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A SIMPLIFIED FIXED-POINT PERTURBATION THEORY AND ITS APPLICATION TO THE COULOMB+SHORT-RANGE POTENTIAL

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1. Introduction

Recently, a renewed interest in diagonalizing the complicated Hamiltonians H (say, by means of the Lanczos (1950) method) appeared in connection with the field-theoretical calculations on the lattice (e.g., Duncan and Roskies 1985). An interesting feature of these calculations seems to lie in the use of the algebraic, non-numerically specified matrix elements of H. This resembles a similar assumption made within the framework of the so-called fixed-point perturbation theory (FPPT, Žnojil 1983, 1984a).

Methodically, the latter approach to the matrix Schrödinger equation

$$H\psi = E\psi \tag{1.1}$$

may be understood as a generalization: in place of the preparatory Lanczos tridiagonalization of H (via an appropriate construction of the basis), we assume that H is a band (2t + 1 - diagonal) matrix. Then, in full analogy with the continued-fractional form of the Lanczos algorithm (Wilkinson 1965), the generalized continued fractions may be used to convert the infinite-dimensional matrix H into its Feshbach (1958) finite (M x M -dimensional) "effective" equivalent H^{eff} (Graffi and Grecchi 1975, Znojil 1983,etc.).

An essence of the FPPT approach to (1.1) lies in a formal decomposition of the Hamiltonian

$$H = H_0 + H_1, \tag{1.2}$$

where H_1 is zero within a variable (M -dimensional) model space and, roughly speaking,

$$(H_0)_{mn} = H_{mn} \times (1 + O(M^{-const}))$$

for m or $n \gtrsim M$.

The detailed illustration of the FPPT treatment of the Hamiltonians

$$H = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) \tag{1.3}$$

has already been given for the trivial (t = 1) example

$$V(r) = r^2 + \frac{\lambda}{1+gr^2}, \quad g > 0 \tag{1.4}$$

(Znojil, 1984b) and for the standard test problem

$$V(r) = r^2 + \lambda r^4 \tag{1.5}$$

(with t = 2: Znojil, et al. 1985, Znojil and Tater 1986). In the present paper, we shall pay attention to the more realistic interaction

$$V(r) = \frac{a}{r} + \frac{b+cr}{1+dr^2} \tag{1.6}$$

with the Coulombic behaviour at $r \approx 0$ and $r \to \infty$.

Besides a phenomenological flexibility of our four-parametric "Padé-screened Coulomb" example (1.6) (able to simulate the non-coulombic interactions, e.g., between the atoms, molecules or nucleons), our choice is also motivated methodically. Indeed, we shall see below that the potential (1.6) gives even simpler results than (1.5). Moreover, the FPPT description of (1.6) will enable us to describe a further improvement of the formalism itself.

In § 2, we shall summarize the preparatory manipulations. First, we change the variables in (1.3) and notice that (1.6) is equivalent to the "Padé-anharmonic" generalization of (1.4),

$$V(r) = r^2 + \frac{\lambda + \mu r^2}{1+gr^4} \tag{1.7}$$

(§ 2.1). Then, we employ the Sturmian basis (cf Whitehead et al., 1982)and obtain the infinite-dimensional matrix representation

$$\sum_{n=m-t}^{m+t} A_{mn}\, \varphi_n = 0, \quad m = 0, 1, \tag{1.8}$$

of eq.(1.1) with t = 2(§ 2.2). Next, we recall the Feshbach (1958) idea of reducing (1.8) to an equivalent finite-dimensional equation (containing merely t^2 unknown "effective matrix elements; § 2.3). Finally, we notice the analogy between t = 2 potentials (1.5)-(1.7) and arrive at an appropriate ansatz for the wave functions (§ 2.4).

The detailed presentation of the simplified FPPT construction of Green's function det A and wave functions φ proceeds then in two steps. In the first one (§ 3), an appropriate change-of-index technique generates immediately an asymptotic-series form of φ. In the next step (§ 4), the finite-dimensional secular equation for energies is obtained, containing a similar asymptotic representation of the effective matrix elements. Summary of these results is given in § 5.

2. The Variable Model Space

2.1. The Change of Variables

In our equation (1.1) with $V(\infty)$ = 0 and with the negative energy $E = -k^2$,

$$\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{a}{r} + \frac{b+cr}{1+dr^2} + k^2\right)\psi(r) = 0 \tag{2.1}$$

$$d > 0, \quad \ell = 0, 1, \dots$$

we may introduce an obvious change of variables as follows:

$$r = x^2, \quad \psi(r) = x^{1/2}\varphi(x), \quad (2\ell+1)^2 = (L+1/2)^2. \tag{2.2}$$

After a scaling $x \to \rho x$ with ρ^4 = 1(4k^2), this leads to a new differential equation

$$\left(H_0 - \frac{\lambda x^2 + \mu x^4}{\eta^2 + x^4} - \nu\right)\varphi(x) = 0$$

$$H_0 = -\frac{d^2}{dx^2} + \frac{L(L+1)}{x^2} + x^2, \quad L = \frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \dots \tag{2.3}$$

where ν = $-2ak^{-1}$ represents a new energy parameter and

$\lambda = -4b/d$, $\mu = -2c/(kd)$ and $\eta = 2k/\sqrt{d} > 0$.

By means of the transition (2.1) → (2.3), we get rid of the continuous part of the spectrum in a way fully analogous to the pure Coulomb case. For the sake of simplicity, we shall simplify also the four-parametric character of (2.3): in what follows, we only consider the $\mu = \nu$ = 0 special case of (2.3) (i.e., $a = c$ = 0 in (2.1)), without any loss of generality of course.

2.2. Recurrences

After an elementary transformation of (2.3)

$$[(x^2+\varepsilon)H_0(x^2-\varepsilon) - \lambda x^2]\varphi(x) = 0, \qquad \varepsilon = i\eta \qquad (2.4)$$

(and similarly also for $\varepsilon = -i\eta$ or $\mu \neq 0 \neq \nu$ if needed), we may expand $\varphi(x)$ in the complete harmonic-oscillator basis $\{|n\rangle\}_{n=0}^{\infty}$ such that

$$\langle n|x^2|n\rangle = a_n, \qquad \langle n|x^2|n+1\rangle = b_n, \qquad H_0|n\rangle = 2a_n|n\rangle$$

and

$$a_{n\pm k} = 2n\left(1+\frac{\alpha\pm k}{n}\right), \qquad \alpha = \frac{1}{2}\left(L+\frac{3}{2}\right) = 1, 2, \qquad (2.5)$$

$$b_{n\pm k} = n\left(1+\frac{1\pm k}{n}\right)^{1/2}\left(1+\frac{2\alpha\pm k}{n}\right)^{1/2}, \qquad n, k = 0, 1, \ldots$$

In this way, equation (2.4) acquires the form (1.8) with $\langle n|\varphi\rangle = \varphi_n$;

$$\sum_{m=-2}^{+2} A_{n\,n+m}\,\varphi_{n+m} = 0, \qquad \varphi_{-1} = \varphi_{-2} = 0 \qquad (2.6)$$

$$A_{n\,n-2} = b_{n-2}\,b_{n-1}\,a_{n-1}, \qquad A_{n\,n+2} = b_n\,b_{n+1}\,a_{n+1}$$

$$A_{n\,n\pm 1} = b_{n-\frac{1}{2}\pm\frac{1}{2}}\left(a^2_{n\pm 1} + a^2_n \mp 2\varepsilon - \frac{1}{2}\lambda\right)$$

$$A_{nn} = a_n^3 + a_{n-1}b^2_{n-1} + a_{n+1}b_n^2 + a_n\eta^2 - \frac{1}{2}\lambda a_n, \qquad n = 0, 1,$$

2.3. The Feshbach Reduction of Recurrences

In the next step of our construction, let us recall the eigenvalue method of Feshbach (1958) and define the "model-space" projector

$$P = \sum_{m=0}^{n+2} |m\rangle\langle m| = 1 - Q. \qquad (2.7)$$

Then, separating (2.6) into an inner and outer part,

$$PA(P+Q)\varphi = 0 \qquad QA(Q+P)\varphi = 0$$

we may eliminate formally $Q\varphi$ from the latter relation,

$$Q\varphi = -\frac{1}{QAQ}\,QAP\varphi.$$

Its insertion into the former equation gives the final formula

$$A^{eff}\,\chi = 0$$

$$A^{eff} = PAP - PAQ\frac{1}{QAQ}QAP, \qquad \chi = P\varphi. \qquad (2.8)$$

Up to the last two rows, the effective form of the pentadiagonal matrix A^{eff} coincides with the original matrix A – we may write

$$\begin{pmatrix} A_{n\,n-2} & A_{n\,n-1} & A_{nn} & A_{n\,n+1} & A_{n\,n+2} \\ 0 & A_{n+1\,n-1} & A_{n+1\,n} & A^{eff}_{n+1\,n+1} & A^{eff}_{n+1\,n+2} \\ 0 & 0 & A_{n+2\,n} & A^{eff}_{n+2\,n+1} & A^{eff}_{n+2\,n+2} \end{pmatrix} \begin{pmatrix} \varphi_{n-2} \\ \varphi_{n-1} \\ \varphi_n \\ \varphi_{n+1} \\ \varphi_{n+2} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \qquad (2.9)$$

We see that a (usually, perturbative) construction of the effective matrix elements

$$\begin{pmatrix} A^{eff}_{n+1\,n+1} & A^{eff}_{n+1\,n+2} \\ A^{eff}_{n+2\,n+1} & A^{eff}_{n+2\,n+2} \end{pmatrix} = \begin{pmatrix} h_1 & h_2 \\ h_2^{*} & h_3 \end{pmatrix} \qquad (2.10)$$

is able to reduce our infinite set of equations (2.6) into a fixed-dimensional matrix equation (2.8). It is solvable exactly on the computer of course.

2.4. Wavefunctions

When we invert the latter argument, we may notice that for a variable index or dimension in (2.7), the n-th row of (2.8) may be reinterpreted as an ordinary difference equation of the fourth order (e.g., Nörlund 1923). Its general solution is a superposition of the four independent components,

$$\varphi_n = c_1\varphi_n^{(1)} + c_2\varphi_n^{(2)} + c_3\varphi_n^{(3)} + c_4\varphi_n^{(4)}. \qquad (2.11)$$

The formal "boundary conditions in the origin"

$$\varphi_{-1} = \varphi_{-2} = 0 \qquad (2.12)$$

are to be combined with the standard physical requirement of normalization,

$$\sum_{n=0}^{\infty} \varphi_n^* \varphi_n < \infty \qquad (2.13)$$

This should fix the $n \to \infty$ asymptotics and energy eigenvalues.

For the present potential (1.6), the four independent asymptotic components (2.11) may be constructed in full analogy with the procedure applied to the quartic anharmonic oscillator (Znojil et al., 1985). Here, the n-th row of (2.8) (i.e., equation (2.6)) may also be given easily the necessary asymptotic-expansion form

$$0 = \sum_{m=-2}^{2} \binom{4}{m+2} \left(1 + \sum_{\ell=1}^{L} \frac{X_{\ell m}}{n^{\ell}} + O\left(\frac{1}{n^{L+1}}\right)\right) \varphi_{n+m}$$

$$X_{1m} = 3\alpha + \frac{3}{2} m , \quad X_{2m} = \frac{(8-3|m|)\alpha^2 + \alpha}{3-|m|} + \frac{13m^2+8}{24} + 3m\alpha + \qquad (2.14)$$

$$+\frac{1}{24}(\lambda + 4\eta^2)\delta_{m0} - \frac{1}{16}(\lambda + 4\varepsilon m)\binom{2}{m+1},$$

$$X_{3m} = \frac{\alpha + \frac{1}{2}m}{3-|m|}\left[(2-|m|)\alpha^2 + (1+m)\alpha + 1 - \frac{1}{4}|m| + \frac{\eta^2}{2}\delta_{m0} + \left(2\alpha m - \frac{\varepsilon m}{4} - \frac{\lambda}{8}\right)\right],$$

$$\ldots, \quad m = -2, -1, 0, 1, 2$$

so that the same general form of the ansatz

$$\varphi_n = (-1)^n \exp\left(a n^{3/4} + b n^{2/4} + c n^{1/4} + d \ln n + e n^{-1/4} + \ldots\right) \qquad (2.15)$$
$$n \gg 1$$

remains applicable.

3. A New Systematic Algebraic Procedure of Solving Equation (3.4)

Let us fix the index n and renormalize $\varphi_{n\pm k}$ in such a way that $const \cdot \varphi_n = 1$. Then, due to the smooth asymptotic behaviour of the projections $(-1)^n \varphi_n$ (cf. (2.15)), we may employ and truncate the Taylor series

$$\varphi_{n\pm k} = \varphi_n \times \left(1 \pm k\Omega_1 + \frac{1}{2!}k^2\Omega_2 \pm \ldots\right), \quad \Omega_\ell = \frac{1}{\varphi_n}\frac{d^\ell}{dn^\ell}\varphi_n . \qquad (3.1)$$

When we compare (3.1) with (2.15), we may also write $(\rho = n^{-1/4})$

$$\Omega_1 = \frac{d}{dn} \ln \varphi_n = \frac{3}{4} a\rho + \frac{2}{4} b\rho^2 + \ldots \qquad (3.2)$$

Now, step-by-step, the coefficients are to be determined algebraically, from the asymptotic form (2.14) of our Schrödinger equation (2.6).

We may notice that

$$\frac{d}{dn} = -\frac{\rho^5}{4}\frac{d}{d\rho}$$

so that the recurrences

$$\Omega_{k+1} = \Omega_k\Omega_1 + \frac{d}{dn}\Omega_k = \Omega_k\Omega_1 - \frac{1}{4}\rho^5\frac{d}{d\rho}\Omega_k \qquad (3.3)$$

i.e.,

$$c_m^{(k+1)} = \sum_{\ell=k}^{m-1} c_\ell^{(k)} c_{m-\ell}^{(1)} + c_{m-4}^{(k)}\left(1 - \frac{1}{4}m\right), \qquad (3.4)$$

in

$$\Omega_k = \sum_{m=k}^{\infty} c_m^{(k)} \rho^m , \qquad c_{k-1}^{(k)} = c_{k-2}^{(k)} = \ldots = 0, \quad k = 1, 2, \ldots$$

determine expansion (3.1) as a power series in the new variable ρ, with $\Omega_k = O(\rho^k)$ for $\rho \ll 1$. In this way, we may insert (3.1) in (2.14) and, comparing the coefficients at each power of the variable ρ, get the identity

$$0 \cdot \rho^0 + 0 \cdot \rho^1 + 0 \cdot \rho^2 + 0 \cdot \rho^3 + \Omega_4 + O(\rho^5) = 0. \qquad (3.5)$$

This is a surprising conclusion - we have to put $c_1^{(1)} = 0$. As a consequence, $\Omega_k = O(\rho^{2k})$ will become a series in the even powers of ρ only. This is an importnat simplification of the formulas when compared with the anharmonic oscillator case.

Due to the above result, an ordering of terms Ω_k as belonging to the ρ^{2k} contributions to the left-hand side of our equation (2.14) must be performed. Thus, in place of (3.5), we get a new, simplified relation

$$0\cdot\rho^0 + 0\cdot\rho^2 + 0\cdot\rho^4 + 0\cdot\rho^6 + \left(\Omega_4 + \frac{\eta^2}{n^2}\right) + $$
$$+ \left(\frac{6\Omega_3}{n} + \frac{2\varepsilon\Omega_1}{n^2}\right) + \tag{3.6}$$
$$+ \left[\frac{1}{6}\Omega_6 + \frac{3\alpha}{n}\Omega_4 + \left(\frac{1}{2}\lambda + 13 + 4\alpha - 4\alpha^2\right)\frac{\Omega_2}{2n^2}\right] + O(\rho^{14}) = 0,$$

where also the higher-order corrections may be added in the same manner. Again, due to the independence of the different powers of the variable ρ^2 , the separate coefficients must be assigned the zero values.

From the lowest nontrivial $O(\rho^8)$ contribution to the left-hand side of equation (3.6), we obtain the requirement

$$\left(c_2^{(1)}\right)^4 + \eta^2 = 0. \tag{3.7}$$

It defines the dominant component of φ_n (cf. (2.15) and (3.2)), so that the ansatz (3.5) proves compatible with our recurrences. All the four general solutions are generated by the formula (3.7) - we may eliminate the two unphysical (non-normalizable) components and write, in (2.15),

$$\frac{3}{4}a = 0, \quad \frac{1}{2}b = \left(\frac{1}{2}\eta\right)^{1/2}(-1 \pm i) = c_2^{(\pm)}. \tag{3.8}$$

These two roots of (3.7) are compatible with our asymptotic "boundary condition" (2.13). In full analogy with the anharmonic oscillator, a superposition of the corresponding wave functions $\varphi_n^{(\pm)}$ will define now the discrete analogue of the standard Jost solutions.

In the next $O(\rho^{10})$ component of (3.6), we come to the condition

$$c_4^{(1)} = -\frac{3}{4} + \frac{i}{2}\left(c_2^{(1)}\right)^2 = -\frac{3}{4} \pm \frac{1}{2} = c_4^{(\pm)}. \tag{3.9}$$

This defines a subdominant factor in φ_n (2.15),

$$\varphi_n^{(\pm)} = (-1)^n\left[\cos(2\eta n)^{1/2} \pm i\sin(2\eta n)^{1/2}\right] \times \exp\left[-(2\eta n)^{1/2}\right]$$
$$\times\, n^{(-3\pm 2)/4} \times \left[1 - \frac{1}{2}c_6^{(1)}n^{-1/2} + O(n^{-1})\right], \quad n >> 1. \tag{3.10}$$

In contrast with our anharmonic methodical guide, our present formula (3.10) defines the two components of the general Jost solution that differ in their asymptotic magnitude. The minus-component is asymptotically suppressed by a factor $1/n << 1$, so that the matching algorithm of Znojil et al. (1985) ceases to be applicable here. Without problems, a reconstruction of A^{eff} seems to be a safe way in a purely numerical context. Preliminarily, the similar conclusion seems to be valid also for the higher anharmonicities (Znojil 1986).

4. The Construction of A^{eff}

The difference equation (2.6) may be understood as a general (say, the last but two) row in equation (2.8) or (2.9). The remaining two rows will be treated now as a direct definition of the matrix elements (2.10) in terms of the wave function asymptotics (3.10) or rather (3.1).

A priori, we may expect that the effective submatrix (2.10) remains symmetric up to the order of magnitude $O(\rho^8)$ when the asymmetric and complex terms enter the original matrix A. Thus, we may use an expansion

$$h_m = h_{m0} + h_{m1}\rho^2 + h_{m2}\rho^4 + O(\rho^6) = h_m^* + O(\rho^8) \tag{4.1}$$
$$m = 1, 2, 3.$$

Of course, the coefficients are to be obtained by the insertion into the truncated definitions (2.9),

$$\left(1 + \frac{3\alpha}{n}\right)\left(-1 + \Omega_1 - \frac{1}{2}\Omega_2\right) + 4\left(1 + \frac{3\alpha + \frac{3}{2}}{n}\right)$$
$$+ h_1\left(-1 - \Omega_1 - \frac{1}{2}\Omega_2\right) + h_2\left(1 + 2\Omega_1 + 2\Omega_2\right) + O(\rho^6) = 0 \tag{4.2}$$
$$\left(1 + \frac{3\alpha + 3}{n}\right) + h_2\left(-1 - \Omega_1 - \frac{1}{2}\Omega_2\right) + h_3\left(1 + 2\Omega_1 + 2\Omega_2\right) + O(\rho^6) = 0,$$

where

$$\Omega_1 = \Omega_1^{(\pm)} = c_2^{(\pm)}\rho^2 + c_4^{(\pm)}\rho^4 + O(\rho^6)$$
$$\Omega_2 = \Omega_2^{(\pm)} = \left(c_2^{(\pm)}\right)^2\rho^4 + O(\rho^6). \tag{4.3}$$

In the leading-order approximation, the set of equations (4.2) (on the O(1) level of precision) is incomplete for a determination of the leading order part of (4.1). Thus, an inclusion of the $O(\rho^2)$ relations is needed to provide the values

$$h_{10} = 5, \qquad h_{20} = 2, \qquad h_{30} = 1. \tag{4.4}$$

Similarly, a partial $O(\rho^2)$ result

$$h_{11} = h_{21} = h_{31} \tag{4.5}$$

may be combined with the $O(\rho^4)$ requirements and gives the first nontrivial contribution

$$h_{11} = h_{21} = h_{31} = (2\eta)^{1/2} > 0. \tag{4.6}$$

An analogous generation of the higher-order contributions to the (infinite, asymptotic, fixed-point - series) representation of A^{eff} may be continued, presumably by means of the symbolic manipulation algorithm on a computer. The preliminary second-order constraints

$$\begin{aligned} h_{12} - h_{22} &= 9\alpha + 6 - \eta \\ h_{22} - h_{32} &= 3\alpha + 3 - \eta \end{aligned} \tag{4.7}$$

follow already from the present $O(\rho^4)$ restriction.

5. Conclusions

The present algebraic construction of the exact and finite-dimensional (Fesbach-projected) Schrödinger equation (2.8) is to be understood, first of all, as an illustration of feasibility of the FPPT expansions. The formalism is extremely consequent. Its presumably asymptotic-series character with the small parameter $(1/M)^{const}$ may be useful in the $M \to \infty$ limit. The change of the separation (1.2) of H is varied, but the whole system (Hamiltonian H) remains unchanged.

A systematic inclusion of the higher-order corrections (at a fixed M) has been shown to be a working algebraic algorithm based on an appropriate ansatz. In this sense, the present simplification of

the procedure becomes straightforward and suitable for further applications to "realistic" H.

With our particular choice of the interaction, we get a negative anharmonic correction near the minimum of (1.6) with $\alpha = \omega = 0$ and $\ell < 0$, etc. This will be interesting in the phenomenological applications. Methodically, we may also emphasize this:

(a) In contrast with the simple example (1.5), solution $\varphi_n^{(-)}$ is suppressed asymptotically. It must be treated with care.

(b) Even with the zero coulombic component, the slow asymptotic decrease of V(x) (1.6) makes the integral $\int x^2 V(x)$ (needed in some general analyses of analyticity- Newton 1982) to diverge.

(c) Our choice of the basis has the following unusual features:

(i) The change of variables (2.2) has changed the scalar product. This may push ψ out of the Hilbert space - the one-dimensional interpretation of (1.1) (with $\ell = -1$) cannot be used here because of this reason.

(ii) In principle, our basis states are the so-called Sturmians discussed briefly by Whitehead et al. (1982). Their properties are closely related to the preceding remark.

(iii) For the general Padé potential treated by means of the present technique, the asymmetry of A will make its truncation questionable in general. This is to be analysed in the future.

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Упрощенная теория возмущений неподвижной точки
и ее применение к кулоновскому+короткодействующему потенциалу

Рассматривается радиальное уравнение Шредингера и его связанные состояния для взаимодействия $V(r) = V_{coulomb} + V_{Padé}$, где $V_{Padé}(r) = (b + cr)/(1 + dr^2)$.

Целью работы является систематическое алгебраическое построение точного эффективного гамильтониана Фешбаха H^{eff}. Для этого используется техника повторяемого вычета неподвижной точки и предлагается ее упрощение. Результаты получаются в форме асимптотических разложений ψ_n и H^{eff}: их первые два слагаемых вычисляются в явном виде. Заключается, что формализм достаточно прост для практических применений и представляет новую технику типа теории возмущений.

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A Simplified Fixed-Point Perturbation Theory
and Its Application to the Coulomb+Short-Range Potential

The radial Schrödinger equation and its bound-state solutions for the interaction $V(r) = V_{coulomb} + V_{Padé}$, where $V_{Padé}(r) = (b + cr)/(1 + dr^2)$ are considered. In order to construct exactly the Feshbach effective Hamiltonian H^{eff}, the fixed-point-subtraction technique is employed and its simplification is proposed. The first two terms in the resulting asymptotic expansions of ψ_n and H^{eff} are calculated and interpreted as a new type of perturbation theory.

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

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