (1.3), the subdominant components (2.8b) may be ignored as irrelevant due to their asymptotic suppression by a huge factor (2.7). For the first $q+1$ components (2.8a), we may repeat the argumentation of our preceding paper[1] – all of them generate superpositions of the growing exponentials. In the $r \gg 1$ asymptotic region, these growing exponentials may cancel in all the $k \leq q$ cases. For the real and positive coefficients $h_n^{(d,q+1)}$, there is no way how to become compatible with the standard normalization requirement $\phi(r) \to 0$ at $r \to \infty$. Indeed, this is very similar to the special harmonic oscillator case with the single root (2.6a) and with the exceptional possibility to obtain $h_n^{(d,q+1)} = 0$ indentically for all $n \geq n_0(E_0)$ (cf., e.g., Flügge, 1971).

As a consequence of the above observation, the coefficients $h_n^{(d,q+1)}$ must be discarded as unphysical from the very beginning. Of course, it is necessary thet their contribution does not become suppressed by the second-order corrections. In fact, this is an important and highly nontrivial assumption. Here, we shall take it for granted – in more detail, it will be analysed in our forthcoming papers.

From the remaining $q+t$ independent solutions (2.8), we may form the general "Jost" asymptotically admissible solution of eq.(2.2),

$$h_n^{(J)} = \sum_{m=1}^{q} a_m h_n^{(d,m)} + \sum_{m=1}^{t} b_m h_n^{(s,m)}, \quad n \geq 0. \qquad (2.9)$$

From the initial values ((2.8) at some large subscripts) it is to be specified for all n by a recurrent use of (2.2). Then, we may expect that its "physical" coefficients a_m and b_m as well as energy E will be fixed by the $q+t$ boundary conditions (2.3) in the origin.

3. THE HESSENBERG "HAMILTONIAN MATRICES"

The difference Schrödinger equation (2.2) may be visualised as an infinite-dimensional matrix diagonalisation

$$Qh = Eh, \quad h = \begin{pmatrix} h_0 \\ h_1 \\ \dots \end{pmatrix} \qquad (3.1)$$

with a $q+t+2$ – diagonal Hessenberg structure of "Hamiltonian",

$$Q = \begin{pmatrix} A_0 & -B_0 & 0 & \dots & & & & & & & \\ C_1^{(1)} & A_1 & -B_1 & 0 & \dots & & & & & & \\ \dots & \dots & & & & & & & & & \\ 0 & \dots & 0 & D^{(t)} & \dots & D^{(1)} & C_n^{(q)} & \dots & C_n^{(1)} & A_n & -B_n & 0 \dots \\ \dots & \dots & & & & & & & & & \end{pmatrix} \qquad (3.2)$$

and E-independent matrix elements ($A_n = (4n + 2\ell + 3)\beta_1$, etc.). Unfortunately, the standard truncation and further manipulations with (3.1) are not permitted in general (cf., e.g., the counterexample by Chaudhuri[4]), due to an absence of its variational background. Here, we intend to connect eq.(3.1) directly with the results of the preceding paragraph.

The special structure of Q implies that each set of the first N+1 coefficients $h_0, \dots, h_N$ satisfies the first N rows of eq.(3.1). The (N+1)-st row defines simply the new coefficient in an explicit manner,

$$h_{N+1} = \frac{h_0}{B_0 B_1 \dots B_N} \det \begin{pmatrix} A_0 - E, & -B_0, & 0, \dots & & 0 \\ & \dots & \dots & & \\ 0 & \dots 0 & D^{(t)} & \dots & A_N - E \end{pmatrix} \qquad (3.3)$$

Hence, an exact restriction of the full equation (3.1) to a finite subspace or "projection"

$$\hat{p}(N)\begin{pmatrix} h_0 \\ h_1 \\ \dots \end{pmatrix} = \hat{p}h = \begin{pmatrix} h_0 \\ \dots \\ h_N \end{pmatrix} \tag{3.4}$$

may be given the $(N+1)\times(N+1)$ - dimensional form

$$Q^{eff(N)}\begin{pmatrix} h_0 \\ \dots \\ h_N \end{pmatrix} = E\begin{pmatrix} h_0 \\ \dots \\ h_N \end{pmatrix} \tag{3.5}$$

with the reduced or "effective" Hamiltonian $Q^{eff(N)}$ and exact energies E. Of course, up to certain similarity to the variational construction of Feshbach[8], an introduction of eq.(3.5) with $Q^{eff(N)}_{m\,n} = Q_{m\,n}$ for $m<N$ and a completely unspecified last row,

$$\begin{aligned}(Q^{eff(N)}_{N\;0}, \dots, Q^{eff(N)}_{N\;N}) = (0, \dots, 0,\; X^{(t)}_N\,(=D^{(t)}),\\ X^{(t-1)}_N, \dots, X^{(1)}_N,\; Y^{(q)}_N, \dots, Y^{(1)}_N,\; Z_N)\end{aligned} \tag{3.6}$$

will prove useful only after taking into account the appropriate boundary conditions at large n.

Let us start from an arbitrary (e.g., asymptotic) Jost solution (2.9) as defined at all subscripts $n \geq M$. In principle, we may define then $h^{(J)}_{M-1}, h^{(J)}_{M-2}, \dots$ from the $(M+q+t-1)$- st, $(M+q+t-2)$ - nd, ... respective rows of eq.(3.1). In practice, this will be an unstable procedure - the subdominant components will spoil the precision of the numerical results after a few steps.

In a symmetrically reverted formulation, the computation of the determinantal coefficients (3.3) "regular in the origin" corresponds to the recurrent process $h_0 \to h_1 \to \dots$ with the numerical instabilities introduced quickly by an admixture of errors proportional to the unphysical coefficients $h^{(d,q+1)}_n$ (cf., e.g., the numerical example given by Tater[9]). Hence, we have to match the pair of boundary conditions (2.3) and (2.9) in a more symmetric manner. In this context, we may recall eq.(3.5), the first $q+t$ rows of which reflect the boundary conditions in the origin, while a flexibility of the dimension N enables us to relate the last row directly to the asymptotic estimates (2.8).

In a concise formulation, the physical solution will be given by eq.(2.9), provided that this formula satisfies eq. (3.5) with some $N \geq q+t$. This is quite a strong requirement - by the construction, the matrix elements X_N, Y_N and Z_N should not vary for any variation in the upper rows of $Q^{eff(N)}$. Of course, the latter variation would change also the coefficients a_m and b_m in (2.9). As a consequence, the last row of eq.(3.5) must be satisfied by all the individual components of $h^{(J)}_n$ separately,

$$\begin{aligned}D^{(t)} h^{(x,k)}_{N-q-t} + \sum_{j=1}^{t-1} X^{(t-j)}_N h^{(x,k)}_{N-q-t+j} + \\ + \sum_{\ell=0}^{q-1} Y^{(q-\ell)}_N h^{(x,k)}_{N-q+\ell} + (Z_N - E)\, h^{(x,k)}_N = 0.\end{aligned} \tag{3.7}$$

With $k = 1, 2, \dots, q$ for $x = d$, and $k = 1, 2, \dots, t$ for $x = s$, this formula is our most important result - as a set of the $q+t$ independent linear a algebraic equations, it defines the $q+t$ unknown effective matrix elements of $Q^{eff(N)}$ in terms of the physical Jost components $h^{(s,j)}_n$ and $h^{(d,j)}_n$ with $j \neq q+1$ and $n \geq N-q-t$.

4. THE HILL DETERMINANTS

In an intermediate domain of indices, $1 \ll n \ll \infty$, a general $(q+t+1)$- parametric solution of (2.2)

$$\sum_{m=0}^{q+t} \alpha_m h^{[m]}_n \tag{4.1}$$

may be specified, e.g., by the requirements

$$h^{[k]}_{M-1} = h^{[k]}_{M-2} = \dots = h^{[k]}_{M-q-t} = 0, \quad M = M_k. \tag{4.2}$$

With some $q+t+1$ different integers $M \gg 1$ ($M_i \neq M_j$ for $i \neq j$), it is easy to derive the small-dimensional determinantal analogues of (3.3) for the separate components $h^{[m]}_n$, and try to match (4.1) to both the boundary conditions (2.3) and (2.9) in an entirely symmetric manner. In a way, the preceding paragraph has described a large-M limit of this procedure. Now, let us consider the opposite case, with $M_0 = 0$ and all $\alpha_m = 0$, $m \neq 0$ due to (2.3). Obviously, an asymptotic matching of the "regular" solution

$$h^{[0]}_n \approx \sum_{m=1}^{q+1} \gamma_m h^{(d,m)}_n + \text{corrections}, \quad n \gg 1 \tag{4.3}$$

will be equivalent now to the condition

$$\gamma_{q+1} = 0 \qquad (4.4)$$

(cf. the text preceding eq.(2.9) above).

After an inclusion of the second order corrections in (4.3), the dominant Jost components $h_n^{(d,m)}$, $m = 1,2,\ldots,q+1$ may be further ordered in accord with their rate of decrease with the increasing index $n \gg 1$. We shall restrict our attention to the cases where $h_n^{(d,q+1)}$ becomes asymptotically dominant in this new sense. In fact, all the solutions considered in the preceding paper [2] and restricted to the "superconfining" potentials belong to this class with

$$|h_n^{(d,q+1)}| \gg |h_n^{(d,m)}|, \quad n \gg 1, \quad m = 1,2,\ldots,q. \qquad (4.5)$$

As a consequence of our assumption (4.5), the physical requirement (4.4) acquires an extremely simple interpretation:

In a vicinity of the binding energy E, the asymptotics (4.3) of coefficients $h_n^{[0]}$ must change sign. Hence, we may identify the energies with roots of determinants $h_{M+1}^{[0]}$ (cf.(3.3)) in the infinite-dimensional limit,

$$\det\begin{pmatrix} A_0 - E, & -B_0, & 0, \ldots, 0 \\ & \ldots & \\ 0, \ldots, 0, & & D^{(t)}, \ldots, A_M - E \end{pmatrix} = 0, \quad M \to \infty \qquad (4.6)$$

In this way, we arrive at the so-called Hill-determonant algorithm as proposed, e.g., by Biswas et al.[10] on the purely intuitive grounds. In the present setting, a rigorous specification of its validity is achieved.

5. SUMMARY

In contrast to the method of paper [2], we started our analysis of the rigorous difference Schrödinger equation (2.2) by emphasizing its asymptotically solvable, two-term character. For an arbitrary polynomial interaction, this enabled us to complement the natural boundary conditions "in the origin" ($h_n = 0$ for $n < 0$) by the rigorous and universal physical boundary conditions "in infinity"($n \to \infty$). In this way, the wavefunctions are transformed in a new, discrete-variable representation $h_n, n \geq 0$, and may be constructed by the straightforward algebraic techniques.

The simple realisation of such a programme was described here as a matching of the "discrete Jost solutions" (correct

at $n \gg 1$), to the boundary conditions imposed at $n = O(1)$.

In the trivial zero-order approximation, this approach degenerates to the simple Hill determinant method if applicable. As a modification of the whole technique, we could obtain and prove [11] also the analytic continued fractional technique of Wilson [12] and Singh et al.[1], as well as its simple-minded generalisations as described in our paper [2].

REFERENCES

1. Singh V., Biswas S.N., Datta K. - Phys.Rev., 1978, D18, p.1901.
2. Znojil M. - J.Phys., 1983, A16, p.213.
3. Ginsburg C.A. - Phys.Rev.Lett., 1982, 48, p.839.
4. Chaudhuri R.N. - Phys.Rev., 1985, D31, p.2687.
5. Znojil M. - Phys.Rev., 1986, D34, p.1224.
6. Newton R.G. Scattering Theory of Waves and Particles, New York, McGraw-Hill, 1982.
7. Flügge S. Practical Quantum Mechanics, Berlin, Springer, 1971.
8. Feshbach H. - Ann.Phys. (N.Y.), 1958, 5, p.357.
9. Tater M. - J.Phys., 1987, A20, p.xxx.
10. Biswas S.N., Datta K., Saxena R.P., Srivastava P.K., Varma V.S. - Phys.Rev., 1971, D4, p.3617.
11. Znojil M.-JINR communication E5-87-480, 1987.
12. Wilson A.H. - Proc.Roy.Soc.London, 1928, Ser. A 118, p.617.

Received by Publishing Department
on June 26, 1987.

Зноил М. E5-87-481

Структура связанных состояний в полиномиальных потенциалах

Обсуждается задача Шредингера для частицы в любом полиномиальном потенциале с целью получить строгое математическое обоснование ее решения при помощи степенных рядов. В рамках так называемого метода Хилла получается полное понимание границ применимости метода и его систематического улучшения.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1987

Znojil M. E5-87-481

The Structure of Bound States in the Polynomial Potentials

For an arbitrary polynomial potential, a rigorous construction of the corresponding difference Schrödinger equation and its non-variational asymptotical physical boundary conditions is given. The two alternative solution methods are also described. If applicable, the method of Hill determinants may be recovered as the simple special case.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1987