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THE ATKINSON-PRÜFER TRANSFORMATION AND THE EIGENVALUE PROBLEM FOR COUPLED SYSTEMS OF THE SCHRÖDINGER EQUATIONS

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1. INTRODUCTION

It is known that the Prüfer transformation[1] is very useful in the investigation of the eigenvalues of the one-dimensional Schrödinger operators (defined, e.g., on the interval $(0, \infty)$) involving potentials represented by a single ("scalar") function of the coordinate (see, e.g., refs.[2,3,4]). In such a case the eigenvalue problem defined originally for the Schrödinger equation may be reformulated in terms of a nonlinear 1st order differential equation for the Prüfer "phase function". The phase function possesses some remarkable properties which facilitate greatly the evaluation of eigenvalues. Moreover, the above-mentioned nonlinear 1st order equation has favourable properties as regards the numerical integration (stability) - see also ref.[4], where a modified Prüfer transformation has been used.

One would like to have an analogous procedure also for the matrix Schrödinger eigenvalue problems. However, much less is known in this case. The corresponding generalization of the Prüfer transformation has been introduced by Atkinson[5], but the discussion in[5] has been restricted to a finite interval only. In paper[6] the Atkinson-Prüfer transformation has been used to develop the oscillation theory for coupled systems of the Schrödinger equations, which was subsequently applied to the numerical evaluation of the eigenvalues. In[6] the corresponding phase functions have been reconstructed by means of a direct integration of the Schrödinger system in question.

The encouraging experience with the method described in ref.[3] (which is based on a direct computation of the phase function by integrating a 1st order differential equation) gave us the motivation to investigate the possibility of extending this method to coupled systems of the "radial" Schrödinger equations defined on the half-axis $\langle 0, \infty)$. As a first step towards the implementation of such a program we study in the present paper the properties of the Atkinson-Prüfer phase functions and find the results analogous to the scalar case. Thus, it is possible to generalize immediately the fundamental theorems giving the connection between asymptotic properties of the phase functions and the eigenvalues.

The second step should consist in analyzing an appropriate system of nonlinear 1st order differential equations which would provide us with the phase functions without referring to the original Schrödinger system. This point will be discussed in detail elsewhere.

The paper is organized as follows. In Sect.2 the relevant phase functions are introduced by means of a matrix of regular solutions of the coupled Schrödinger system. In Sect.3 the properties of the phase functions are investigated. Theorems on the eigenvalues, formulated in terms of the asymptotic behaviour of the phase functions, are given in Sect.4. Some concluding remarks and an outlook are contained in Sect.5.

2. BASIC DEFINITIONS AND PRELIMINARIES

Let us consider the following system of the coupled radial Schrödinger equations defined on the interval $<0, \infty)$

$$-\frac{d^2u}{dx^2} + (\mathcal{C}(x) - \epsilon)u = 0, \tag{2.1}$$

where $u \equiv u(x, \epsilon)$ is a column vector, $\mathcal{C}$ is a real symmetric $n{\times}n$ potential matrix and ϵ is a real parameter, $\epsilon = -\kappa^2$, $\kappa > 0$. For simplicity we suppose that

(i) for any i,j the matrix element $\mathcal{C}_{ij}(x)$ is continuous for $x \in <0, \infty)$;

(ii) for $x \to \infty$ the absolute values of the matrix elements $\mathcal{C}(x)$ with $i \neq j$ decay faster than $1/x^2$, whereas $\mathcal{C}_{ii}(x)$ may contain a term d_i/x^2 with $d_i > 0$.

We look for the solutions of eq. (2.1) satisfying the boundary conditions

$$u(0, \epsilon) = u(\infty, \epsilon) = 0. \tag{2.2}$$

The value of ϵ for which such a solution exists is an eigenvalue of the Schrödinger operator corresponding to eq. (2.1).

Any solution of eq. (2.1) satisfying $u(0, \epsilon) = 0$ will be called regular in what follows. The existence of such solutions is guaranteed by the following theorem (see ref. /7/):

Theorem 2.1. For $\mathcal{C}$ satisfying the condition (i) and $\epsilon = -\kappa^2$, $\kappa > 0$, there is a fundamental system $G(x, \kappa)$, $H(x, \kappa)$ of the solutions of eq. (2.1) (G,H are $n{\times}n$ matrices formed by columns which are linearly independent solutions of (2.1)) such that for some $\delta > 0$ it holds

$$G(x, \kappa) = x(I + o(x^\delta)), \qquad H(x, \kappa) = I + o(x^\delta);\ I = \text{unit matrix} \tag{2.3}$$

for $x \to 0+$ and the relations (2.3) may be differentiated.

In the following we shall also need a theorem on the asymptotic behaviour of solutions of eq. (2.1) for $x \to \infty$ (cf. again /7/).

Theorem 2.2. For $\mathcal{C}$ satisfying the condition (ii) and $\epsilon = -\kappa^2$, $\kappa > 0$ there exists a fundamental system $\Phi^{(-)}(x, \kappa)$, $\Phi^{(+)}(x, \kappa)$ (in the matrix form) of solutions of eq. (2.1) such that

$$\Phi^{(-)}(x, \kappa) = e^{-\kappa x}(I + o(1)), \qquad \Phi^{(+)}(x, \kappa) = e^{+\kappa x}(I + o(1)) \tag{2.4}$$

for $x \to \infty$ and the relations (2.4) may be differentiated.

Let now $U = U(x, \epsilon)$ be a $n{\times}n$ matrix of regular solutions of eq. (2.1), i.e., the columns of U are n arbitrary linearly independent regular solutions of eq. (2.1). Obviously, U also satisfies eq. (2.1), i.e., (the prime denotes the derivative w.r.t. x)

$$V'(x, \epsilon) + Q(x, \epsilon)\,U(x, \epsilon) = 0, \tag{2.5}$$

where $V(x, \epsilon) \equiv U'(x, \epsilon)$ and $Q(x, \epsilon) \equiv \epsilon - \mathcal{C}(x)$. It is easy to show that U may be expressed in terms of G (cf. Theorem 2.1)

$$U = G \cdot C, \tag{2.6}$$

where C is a constant nonsingular matrix. We shall define, according to ref. /5/

$$W(x, \epsilon) = (V + iU)(V - iU)^{-1}. \tag{2.7}$$

In ref. /5/ a theorem is proved, stating that the existence of the unitary matrix W is guaranteed for any x, provided that U^+V is Hermitean (U^+ means Hermitean conjugate of U) and $(V - iU)^{-1}$ exists for some x (see Theorem 10.2.2, p. 305 in ref. /5/). In our case obviously $x = 0$ has the desired properties owing to (2.3) and (2.6). Also, it follows immediately from (2.6) that W does not depend on the particular choice of the regular solutions forming the matrix U. It is interesting to note that W is also symmetric, owing to the symmetry of Q in eq. (2.5). To see this, one has to use the identity ($\tilde{U}$ means the transposition of U)

$$\tilde{U}V = \tilde{V}U \tag{2.8}$$

which can be easily obtained from (2.5) for any regular U. The symmetry of W follows immediately from the definition (2.7) and the relation (2.8). The above results can be thus summarized as follows:

Theorem 2.3. Let U be a matrix made up of n linearly independent regular solutions of eq. (2.1). Then

a) W defined by (2.7) exists for any $x \in <0, \infty)$.

b) W is symmetric and unitary for $x \in <0, \infty)$.

c) W is independent of the particular choice of the corresponding regular solutions.

In the subsequent discussion we shall also need some important differential equations valid for the matrix $W = W(x, \epsilon)$ defined by (2.7) for regular U, namely:

$$\frac{\partial}{\partial x} W(x, \epsilon) = iW(x, \epsilon)\,\Omega(x, \epsilon), \tag{2.9}$$

where

$$\Omega = 2(V^+ + iU^+)^{-1}\,(V^+V + U^+QU)\,(V - iU)^{-1} \tag{2.10}$$

and

$$\frac{\partial}{\partial \epsilon} W(x, \epsilon) = iW(x, \epsilon)\,\bar{\Omega}(x, \epsilon), \tag{2.11}$$

where

$$\bar{\Omega} = 2(V^+ + iU^+)^{-1}\,[\int_0^x U^+(t, \epsilon)\,U(t, \epsilon)dt]\,(V - iU)^{-1}. \tag{2.12}$$

The relations (2.9) through (2.12) may be proved in full analogy with ref./5/ - cf. Theorem 10.2.2, p. 305 and Theorem 10.2.3, p. 307 therein. Evidently, both Ω and $\bar{\Omega}$ are Hermitean. Note also that Ω may be expressed in terms of W and then (2.9) takes the form (cf. also the relations (10.2.19) and (10.4.19) in ref./5/)

$$W' = \frac{i}{2}[(I + W)^2 - (I - W)\,Q(I - W)]. \tag{2.13}$$

We now come to the definition of the phase functions. Since $W(x, \epsilon)$ is unitary for any x, its eigenvalues $\omega_1(x, \epsilon), \ldots, \omega_n(x, \epsilon)$ may be written as

$$\omega_1(x, \epsilon) = e^{i\phi_1(x,\epsilon)}, \ldots, \omega_n(x, \epsilon) = e^{i\phi_n(x,\epsilon)}. \tag{2.14}$$

Further, $W(0, \epsilon) = I$, so we may set

$$\phi_1(0, \epsilon) = \ldots = \phi_n(0, \epsilon) = 0. \tag{2.15}$$

According to ref./5/ it may be shown that $\phi_j(x, \epsilon)$, $j = 1, 2, \ldots, n$, can be continued uniquely and continuously so that

$$\phi_1(x, \epsilon) \le \phi_2(x, \epsilon) \le \ldots \le \phi_n(x, \epsilon) \le \phi_1(x, \epsilon) + 2\pi. \tag{2.16}$$

Although other conventions are also possible, we shall use (2.16) in the present paper. The passage from the matrix U of the regular solutions of the coupled Schrödinger system to the matrix W given by (2.7) or, eventually, to the phase functions (2.14), (2.15), will be called the Atkinson-Prüfer transformation henceforth. Clearly, the Prüfer phase function z encountered in the scalar case is just $\phi/2$.

The phase functions posses a set of remarkable properties, which will be described in the next section.

3. PROPERTIES OF THE PHASE FUNCTIONS

We shall denote the relevant properties of the phase functions consecutively by P1 through P5.

P1: Let $\epsilon = -\kappa^2$, $\kappa > 0$ be fixed. Let $x \in \langle 0, \infty)$ and $e^{i\phi_k(x_0, \epsilon)} = 1$ for some k, $1 \le k \le n$. Then ϕ_k is increasing function of x at $x = x_0$.

Proof can be found in ref./5/ and is based on eq. (2.9). The point is that for any vector w, $w \neq 0$, such that $W(x_0, \epsilon)w = w$ it can be proved $w^+\Omega(x_0, \epsilon)w = 2w^+w$, where $\Omega(x, \epsilon)$ is given by (2.10). That is, $\Omega(x_0, \epsilon)$ is positive definite when acting on w. Taking into account eq. (2.9), P1 then immediately follows from Theorem V.6.2, p. 469 in ref./5/.

P2: Let $\epsilon = -\kappa^2$, $\kappa > 0$. There exists $x_0(\epsilon)$ such that if for some k, $1 \le k \le n$ and for some $x_1 > x_0(\epsilon)$ one has

$$e^{i\phi_k(x_1, \epsilon)} = -1 \tag{3.1}$$

then ϕ_k is decreasing function of x at $x = x_1$.

Proof is again based on eq. (2.9). In analogy with the preceding case it is not difficult to show that for any nontrivial vector w satisfying $W(x_1, \epsilon)w = -w$ (cf. (3.1)) one has

$$w^+\Omega(x, \epsilon)w = 2w^+Q(x_1, \epsilon)w. \tag{3.2}$$

However, with $\epsilon = -\kappa^2$, $Q(x, \kappa) = -\kappa^2 + \mathcal{C}(x)$ and $\lim_{x\to\infty}\mathcal{C}(x) = 0$. Thus, it is easy to prove that for a fixed $\kappa > 0$ there exists $x_0(\kappa) = x_0(\epsilon)$ such that $Q(x, \kappa)$ is negative definite for $x > x_0(\kappa)$. (To see this one has to employ the min-max principle for the eigenvalues of $\mathcal{C}$). Thus, the l.h.s. of eq. (3.2) is negative for $x > x_0(\kappa)$ and P2 then immediately follows from the Theorem V.6.2 in ref./5/.

P3: Let $x_0 > 0$ be fixed. Then any phase $\phi_k(x_0, \epsilon)$, $1 \le k \le n$, is a continuous increasing function of ϵ (i.e., for $\epsilon = -\kappa^2$ $\phi_k(x_0, \kappa)$ is a continuous decreasing function of κ).

Proof is based on eq. (2.11) and is given in ref./5/ (see p. 308 and Theorem V.6.1 therein - the point is that the matrix $\bar{\Omega}(x, \epsilon)$ is positive definite).

P4: Choose some $\epsilon = -\kappa^2$. ϵ is a k-fold degenerate eigenvalue, $0 \le k \le n$ ($k = 0$ denoting the case when ϵ is not an eigenvalue) if and only if there are just k phase functions $\phi_j(x, \epsilon)$, $1 \le j \le k$, for which

$$\lim_{x\to\infty} \operatorname{tg}\frac{1}{2}\phi_j(x, \kappa) = -\frac{1}{\kappa} \tag{3.3}$$

and for the remaining $(n-k)$ phases

$$\lim_{x\to\infty} \mathrm{tg}\frac{1}{2}\phi_j(x,\kappa) = +\frac{1}{\kappa}. \tag{3.4}$$

Proof: It is sufficient to prove the assertion in one direction only; the inverse can be then immediately proved by contradiction.

Suppose that $\epsilon = -\kappa^2$ is a k-fold degenerate eigenvalue, e.g., $1 \le k < n$ (the modifications for $k = 0$ or $k = n$ will be obvious). This means that there are just k linearly independent regular solutions $u_i^{(-)}(x,\epsilon)$ of eq. (2.1), which are linear combinations of the columns of the matrix $\Phi^{(-)}$ defined in (2.4). In the rest of this proof we shall employ the parameter κ instead of ϵ. Denote these columns by $\phi_1^{(-)}(x,\kappa), \ldots, \phi_n^{(-)}(x,\kappa)$ and, similarly, the columns of $\Phi^{(+)}(x,\kappa)$ in eq. (2.4) by $\phi_1^{(+)}(x,\kappa), \ldots, \phi_n^{(+)}(x,\kappa)$. Thus

$$u_i^{(-)}(x,\kappa) = \sum_{j=1}^{n} A_{ji}\,\phi_j^{(-)}(x,\kappa); \qquad i = 1,2,\ldots,k. \tag{3.5}$$

The remaining $(n-k)$ linearly independent regular solutions are then of the type

$$u_i^{(+)}(x,\kappa) = \sum_{j=1}^{n} A_{ji}\,\phi_j^{(+)}(x,\kappa) + \text{terms with } \phi_j^{(-)}; \qquad i = k+1,\ldots,n. \tag{3.6}$$

It is easy to see that the linear independence of the solutions (3.5) and (3.6) implies linear independence of the columns $\{A_{ji}\}_{j=1}^{n}$ of the matrix $A = \{A_{ji}\}$ for $i = 1,\ldots,k$ and $i = k+1,\ldots,n$, separately. Let us now prove that, in fact, they are all linearly independent, and, consequently

$$\det A \neq 0. \tag{3.7}$$

To this end, we shall employ the identity (2.8) which means that for any pair a, b of regular solutions of eq. (2.1) one has, for $x \in \langle 0,\infty)$

$$\hat{a}b' - \hat{a}'b = 0. \tag{3.8}$$

When (3.8) is applied to an arbitrary pair of the type

$$a \equiv u_i^{(-)}, \quad 1 \le i \le k; \qquad b \equiv u_j^{(+)}, \quad k+1 \le j \le n, \tag{3.9}$$

then, using eqs. (3.5), (3.6) and Theorem 2.2 and performing the limit $x \to \infty$, we obtain the relation

$$\sum_{r=1}^{n} A_{ri} A_{rj} = 0; \quad i = 1,\ldots,k, \quad j = k+1,\ldots,n. \tag{3.10}$$

Since the columns of the matrix A must be nontrivial, the orthogonality relation (3.10) implies the linear independence of $\{A_{ki}\}_{k=1}^{n}$, $\{A_{kj}\}_{k=1}^{n}$ for any pair i, j satisfying (3.9). This, in conjunction with the statement following the relation (3.6), leads to the desired result (3.7). Note that for $k = 0$ or $k = n$ the relation (3.7) is obvious.

Let us now consider the characteristic polynom of W

$$P(\lambda,x,\kappa) \equiv \det(W-\lambda I) = \det[(V+iU)(V-iU)^{-1} - \lambda(V-iU)(V-iU)^{-1}] = \det\{[(1-\lambda)V + i(1+\lambda)U](V-iU)^{-1}\}. \tag{3.11}$$

Using the fact that W does not depend on the particular choice of U (see Theorem 2.3), we may choose U so that the first k columns are just $u_i^{(-)}$, $i = 1,\ldots,k$ and the last $(n-k)$ columns are just $u_i^{(+)}$, $i = k+1,\ldots,n$. Then, using Theorem 2.2 and eqs. (3.5), (3.6), eq. (3.11) may be rewritten, after some manipulations, as follows:

$$P(\lambda,x,\kappa) = \frac{[e^{-\kappa x}(-\kappa(1-\lambda)+i(1+\lambda))]^k\,[e^{\kappa x}(\kappa(1-\lambda)+i(1+\lambda))]^{n-k}}{[e^{-\kappa x}(-\kappa-i)]^k\,[e^{\kappa x}(\kappa-i)]^{n-k}} \times \frac{\det(A+\Delta)}{\det(A+\delta)} =$$

$$= \left(\frac{\kappa-i}{\kappa+i} - \lambda\right)^k \left(\frac{\kappa+i}{\kappa-i} - \lambda\right)^{n-k} \frac{\det(A+\Delta)}{\det(A+\delta)}, \tag{3.12}$$

where $\Delta \equiv \Delta(\lambda,x,\kappa)$, $\delta \equiv \delta(\lambda,x,\kappa)$ are some $n{\times}n$ matrices such that $\lim_{x\to\infty}\Delta(\lambda,x,\kappa) = \lim_{x\to\infty}\delta(\lambda,x,\kappa) = 0$. Note that (3.12) holds for any k, $0 \le k \le n$. Obviously, (3.7) now implies that

$$\lim_{x\to\infty} \frac{\det(A+\Delta)}{\det(A+\delta)} = 1 \tag{3.13}$$

and from (3.12), (3.13) we then get for any λ

$$\lim_{x\to\infty} P(\lambda,x,\kappa) = \left(\frac{\kappa-i}{\kappa+i} - \lambda\right)^k \left(\frac{\kappa+i}{\kappa-i} - \lambda\right)^{n-k}. \tag{3.14}$$

Thus, assuming the existence of the limits for $x \to \infty$ of the eigenvalues of $W(x,\kappa)$, from (3.14) easily follow the desired relations (3.3) and (3.4). However, the existence of the limits in question is guaranteed by the existence of the limits for $x \to \infty$ of the coefficients of the characteristic polynomial $P(\lambda,x,\kappa)$ (i.e. by (3.14))*. The property P4 is thereby proved.

*We are grateful to B.Lonek for communicating this result to us.

P5: For any phase function $\phi_j(x,\epsilon)$, $1 \le j \le n$, there exists ϵ_0 such that for $\epsilon < \epsilon_0$, $\phi_j(x,\epsilon) < \pi$ for $x \in <0,\infty)$.

Proof: The conditions (i), (ii) imposed on the potential matrix $\mathbb{C}$ imply that the matrix elements of $\mathbb{C}$ are bounded for $x \in <0,\infty)$. Consequently, there exists κ_0 so large that $Q(x,\kappa_0) = -\kappa_0^2 - \mathbb{C}(x)$ is negative definite for any $x \in <0,\infty)$ (cf. the proof of P2). Since ϕ_j is continuous w.r.t. x and the condition (2.15) holds, from the proof of P2 then immediately follows that for any $j = 1,\dots,n$, $\phi_j(x,\epsilon_0)$ with $\epsilon_0 = -\kappa_0^2$ must stay below π for $x \in <0,\infty)$. Finally, according to P3, for any $x \in (0,\infty)$ we have $\phi_j(x,\epsilon) < \phi_j(x,\epsilon_0) < \pi$ if $\epsilon < \epsilon_0$, and P5 is thus proved.

We see that the phase functions possess the properties analogous to those of the Prüfer phase function relevant in the scalar case (notice the correspondence $\phi/2 \to z$). This leads us to a straightforward generalization of the theorems relating asymptotic properties of the phase functions to the bounds for the eigenvalues of the original Schrödinger system, which for the scalar case have been proved in ref./3/. Such a generalization will be the subject of the next section.

4. PHASE FUNCTIONS AND THE EIGENVALUE PROBLEM

Theorem 4.1. Let ϵ_0 be fixed. Denote $\phi_1(\infty,\epsilon),\dots,\phi_n(\infty,\epsilon)$ the limits $\lim_{x\to\infty}\phi_1(x,\epsilon),\dots,\lim_{x\to\infty}\phi_n(x,\epsilon)$. Then

I. There exists a positive integer m and a set of three nonnegative integers $\{n_1, n_2, n_3\}$ satisfying

$$0 \le n_1 \le n_2 \le n_3 \le n, \tag{4.1}$$

$$\text{if } n_1 \ge 1 \text{ then } n_3 = n \tag{4.2}$$

such that

$$\frac{1}{2}\phi_j(\infty,\epsilon_0) = (m-1)\pi + \operatorname{arctg}\frac{1}{\sqrt{-\epsilon_0}}, \quad j = 1,\dots,n_1, \tag{4.3}$$

$$\frac{1}{2}\phi_j(\infty,\epsilon_0) = m\pi - \operatorname{arctg}\frac{1}{\sqrt{-\epsilon_0}}, \quad j = n_1+1,\dots,n_2, \tag{4.4}$$

$$\frac{1}{2}\phi_j(\infty,\epsilon_0) = m\pi + \operatorname{arctg}\frac{1}{\sqrt{-\epsilon_0}}, \quad j = n_2+1,\dots,n_3, \tag{4.5}$$

$$\frac{1}{2}\phi_j(\infty,\epsilon_0) = (m+1)\pi - \operatorname{arctg}\frac{1}{\sqrt{-\epsilon_0}}, \quad j = n_3+1,\dots,n^*. \tag{4.6}$$

* Eqs. (4.3)-(4.6) are to be understood in the following sense: If it happens that at least one equality in (4.1) occurs, e.g., $n_1 = n_2$, then there is no phase function with the corresponding property, i.e., for $n_1 = n_2$ there is no ϕ_j satisfying (4.4), etc.

II. ϵ_0 is an eigenvalue with the $(n_2 - n_1 + n - n_3)$ - fold degeneracy iff $n_2 - n_1 + n - n_3 > 0$.

III. ϵ_0 is not an eigenvalue iff $n_2 - n_1 + n - n_3 = 0$.

IV. There are $n(\epsilon_0) = n \cdot m - n_2$ eigenvalues less than ϵ_0 if each of the different eigenvalues is counted together with its degeneracy.

Proof is based on eqs. (2.15), (2.16) and the properties P1-P5. Now, keep ϵ_0 fixed and consider the functions $\phi_1(\infty,\epsilon),\dots,\phi_n(\infty,\epsilon)$ in the interval $I_{\epsilon_0} = (-\infty,\epsilon_0>$. It holds

Theorem 4.2. I. For each $j = 1,\dots,n$ the function $\phi_j(\infty,\epsilon)$ is positive, increasing and piecewise continuous in I_{ϵ_0}.

II. $\tilde{\epsilon} \in I_{\epsilon_0}$ is an eigenvalue iff $\tilde{\epsilon}$ is a discontinuity point of at least one of the functions $\phi_1(\infty,\epsilon),\dots,\phi_n(\infty,\epsilon)$.

III. Supposing $\tilde{\epsilon}$ is a discontinuity point of a function $\phi_j(\infty,\epsilon)$, $1 \le j \le n$, it holds

$$\lim_{\eta\to 0+}\left[\frac{1}{2}\phi_j(\infty,\epsilon+\eta) - \frac{1}{2}\phi_j(\infty,\epsilon-\eta)\right] = \pi. \tag{4.7}$$

Proof follows from the properties P1-P5, in analogy with the scalar case; cf. ref./3/.

Thus, all the eigenvalues contained in I_{ϵ_0} could in principle be determined if the functions $\phi_1(\infty,\epsilon),\dots,\phi_n(\infty,\epsilon)$ were reconstructed in I_{ϵ_0} and their discontinuities found. Since we are not able to compute the functions $\phi_1(\infty,\epsilon),\dots,\phi_n(\infty,\epsilon)$ numerically, it is a crucial point that the properties of these functions are signalled already by the behaviour of functions $\phi_1(x_0,\epsilon),\dots,\phi_n(x_0,\epsilon)$ with a suitably large but finite x_0.

Theorem 4.3. Let $\epsilon = \epsilon_0$ be fixed and $\tilde{x}$ be such that for $x > \tilde{x}$ the matrix $(\epsilon_0 - \mathbb{C}(x))$ is negative definite when applied to eigenvectors of $W(x,\epsilon_0)$ associated with an eigenvalue -1 (cf. the proof of P2). Choose some $x_0 \in (\tilde{x},\infty)$. Then

I. There exists a positive integer m and a set of nonnegative integers $\{n_1, n_2, n_3\}$ with the properties (4.1), (4.2) such that

$$\frac{1}{2}\phi_j(x_0,\epsilon_0) \in <(m-1)\pi, m\pi - \frac{\pi}{2}>, \quad j = 1,\dots,n_1, \tag{4.3'}$$

$$\frac{1}{2}\phi_j(x_0,\epsilon_0) \in (m\pi - \frac{\pi}{2}, m\pi), \quad j = n_1+1,\dots,n_2, \tag{4.4'}$$

$$\frac{1}{2}\phi_j(x_0,\epsilon_0) \subset <m\pi, m\pi + \frac{\pi}{2}>, \quad j = n_2+1,\dots,n_3, \tag{4.5'}$$

$$\frac{1}{2}\phi_j(x_0,\epsilon_0) \in (m\pi + \frac{\pi}{2}, (m+1)\pi), \quad j = n_3+1,\dots,n. \tag{4.6'}$$

(A remark analogous to the footnote concerning eqs. (4.3)-(4.6) applies also here).

II. There are $n(\epsilon_0)$ eigenvalues less than ϵ_0, $n(\epsilon_0)$ being a nonnegative integer which can take on one of the values $n\cdot m - n_2$, $n\cdot m - n_2 + 1, \dots, n(m+1) - n_1 - n_3$.

Thus, from the values of the phase functions $\phi_1(x,\epsilon_0),\dots,\phi_n(x,\epsilon_0)$ at the point x_0 one obtains the information on the number of eigenvalues less than ϵ_0. Moreover, reconstructing functions $\phi_1(x_0,\epsilon),\dots,\phi_n(x_0,\epsilon)$ in the interval I_{ϵ_0} for a given x_0 (with the properties required in Theorem 4.3) one finds upper and lower bounds on each eigenvalue less than ϵ_0. It holds

Theorem 4.4. Let ϵ_0, x_0, m, $\{n_1, n_2, n_3\}$ be the same as in Theorem 4.3. Suppose $n\cdot m - n_2 \geq 1$, i.e., there is at least one eigenvalue less than ϵ_0, and consider the functions $\phi_1(x_0,\epsilon),\dots,\phi_n(x_0,\epsilon)$ with x_0 fixed and ϵ varying within I_{ϵ_0}. For each j, $1 \leq j \leq n$, such that $\phi_j(x_0,\epsilon_0) \geq 2\pi$, define a set of intervals $\{I^j_k\}$, satisfying $I^j_k \subset I_{\epsilon_0}$, by the relations

$$I^j_k = \langle \bar{\epsilon}^j_k, \bar{\bar{\epsilon}}^j_k \rangle; \tag{4.8}$$

$$\frac{1}{2}\phi_j(x_0, \bar{\epsilon}^j_k) = k\pi - \frac{1}{2}\pi, \tag{4.9}$$

$$\frac{1}{2}\phi_j(x_0, \bar{\bar{\epsilon}}^j_k) = k\pi. \tag{4.10}$$

In this definition, for a given j, k is varying in the range $1,2,\dots,n_j$, where $\sum_j n_j = n\cdot m - n_2$. The intervals I^j_k have the following properties:

I. Each I^j_k contains just one eigenvalue $\epsilon^j_k < \epsilon_0$.

II. When x_0 is increased, the length of each of the intervals I^j_k decreases. In the limit $x_0 \to \infty$ each of the intervals I^j_k degenerates into one point which is just one of the eigenvalues $\epsilon^j_k < \epsilon_0$.

Proofs of Theorems 4.3., 4.4 are based on eqs. (2.15), (2.16) and the properties P1-P5 in analogy with what has been done in ref./3/ for the scalar case.

According to Theorem 4.4 one can find intervals, each of which contains just one eigenvalue less than ϵ_0, by reconstructing the functions $\phi_1(x_0,\epsilon),\dots,\phi_n(x_0,\epsilon)$ for $\epsilon \in I_{\epsilon_0}$. By increasing x_0 one can in principle make the "eigenvalue intervals" small enough to determine the eigenvalues with the desired accuracy. This is a conclusion completely analogous to that obtained earlier for the scalar case (see, e.g., the last two papers in ref. /3/). Of course, in the matrix case discussed in the present paper the situation is complicated by the possible degeneracy of the eigenvalues.

5. CONCLUDING REMARKS AND AN OUTLOOK

We have discussed the phase functions defined by means of the Atkinson-Prüfer transformation for a coupled system of the radial Schrödinger equations. We have shown how the asymptotic behaviour of the phase functions can be employed to find the eigenvalues of the original Schrödinger system. The results are analogous to the scalar case except that in the matrix case, instead of one, several phase functions have to be investigated simultaneously and degenerate eigenvalues may occur.

The next step should be the practical determination of the phase functions. Motivated by the scalar case, we propose to employ a suitable system of 1st order nonlinear equations either for the matrix $W(x,\epsilon)$ or the phase functions themselves.

As regards the first possibility, one may use the Riccati-type eq. (2.13) together with the initial condition $W(0,\epsilon) = I$. Standard theorems on the uniqueness of the solution of differential equations then obviously guarantee the one-to-one correspondence between eq. (2.13) supplemented with the above-mentioned initial condition and the original Schrödinger system. In such an approach, the matrix W should be diagonalized in the course of the integration of eq. (2.13) and the phase functions reconstructed to be continuous w.r.t. x and (eventually) satisfy (2.16).

As to the second alternative (finding a system of equations for the phase functions), it may be implemented at least in the case of 2x2 potential matrices, when W can be easily diagonalized explicitly. Nevertheless, the situation is somewhat more complicated than in the scalar case and the corresponding nonlinear 1st order differential system as well as the results of numerical calculations will be discussed elsewhere. Note that a system of nonlinear 1st order equations based on an alternative transformation of the original Schrödinger system has been already discussed in ref./8/.

Finally, we would like to add the following comment. In this paper we have considered, mostly for the sake of technical simplicity, only the regular potential matrices satisfying (i), (ii). Of course, physically interesting examples are described by potential matrices singular at the origin (due to Coulomb-like terms or the "centrifugal" terms $\propto 1/x^2$, etc.). However, we have reasons to expect that our results are relevant also for singular potentials. Firstly, we have checked explicitly that the theorems given here apply, e.g., also to the 2x2 potential matrices involving Coulomb-like and centrifugal singularities (the corresponding analysis will appear elsewhere). Secondly, working up a problem with a singular potential numerically and trying to avoid computational complications, some authors /9/ utilize the approach based on regularizing the original potential near the origin so as to satisfy (i), (ii). Then, the results of the present analysis are directly applicable.

Note that the mentioned approach is justifiable only if the sought solutions of the corresponding differential equations are asymptotically stable (we have in mind the asymptotic stability discussed, e.g., in [10]). This stability property is necessary to ensure that the solutions obtained by the numerical integration of the equation with the potential regularized at the origin approach the proper solutions, corresponding to the original singular potential, for large x. Motivated by our experience with the scalar eigenvalue problems, as far as the stability properties are concerned (see the last reference in [3]), we expect that the relevant solutions of the 1st order nonlinear equations discussed in the present paper are asymptotically stable. Work on these problems is in progress.

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Преобразование Аткинсона-Прюфера и проблема собственных значений для систем уравнений Шредингера

Матричное обобщение преобразования Прюфера, введенное Аткинсоном, применяется к системе радиальных уравнений Шредингера. Показано, что фазовые функции, соответствующие матричному случаю, обладают свойствами, аналогичными свойствам фазовой функции Прюфера в скалярном случае. Установлены строгие теоремы, на основе которых можно определить собственные значения для системы уравнений Шредингера по асимптотическому поведению фазовых функций. Обсуждается возможность получения фазовых функций при помощи интегрирования некоторой системы нелинейных дифференциальных уравнений первого порядка.

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The Atkinson-Prüfer Transformation and the Eigenvalue Problem for Coupled Systems of the Schrödinger Equations

The matrix generalization of the Prüfer transformation introduced by Atkinson is applied to a coupled system of the radial Schrödinger equations. It is shown that the phase functions corresponding to the matrix case exhibit properties analogous to those of the Prüfer phase function encountered in the scalar case. Rigorous theorems are established which allow one to determine the eigenvalues of the original Schrödinger system with an arbitrary accuracy provided that the asymptotic behaviour of the phase functions is known. The possibility of obtaining the phase functions by means of the integration of an appropriate system of nonlinear 1st order differential equations is briefly discussed.

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

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