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1984 J. Phys. A: Math. Gen. 17 2621

(http://iopscience.iop.org/0305-4470/17/13/014)

J. Phys. A: Math. Gen. 17 (1984) 2621–2631. Printed in Great Britain

The Atkinson–Prüfer transformation and the eigenvalue problem for coupled systems of Schrödinger equations

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Received 23 January 1984

Abstract. The matrix generalisation of the Prüfer transformation introduced by Atkinson is applied to a coupled system of 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 us 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 first-order differential equations is briefly discussed.

1. Introduction

It is known that the Prüfer transformation (PT) (Prüfer 1926) 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. Bailey 1978, Úlehla and Havlíček 1980, Úlehla *et al* 1981, Adamová 1981, Adamová and Úlehla 1983, Crandall 1983). In such a case the eigenvalue problem defined originally for the Schrödinger equation (SE) may be reformulated in terms of a nonlinear first-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 first-order equation has favourable properties as regards the numerical integration (stability)—see also Crandall (1983), where a modified PT has been used.

One would like to have an analogous procedure also for a matrix Schrödinger eigenvalue problem. However, much less is known in this case. The corresponding form of the PT has been introduced by Atkinson (1964) but he has restricted the analysis to a finite interval only. Calvert and Davison (1969) have used the Atkinson–Prüfer transformation (APT) to develop the oscillation theory for coupled systems of SE and applied their results to the numerical evaluation of the eigenvalues. Calvert and Davison (1969) have reconstructed the corresponding phase functions by means of a direct integration of the Schrödinger system in question.

The encouraging experience with the method described briefly by Úlehla *et al* (1981) and in more detail by Adamová (1981) (which is based on a direct computation

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of the phase function by integrating a first-order differential equation) gave us the motivation to investigate the possibility of extending this method to coupled systems of radial SE defined on the half-axis $\langle 0, \infty)$. As a first step towards the implementation of such a programme we study in the present paper the properties of the Atkinson–Prüfer (AP) phase functions and find results analogous to the scalar case. Thus, it is possible to generalise immediately the fundamental theorems giving the connection between asymptotic properties of the phase functions and the eigenvalues.

The second step should consist in analysing an appropriate system of nonlinear first-order differential equations which would provide us with the phase functions without referring to the original system of SE. This point will be discussed elsewhere.

The paper is organised as follows. In § 2 the relevant phase functions are introduced by means of a matrix of regular solutions of the coupled system of SE. In § 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 § 4. Some concluding remarks and an outlook are contained in § 5.

2. Basic definitions and preliminaries

Let us consider the following system of coupled radial SE defined on the interval $\langle 0, \infty)$:

$$-\mathrm{d}^2\boldsymbol{u}/\mathrm{d}x^2+(\boldsymbol{\mathcal{V}}(x)-\varepsilon)\boldsymbol{u}=0 \tag{2.1}$$

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

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

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

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

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

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

Any solution of (2.1) satisfying $\boldsymbol{u}(0, \varepsilon)=0$ will be called regular in what follows. The existence of such solutions is guaranteed by the following theorem (Agranovich and Marchenko 1963).

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

$$\boldsymbol{G}(x, \varkappa)=x(\boldsymbol{I}+\mathrm{o}(x^\delta)), \qquad \boldsymbol{H}(x, \varkappa)=\boldsymbol{I}+\mathrm{o}(x^\delta) \tag{2.3}$$

($\boldsymbol{I}$ = unit matrix) 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 (2.1) for $x\to\infty$ (cf again Agranovich and Marchenko 1963).

Theorem 2.2. For $\boldsymbol{\mathcal{V}}$ satisfying the condition (ii) and $\varepsilon=-\varkappa^2$, $\varkappa>0$, there exists a fundamental system $\boldsymbol{\phi}^-(x, \varkappa)$, $\boldsymbol{\phi}^+(x, \varkappa)$ (in the matrix form) of solutions of (2.1) such that

$$\boldsymbol{\phi}^{-}(x, \varkappa) = \mathrm{e}^{-\varkappa x}(\boldsymbol{I} + \mathrm{o}(1))., \qquad \boldsymbol{\phi}^{+}(x, \varkappa) = \mathrm{e}^{+\varkappa x}(\boldsymbol{I} + \mathrm{o}(1)), \tag{2.4}$$

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

Let now $\boldsymbol{U} \equiv \boldsymbol{U}(x, \varepsilon)$ be an $n \times n$ matrix of regular solutions of (2.1), i.e. the columns of $\boldsymbol{U}$ are n arbitrary linearly independent regular solutions of (2.1). Obviously, $\boldsymbol{U}$ also satisfies (2.1), i.e. (the prime denotes the derivative with respect to x)

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

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

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

where $\boldsymbol{C}$ is a constant non-singular matrix. We shall define according to Atkinson (1964) (we shall refer to this work as A hereafter)

$$\boldsymbol{W}(x, \varepsilon) = (\boldsymbol{V} + \mathrm{i}\boldsymbol{U})(\boldsymbol{V} - \mathrm{i}\boldsymbol{U})^{-1}. \tag{2.7}$$

In A a theorem is proved stating that the existence of the unitary matrix $\boldsymbol{W}$ is guaranteed for any x provided that $\boldsymbol{U}^{+}\boldsymbol{V}$ is Hermitian ($\boldsymbol{U}^{+}$ means Hermitian conjugate of $\boldsymbol{U}$) and $(\boldsymbol{V} - \mathrm{i}\boldsymbol{U})^{-1}$ exists for some x (see theorem 10.2.2, p 305 in A). 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 the form of $\boldsymbol{W}$ does not depend on the particular choice of the regular solutions forming the matrix $\boldsymbol{U}$. It is interesting to note that $\boldsymbol{W}$ is also symmetric owing to the symmetry of $\boldsymbol{Q}$ in (2.5). To see this, one has to use the identity ($\tilde{\boldsymbol{U}}$ means the transposition of $\boldsymbol{U}$)

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

which can be easily obtained from (2.5) for any regular $\boldsymbol{U}$. The symmetry of $\boldsymbol{W}$ follows immediately from the definition (2.7) and the relation (2.8). Thus, we can summarise:

Theorem 2.3. Let $\boldsymbol{U}$ be a matrix made up from n linearly independent regular solutions of (2.1). Then:

(a) $\boldsymbol{W}$ defined by (2.7) exists for any $x \in \langle 0, \infty)$;

(b) $\boldsymbol{W}$ is symmetric and unitary for $x \in \langle 0, \infty)$;

(c) the form of $\boldsymbol{W}$ does not depend on the particular choice of the corresponding regular solutions.

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

$$(\partial/\partial x)\boldsymbol{W}(x, \varepsilon) = \mathrm{i}\boldsymbol{W}(x, \varepsilon)\boldsymbol{\Omega}(x, \varepsilon) \tag{2.9}$$

where

$$\boldsymbol{\Omega} \equiv 2(\boldsymbol{V}^{+} + \mathrm{i}\boldsymbol{U}^{+})^{-1}(\boldsymbol{V}^{+}\boldsymbol{V} + \boldsymbol{U}^{+}\boldsymbol{Q}\boldsymbol{U})(\boldsymbol{V} - \mathrm{i}\boldsymbol{U})^{-1} \tag{2.10}$$

and

$$(\partial/\partial\varepsilon)\boldsymbol{W}(x, \varepsilon) = \mathrm{i}\boldsymbol{W}(x, \varepsilon)\bar{\boldsymbol{\Omega}}(x, \varepsilon) \tag{2.11}$$

where

$$\bar{\boldsymbol{\Omega}} \equiv 2(\boldsymbol{V}^{+} + \mathrm{i}\boldsymbol{U}^{+})^{-1}\left(\int_0^x \boldsymbol{U}^{+}(t, \varepsilon)\boldsymbol{U}(t, \varepsilon)\,\mathrm{d}t\right)(\boldsymbol{V} - \mathrm{i}\mathrm{U})^{-1}. \tag{2.12}$$

The relations (2.9)–(2.12) may be proved in full analogy with the proofs given in A—cf theorem 10.2.2, p 305 and theorem 10.2.3, p 307 therein. Evidently, both $\boldsymbol{\Omega}$ and $\bar{\boldsymbol{\Omega}}$ are Hermitian. Note also that $\boldsymbol{\Omega}$ may be expressed in terms of $\boldsymbol{W}$ and then (2.9) takes the form (cf also the relations (10.2.19) and (10.4.19) in A)

$$\boldsymbol{W}' = \tfrac{1}{2}\mathrm{i}[(\boldsymbol{I}+\boldsymbol{W})^2 - (\boldsymbol{I}-\boldsymbol{W})\boldsymbol{Q}(\boldsymbol{I}-\boldsymbol{W})]. \tag{2.13}$$

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

$$\omega_1(x, \varepsilon) = \mathrm{e}^{\mathrm{i}\varphi_1(x,\varepsilon)}, \ldots, \omega_n(x, \varepsilon) = \mathrm{e}^{\mathrm{i}\varphi_n(x,\varepsilon)}. \tag{2.14}$$

Further, $\boldsymbol{W}(0, \varepsilon) = \boldsymbol{I}$, so we may set

$$\varphi_1(0, \varepsilon) = \ldots = \varphi_n(0, \varepsilon) = 0. \tag{2.15}$$

According to A it may be shown that $\varphi_j(x, \varepsilon)$, $j = 1, 2, \ldots, n$, can be continued uniquely and continuously so that

$$\varphi_1(x, \varepsilon) \leqslant \varphi_2(x, \varepsilon) \leqslant \ldots \leqslant \varphi_n(x, \varepsilon) \leqslant \varphi_1(x, \varepsilon) + 2\pi. \tag{2.16}$$

Although other conventions are also possible, we shall use (2.16) in what follows.

The phase functions defined by (2.14)–(2.16) possess a set of remarkable properties which will be described in § 3.

3. Properties of the phase functions

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

P1. Let $\varepsilon = -\varkappa^2$, $\varkappa > 0$ be fixed. Let $x_0 \in \langle 0, \infty)$ and $\exp[\mathrm{i}\varphi_k(x_0, \varepsilon)] = 1$ for some k, $1 \leqslant k \leqslant n$. Then φ_k is an increasing function of x at $x = x_0$.

The proof can be found in A and is based on (2.9). The point is that for any vector $\boldsymbol{w}$, $\boldsymbol{w} \neq 0$, such that $\boldsymbol{W}(x_0, \varepsilon)\boldsymbol{w} = \boldsymbol{w}$ it can be proved that

$$\boldsymbol{w}^+\boldsymbol{\Omega}(x_0, \varepsilon)\boldsymbol{w} = 2\boldsymbol{w}^+\boldsymbol{w}$$

where $\boldsymbol{\Omega}(x, \varepsilon)$ is given by (2.10). That is, $\boldsymbol{\Omega}(x_0, \varepsilon)$ is positive definite when acting on $\boldsymbol{w}$. Taking into account (2.9), P1 then immediately follows from theorem V.6.2, p 469 in A.

P2. Let $\varepsilon = -\varkappa^2$, $\varkappa > 0$. There exists $x_0(\varepsilon)$ such that if for some k, $1 \leqslant k \leqslant n$, and for some $x_1 \geqslant x_0(\varepsilon)$ one has

$$\exp[\mathrm{i}\varphi_k(x_1, \varepsilon)] = -1 \tag{3.1}$$

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

The proof is again based on (2.9). In analogy with the preceding case it is not difficult to show that for any non-trivial vector $\boldsymbol{w}$ satisfying $\boldsymbol{W}(x_1, \varepsilon)\boldsymbol{w} = -\boldsymbol{w}$ (cf (3.1)) one has

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

However, with $\varepsilon = -\varkappa^2$, $\boldsymbol{Q}(x, \varkappa) = -\varkappa^2 - \mathscr{V}(x)$ and $\lim_{x\to\infty} \mathscr{V}(x) = 0$. Thus, it is easy to prove that for a fixed $\varkappa > 0$ there exists $x_0(\varkappa) = x_0(\varepsilon)$ such that $\boldsymbol{Q}(x, \varkappa)$ is negative definite for $x \geq x_0(\varkappa)$. (To see this one has to employ the min–max principle for the eigenvalues of $\mathscr{V}$.) Thus, the LHS of (3.2) is negative for $x \geq x_0(\varepsilon)$ and P2 then again follows immediately from theorem V.6.2 in A.

P3. Let $x_0 > 0$ be fixed. Then any phase $\varphi_k(x_0, \varepsilon)$, $1 \leq k \leq n$, is a continuous increasing function of ε (i.e. for $\varepsilon = -\varkappa^2$, $\varphi_k(x_0, \varkappa)$ is a continuous decreasing function of $\varkappa$).

The proof is based on (2.11) and is given in A (see p 308 and theorem V.6.1 therein; the point is that the matrix $\tilde{\boldsymbol{\Omega}}(x, \varepsilon)$ is positive definite.)

P4. Choose some $\varepsilon = \varepsilon_0 = -\varkappa_0^2$. ε_0 is a k-fold degenerate eigenvalue, $0 \leq k \leq n$ ($k = 0$ denoting the case when ε_0 is not an eigenvalue) iff there are just k phase functions $\varphi_j(x, \varepsilon_0)$, $1 \leq j \leq k$, for which

$$\lim_{x\to\infty} \tan(\tfrac{1}{2}\varphi_j(x, \varkappa_0)) = -1/\varkappa_0 \tag{3.3}$$

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

$$\lim_{x\to\infty} \tan(\tfrac{1}{2}\varphi_j(x, \varkappa_0)) = +1/\varkappa_0. \tag{3.4}$$

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

Suppose that $\varepsilon_0 = -\varkappa_0^2$ is a k-fold degenerate eigenvalue, e.g. $1 \leq k < n$ (modifications for $k = 0$ or $k = n$ will be obvious). This means that there are just k linearly independent regular solutions $\boldsymbol{u}_i^-(x, \varepsilon_0)$ of (2.1) that are linear combinations of the columns of the matrix $\boldsymbol{\phi}^-$ defined by (2.4). In the rest of this proof we shall employ the parameter $\varkappa_0$ instead of ε_0. Denote the mentioned columns by $\boldsymbol{\varphi}_1^-(x, \varkappa_0), \ldots, \boldsymbol{\varphi}_n^-(x, \varkappa_0)$ and, similarly, the columns of $\boldsymbol{\phi}^+(x, \varkappa_0)$ in (2.4) by $\boldsymbol{\varphi}_1^+(x, \varkappa_0), \ldots, \boldsymbol{\varphi}_n^+(x, \varkappa_0)$. Thus

$$\boldsymbol{u}_i^-(x, \varkappa_0) = \sum_{j=1}^{n} A_{ji}\boldsymbol{\varphi}_j^-(x, \varkappa_0), \qquad i = 1, 2, \ldots, k. \tag{3.5}$$

The remaining $(n-k)$ linearly independent regular solutions $\boldsymbol{u}_i^+(x, \varkappa_0)$ are of the type

$$\boldsymbol{u}_i^+(x, \varkappa_0) = \sum_{j=1}^{n} A_{ji}\boldsymbol{\varphi}_j^+(x, \varkappa_0) + \text{terms with } \boldsymbol{\varphi}_j^-(x, \varkappa_0), \qquad i = k+1, \ldots, n. \tag{3.6}$$

It is easy to see that the linear independence of the solutions (3.5) and (3.6) implies the linear independence of the columns $\{A_{ji}\}_{j=1}^n$ of the matrix $\boldsymbol{A} \equiv \{A_{ji}\}$ for $i = 1, 2, \ldots, k$ and $i = k+1, \ldots, n$ separately. Let us now prove that, in fact, they are all linearly independent and, consequently,

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

To this end, we shall employ the identity (2.8) that means that for any pair $\boldsymbol{a}$, $\boldsymbol{b}$ of regular solutions of (2.1) one has

$$\tilde{\boldsymbol{a}}\boldsymbol{b}' - \tilde{\boldsymbol{a}}'\boldsymbol{b} = 0 \tag{3.8}$$

for $x \in \langle 0, \infty)$.

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

$$\boldsymbol{a} \equiv \boldsymbol{u}_i^-, \qquad 1 \leq i \leq k; \qquad \boldsymbol{b} \equiv \boldsymbol{u}_j^+, \qquad k+1 \leq j \leq n, \tag{3.9}$$

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

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

Since the columns of the matrix A must be non-trivial, 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 conjuction 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 polynomial of $W(x, \varkappa_0)$

$$\begin{aligned} P(\lambda, x, \varkappa_0) &= \det(W - \lambda I) \\ &= \det[(V + \mathrm{i}U)(V - \mathrm{i}U)^{-1} - \lambda (V - \mathrm{i}U)(V - \mathrm{i}U)^{-1}] \\ &= \det\{[(1-\lambda)V + \mathrm{i}(1+\lambda)U](V - \mathrm{i}U)^{-1}\}. \end{aligned} \tag{3.11}$$

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 equations (3.5), (3.6), equation (3.11) may be rewritten, after some manipulations, as follows:

$$\begin{aligned} P(\lambda, x, \varkappa_0) &= \frac{\{\mathrm{e}^{-\varkappa_0 x}[-\varkappa_0(1-\lambda) + \mathrm{i}(1+\lambda)]\}^k}{[\mathrm{e}^{-\varkappa_0 x}(-\varkappa_0 - \mathrm{i})]^k} \\ &\quad \times \frac{\{\mathrm{e}^{+\varkappa_0 x}[\varkappa_0(1-\lambda) + \mathrm{i}(1+\lambda)]\}^{n-k}}{[\mathrm{e}^{+\varkappa_0 x}(\varkappa_0 - \mathrm{i})]^{n-k}} \det(A + \Delta)/\det(A + \delta) \\ &= \left(\frac{\varkappa_0 - \mathrm{i}}{\varkappa_0 + \mathrm{i}} - \lambda\right)^k \left(\frac{\varkappa_0 + \mathrm{i}}{\varkappa_0 - \mathrm{i}} - \lambda\right)^{n-k} \det(A + \Delta)/\det(A + \delta) \end{aligned} \tag{3.12}$$

where $\Delta \equiv \Delta(\lambda, x, \varkappa_0)$, $\delta \equiv \delta(\lambda, x, \varkappa_0)$ are some $n \times n$ matrices such that $\lim_{x\to\infty} \Delta(\lambda, x, \varkappa_0) = \lim_{x\to\infty} \delta(\lambda, x, \varkappa_0)$. Note that (3.12) holds for any k, $0 \leqslant k \leqslant n$. Obviously, (3.7) now implies that

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

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

$$\lim_{x\to\infty} P(\lambda, x, \varkappa_0) = \left(\frac{\varkappa_0 - \mathrm{i}}{\varkappa_0 + \mathrm{i}} - \lambda\right)^k \left(\frac{\varkappa_0 + \mathrm{i}}{\varkappa_0 - \mathrm{i}} - \lambda\right)^{n-k}. \tag{3.14}$$

Thus, assuming the existence of the limits for $x \to \infty$ of the eigenvalues of $W(x, \varkappa_0)$, from (3.14) we easily obtain 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 $P(\lambda, x, \varkappa_0)$ (i.e. by (3.14))†.

P5. For any phase function $\varphi_j(x, \varepsilon)$, $1 \leqslant j \leqslant n$, there exists ε_0 such that for $\varepsilon < \varepsilon_0$, $\varphi_j(x, \varepsilon) < \pi$ for $x \in \langle 0, \infty)$.

Proof. The conditions (i), (ii) imposed on the potential matrix $\mathscr{V}$ imply that the matrix elements of $\mathscr{V}$ are bounded for $x \in \langle 0, \infty)$. Consequently, there exists $\varkappa_0$ so large that

† We are grateful to B Lonek for explaining this point to us.

$Q(x, \varkappa_0) = -\varkappa_0^2 - \mathscr{V}(x)$ is negative definite for any $x \in \langle 0, \infty)$ (cf the proof of P2). Since φ_j is continuous with respect to x and the condition (2.15) holds, it follows from the proof of P2 that for any $j = 1, \ldots, n$, $\varphi_j(x, \varepsilon_0)$ with $\varepsilon_0 = -\varkappa_0^2$ must stay below π for $x \in \langle 0, \infty)$. Finally, according to P3, for any $x \in (0, \infty)$ we have $\varphi_j(x, \varepsilon) < \varphi_j(x, \varepsilon_0) < \pi$ if $\varepsilon < \varepsilon_0$, and P5 is thereby proved.

We see that the phase functions possess the properties analgous to those of the Prüfer phase function z relevant in the scalar case (notice the correspondence $\frac{1}{2}\varphi \leftrightarrow z$). This leads us to a straightforward generalisation of the theorems relating asymptotic properties of the phase functions to the bounds for the eigenvalues of the original system of SE, which for the scalar case have been proved by Úlehla and Havlíček (1980), Adamová (1981) and Adamová and Úlehla (1983). Such a generalisation will be the subject of § 4.

4. Phase functions and the eigenvalue problem

Theorem 4.1. Let ε_0 be fixed. Denote by $\varphi_1(\infty, \varepsilon), \ldots, \varphi_n(\infty, \varepsilon)$ the limits $\lim_{x\to\infty} \varphi_1(x, \varepsilon), \ldots, \lim_{x\to\infty} \varphi_n(x, \varepsilon)$. Then:

(I) There exists a positive integer m and a set of three non-negative integers $\{n_1, n_2, n_3\}$ satisfying

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

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

(recall that n is the dimension of the system in (2.1)), such that

$$\tfrac{1}{2}\varphi_j(\infty, \varepsilon_0) = (m-1)\pi + \tan^{-1}(1/\sqrt{-\varepsilon_0}), \qquad j = 1, \ldots, n_1, \tag{4.3}$$

$$\tfrac{1}{2}\varphi_j(\infty, \varepsilon_0) = m\pi - \tan^{-1}(1/\sqrt{-\varepsilon_0}), \qquad j = n_1 + 1, \ldots, n_2, \tag{4.4}$$

$$\tfrac{1}{2}\varphi_j(\infty, \varepsilon_0) = m\pi + \tan^{-1}(1/\sqrt{-\varepsilon_0}), \qquad j = n_2 + 1, \ldots, n_3, \tag{4.5}$$

$$\tfrac{1}{2}\varphi_j(\infty, \varepsilon_0) = (m+1)\pi - \tan^{-1}(1/\sqrt{-\varepsilon_0}), \qquad j = n_3 + 1, \ldots, n\dagger. \tag{4.6}$$

(II) ε_0 is an eigenvalue with $(n_2 - n_1 + n - n_3)$-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 $n(\varepsilon_0) = nm - n_2$ eigenvalues less than ε_0, $n(\varepsilon_0)$ involving each of the different eigenvalues according to its degeneracy.

The proof is based on (2.15), (2.16) and the properties P1–P5.

Now, keep ε_0 fixed and consider the functions $\varphi_1(\infty, \varepsilon), \ldots, \varphi_n(\infty, \varepsilon)$ in the interval $I(\varepsilon_0) = (-\infty, \varepsilon_0\rangle$. The following holds.

Theorem 4.2. (I) For each $j = 1, \ldots, n$ the function $\varphi_j(\infty, \varepsilon)$ is positive, increasing and piecewise continuous in $I(\varepsilon_0)$.

(II) $\tilde{\varepsilon} \in I(\varepsilon_0)$ is an eigenvalue iff $\tilde{\varepsilon}$ is a discontinuity point of at least one of the functions $\varphi_1(\infty, \varepsilon), \ldots, \varphi_n(\infty, \varepsilon)$.

† Equations (4.3)–(4.6) are to be understood in the following sense: if it happens that at least one equality in (4.1) takes place, 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).

(III) Supposing $\tilde{\varepsilon}$ is a discontinuity point of a function $\varphi_j(\infty, \varepsilon)$, $1 \leq j \leq n$, it holds that

$$\lim_{\eta \to 0^+} [\tfrac{1}{2}\varphi_j(\infty, \tilde{\varepsilon} + \eta) - \tfrac{1}{2}\varphi_j(\infty, \tilde{\varepsilon} - \eta)] = \pi. \tag{4.7}$$

The proof follows from the properties P1–P5 and can be carried out in analogy with the scalar case (see Adamová 1981).

Thus, all the eigenvalues contained in $I(\varepsilon_0)$ could in principle be determined if the functions $\varphi_1(\infty, \varepsilon), \ldots, \varphi_n(\infty, \varepsilon)$ were reconstructed in $I(\varepsilon_0)$ and their discontinuities found. Since we are not able to reconstruct the functions $\varphi_1(\infty, \varepsilon), \ldots, \varphi_n(\infty, \varepsilon)$ numerically, it is a crucial point that the properties of these functions are signalled already by the behaviour of functions $\varphi_1(x_0, \varepsilon), \ldots, \varphi_n(x_0, \varepsilon)$ with a suitably large but finite x_0.

Theorem 4.3. Let $\varepsilon = \varepsilon_0$ be fixed and $\tilde{x}$ be such that for $x > \tilde{x}$ the matrix $(\varepsilon_0 - \mathscr{V}(x))$ is negative definite when applied to eigenvectors of $\boldsymbol{W}(x, \varepsilon)$, $\varepsilon \leq \varepsilon_0$, associated with the 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 non-negative integers $\{n_1, n_2, n_3\}$ with the properties (4.1), (4.2) such that

$$\tfrac{1}{2}\varphi_j(x_0, \varepsilon_0) \in \langle (m-1)\pi, m\pi - \tfrac{1}{2}\pi \rangle, \qquad j = 1, 2, \ldots, n_1, \tag{4.3'}$$

$$\tfrac{1}{2}\varphi_j(x_0, \varepsilon_0) \in (m\pi - \tfrac{1}{2}\pi, m\pi), \qquad j = n_1 + 1, \ldots, n_2, \tag{4.4'}$$

$$\tfrac{1}{2}\varphi_j(x_0, \varepsilon_0) \in \langle m\pi, m\pi + \tfrac{1}{2}\pi \rangle, \qquad j = n_2 + 1, \ldots, n_3, \tag{4.5'}$$

$$\tfrac{1}{2}\varphi_j(x_0, \varepsilon_0) \in (m\pi + \tfrac{1}{2}\pi, (m+1)\pi), \qquad j = n_3 + 1, \ldots, n. \tag{4.6'}$$

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

(II) There are $n(\varepsilon_0)$ eigenvalues less than ε_0, $n(\varepsilon_0)$ being a non-negative integer which can take on one of the values $nm - n_2$, $nm - n_2 + 1, \ldots, n(m+1) - n_1 - n_3$.

Thus, from the values of the phase functions $\varphi_1(x, \varepsilon_0), \ldots, \varphi_n(x, \varepsilon_0)$ at the point x_0 one obtains the information on the number of eigenvalues less than ε_0. Moreover, reconstructing functions $\varphi_1(x_0, \varepsilon), \ldots, \varphi_n(x_0, \varepsilon)$ in the interval $I(\varepsilon_0)$ 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. The following 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 $nm - n_2 \geq 1$, i.e. there is at least one eigenvalue less than ε_0, and consider the functions $\varphi_1(x_0, \varepsilon), \ldots, \varphi_n(x_0, \varepsilon)$ with x_0 fixed and ε varying within $I(\varepsilon_0)$. For each j, $1 \leq j \leq n$, such that $\varphi_j(x_0, \varepsilon_0) \geq 2\pi$ define a set of intervals $\{I_k^j\}$ satisfying $I_k^j \subset I(\varepsilon_0)$, by the relations

$$I_k^j = \langle \bar{\varepsilon}_k^j, \bar{\bar{\varepsilon}}_k^j \rangle, \tag{4.8}$$

$$\tfrac{1}{2}\varphi_j(x_0, \bar{\varepsilon}_k^j) = k\pi - \tfrac{1}{2}\pi, \tag{4.9}$$

$$\tfrac{1}{2}\varphi_j(x_0, \bar{\bar{\varepsilon}}_k^j) = k\pi. \tag{4.10}$$

In this definition, for a given j, k is varying in the range $1, 2, \ldots, n_j$ where $\Sigma_j\, n_j = nm - n_2$. The intervals I_k^j have the following properties.

(I) Each I_k^j contains just one eigenvalue $\varepsilon_k^j < \varepsilon_0$.

(II) When x_0 is increased the length of each of the intervals I_k^j decreases. In the limit $x_0 \to \infty$ each of the intervals I_k^j degenerates into one point which is just one of the eigenvalues $\varepsilon_k^j < \varepsilon_0$.

The proofs of theorems 4.3, 4.4 are based on (2.15), (2.16) and the properties P1–P5 in analogy with what has been done for the scalar case (Adamová 1981).

According to theorem 4.4 one can find intervals each of which contains just one eigenvalue less than ε_0, by reconstructing the functions $\varphi_1(x_0, \varepsilon), \ldots, \varphi_n(x_0, \varepsilon)$ for $\varepsilon \in I(\varepsilon_0)$. 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. Úlehla *et al* 1981, Adamová 1981). Of course, in the matrix case discussed in the present paper the situation is complicated by the possible degeneracy of the eigenvalues.

We conclude this section with a remark concerning the role of the x_0 value. Mostly, already the first choice of x_0 such that $(\mathcal{V}(x) - \varepsilon_0)$ is positive definite for $x \geqslant x_0$ provides one with eigenvalue intervals small enough, i.e. for a given eigenvalue ε one gets a lower bound $\varepsilon_{\min}$ and an upper bound $\varepsilon_{\max}$ the distance of which is smaller than a required accuracy. Increasing x_0 one obtains a lower bound $\varepsilon'_{\min}$ and an upper bound $\varepsilon'_{\max}$ and it holds that $\varepsilon'_{\min} \geqslant \varepsilon_{\min}$, $\varepsilon'_{\max} \leqslant \varepsilon_{\max}$.

It may happen that the x_0 value necessary for reaching a desired accuracy is unsuitably large. Then, it is convenient to perform the transformation $x \to ay$, $\mathcal{V}(x) \to \mathcal{W}(y) = a^2\mathcal{V}(ay)$, $\varepsilon \to E = a^2\varepsilon$, where a is a sufficiently large constant, and use the new variable y in the numerical calculations.

We have performed a great number of eigenvalue calculations for the scalar as well as for the matrix (2×2) cases and always obtained eigenvalues with a desired accuracy (e.g. to seven or more digits) for reasonably large x_0 values.

5. Concluding remarks and an outlook

We have discussed the phase functions defined by means of the APT of a coupled system of radial SE. 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 first-order nonlinear equations either for the matrix $\boldsymbol{W}(x, \varepsilon)$ or for the phase functions themselves.

As regards the first possibility, one may use the Riccati-type equation (2.13) together with the initial condition $\boldsymbol{W}(0, \varepsilon) = \boldsymbol{I}$. Standard theorems on the uniqueness of the solutions of differential equations then obviously guarantee the one-to-one correspondence between (2.13) supplemented with the above-mentioned initial condition and the original system of SE. In such an approach the matrix $\boldsymbol{W}$ should be diagonalised in the course of the integration of (2.13) and the phase functions reconstructed to be continuous with respect to 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 2×2 potential matrices, when $\boldsymbol{W}$ can be easily diagonalised explicitly. Nevertheless, the situation is somewhat more complicated than in the scalar case and the corresponding nonlinear first-order differential system as well as the results of numerical calculation will be discussed elsewhere. Note that a system of nonlinear first-order equations based on an alternative transformation of the original system of SE has been already discussed by Úlehla (1982).

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, a number of physically interesting examples are described by potential matrices with singularities of various types, e.g. due to Coulomb-like or 'centrifugal' ($\sim 1/x^2$) terms singular at the origin, or due to 'confining' terms ($\sim x^\alpha$, $\alpha > 0$) singular for $x \to \infty$. We have investigated also some of these singular problems (the corresponding analysis will appear elsewhere).

Firstly, we have analysed the asymptotic behaviour of the phase functions for $x \to \infty$ for potential matrices with confining terms at the diagonal. In this case each of the phase functions goes to a multiple of 2π for $x \to \infty$ and a given ε is a k-fold degenerate eigenvalue iff k of the phase functions approach their limits for $x \to \infty$ from below and $(n-k)$ from above.

Secondly, we have investigated problems with 2×2 potential matrices involving Coulomb-like and centrifugal singularities at the origin and checked that the theorems given in the present paper apply also to this case.

Generally, considering problems with $n \times n$ potentials singular at the origin, $n \geqslant 2$, we expect that the results given in the present paper are relevant also in these cases. It is known that some authors, working up a problem with such a potential numerically and trying to avoid computational difficulties, utilise the approach based on regularising the original potential near the origin so as to satisfy (i), (ii) (see e.g. Reid 1968, Pham and Richard 1977 and references therein). Then the results of the present paper are directly applicable.

Note that this 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. by Bellman and Cooke (1963)). This stability property is necessary to ensure that the solutions obtained by the numerical integration of the equations with the regularised potential 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 (Adamová and Úlehla 1983) we expect that the relevant solutions of the first-order nonlinear equations discussed in the present paper are asymptotically stable. Work on these problems is in progress.

Acknowledgment

We are grateful to Dr M Havlíček for a careful reading of the manuscript and for numerous discussions concerning the subject of this paper.

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