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1990 J. Phys. A: Math. Gen. 23 2055

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Transformations in quantum action variable theory

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Received 1 August 1989

Abstract. The transformed quantum momentum function (QMF) equation presented here is derived by transforming the quantum momentum function while keeping the form of its equation and the action variable integral unchanged. This new transformed equation is suitable for solving quantum systems having complex turning points and more than two turning points. New forms of boundary conditions in the QMF are obtained and several applications of this transformed QMF equation are given.

1. Introduction/overview

In an earlier work [1, 2], quantum action variable theory is shown to be an alternative method of obtaining boundstate energy eigenvalues without finding the system wavefunctions. In one dimension, the quantum action variable, the quantum analogue of the classical action variable, is defined as a contour integral

$$J = \frac{1}{2\pi} \int_C p(x) dx \quad (1.1)$$

where the quantum momentum function (QMF), $p(x)$, is the solution of the quantum momentum function equation (QMF equation),

$$\frac{\hbar}{i} \left(\frac{dp(x)}{dx} \right) + p^2(x) = p_c^2(x). \quad (1.2)$$

$p_c(x)$ is the classical momentum function defined as $p_c(x) = \sqrt{E - v(x)}$. The contour C in equation (1.1) encloses the two physical turning points of $p_c(x)$. The boundstate boundary condition imposed upon QMF $p(x)$ is

$$p(x) \rightarrow p_c(x) \quad \text{as} \quad \hbar \rightarrow 0. \quad (1.3)$$

The quantum action variable J can be used to obtain the energy eigenvalues without solving the QMF equation (1.2) as shown in [1] and [2].

In three dimensions, if the potential is central, the QMF can be separated, and the radial QMF equation [2] is

$$\frac{\hbar}{i} \left[\frac{1}{r^2} \left(\frac{d}{dr} (r^2 p_r(r)) \right) \right] + p_r^2(r) = p_{rc}^2(r) \quad (1.4)$$

where $p_{rc}(r)$ is $\sqrt{E - v(r) - [l(l+1)\hbar^2/r^2]}$ and $p_r(r)$ is the radial QMF. As in one dimension, the radial quantum action variable J_r in three dimensions is

$$J_r = \frac{1}{2\pi} \int_{C_r} p_r(r) dr \quad (1.5)$$

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where C_r encloses the two turning points of $p_{rc}(r)$. The boundary condition on radial QMF is

$$p_r(r) \rightarrow p_{rc}(r) \quad \text{as} \quad \hbar \rightarrow 0. \quad (1.6)$$

All the exactly solvable quantum systems discussed in [1] and [2] have following properties:

- (1) all the turning points (both physical and unphysical) are real;
- (2) all the systems have two turning points, except in one system.

The exception ($v(x) = a/x + x^2$), which has four turning points, has been solved by using symmetric properties. The major problem of solving those systems which have more than two turning points is in locating the moving poles of the quantum momentum function. When the turning points are complex, the problem becomes more difficult.

In this paper we show how to solve quantum systems having more than two turning points and complex turning points. In section 2, we discuss the new boundary conditions for the QMF which can be used to evaluate the quantum action variable J . Section 3 shows how to make transformations on a QMF equation to eliminate the complex turning points and to reduce the number of turning points in the system, whilst keeping the contour integral J and the form of the quantum momentum function equation unchanged. Sections 4 and 5 contain a number of illustrations for the use of transformations discussed in section 3. Finally, in section 6, we discuss the limitations of this transformation method and make concluding remarks.

2. Boundary conditions

The boundary condition imposed upon the QMF in [1] and [2] is $p \rightarrow p_c$ as $\hbar \rightarrow 0$ for both one- and three-dimensional systems. In this section, we obtain new boundary conditions on the QMF which are equivalent to the boundary conditions on Schrödinger's wavefunction u and the normalisation condition. It can be shown that these new boundary conditions are equivalent to the old boundary condition $p \rightarrow p_c$ as $\hbar \rightarrow 0$.

Consider the transformation

$$p(x) = \frac{\hbar}{i} \left(\frac{du/dx}{u} \right) \quad (2.1)$$

or

$$u = \exp\left(\frac{i}{\hbar} \int p(x) dx\right). \quad (2.2)$$

Substituting equation (2.1) in the one-dimensional QMF equation (1.2), we get the one-dimensional Schrödinger equation ($2m = 1$)

$$\hbar^2 \left(\frac{d^2 u}{dx^2} \right) + p_c^2(x) u = 0 \quad (2.3)$$

where $p_c(x) = \sqrt{E - v(x)}$. The boundstate boundary condition on equation (2.3) is

$$u \rightarrow 0 \quad \text{as} \quad x \rightarrow \infty. \quad (2.4)$$

Using equation (2.2), the equivalent condition on $p(x)$ is

$$\frac{i}{\hbar} \int p(x) dx \rightarrow -\infty \quad \text{as} \quad x \rightarrow \infty. \quad (2.5)$$

Now consider the points where $p_c(x)$ has real poles. The normalisation condition on wavefunction u demands that

$$\frac{i}{\hbar} \int p(x) dx \rightarrow -\infty \tag{2.6}$$

as $x \rightarrow$ real poles of $p_c(x)$. Otherwise wavefunction u will not be finite.

For three-dimensional radial potentials, similar boundary conditions can be derived on the radial QMF $p_r(r)$. They are

$$\frac{i}{\hbar} \int p_r(r) dr \rightarrow -\infty \quad \text{as} \quad r \rightarrow 0 \quad \text{and} \quad r \rightarrow \infty \tag{2.7}$$

and

$$\frac{i}{\hbar} \int p_r(r) dr \rightarrow -\infty \tag{2.8}$$

as $r \rightarrow$ real poles of classical momentum function $p_{cr}(r)$.

The boundary conditions derived on the QMF in this section are useful in deriving boundary conditions for the transformed quantum momentum function as shown in the next section.

3. Simple transformations on the QMF equation

In order to evaluate the quantum action variable J , one must know the locations and the distribution of the poles of the QMF. The locations and distribution of the moving poles of QMF $p(x)$ (these are the poles of $p(x)$ which are not the poles of $p_c(x)$) are found by using the oscillatory theorems given in the appendix. When the systems have complex turning points or have more than two turning points, finding the locations and the distribution of the moving poles of $p(x)$, and hence the evaluation of quantum action variable J becomes impossible. In this section we show how to reduce the number of turning points and eliminate complex poles by transformations.

Consider the one-dimensional QMF equation. Suppose the transformation $x = g(y)$ changes the $p_c(x)$ to a 'simple' form (for examples, see sections 4 and 5), where y is the new variable in the quantum momentum function equation. This changes the form of QMF equation (1.2) and the contour integral (1.1). The form of the QMF equation (1.2) is important to locate the poles of the QMF by theorems given in the appendix and the form of the contour integral (1.1) is necessary to use the residue theorem to evaluate J . In order to keep the form of (1.1) and (1.2) unchanged, the quantum momentum function has to be transformed. Consider the transformation

$$p(y) = a(y)P(y) + b(y) \tag{3.1}$$

where $p(y)$ and $P(y)$ are the old and new quantum momentum functions respectively. The functions $a(y)$ and $b(y)$ are found by substituting (3.1) in (1.1) and (1.2) and imposing the condition that the forms of the contour integral (1.1) and the equation (1.2) are invariant. This results in

$$a(y) = \frac{1}{g'(y)} \tag{3.2}$$

and

$$b(y) = \frac{\hbar}{2i} \left(\frac{g''}{g'^2} \right). \tag{3.3}$$

Hence the transformed QMF equation becomes

$$\frac{\hbar}{i} \left(\frac{dP(y)}{dy} \right) + P^2(y) = \left[[E - vg(y)]g'^2 + \frac{\hbar g'''}{2g'} - \frac{3\hbar^2}{4} \left(\frac{g''}{g'} \right)^2 \right] = P_c^2(y) \tag{3.4}$$

and the quantum action variable integral becomes

$$J = \frac{1}{2\pi} \int_{C_y} P(y) dy \tag{3.5}$$

where the contour C_y encloses the two physical turning points of the new $P_c(y)$.

Consider the transformations $r = g(y)$ and $P(y) = a(y)p(y) + b(y)$ on the three-dimensional radial QMF equation. Imposing the condition that the form of the radial QMF equation and the contour integral for J_r are unchanged, we obtain the transformed radial quantum momentum function equation

$$\frac{\hbar}{i} \left(\frac{dP(y)}{dy} \right) + P^2(y) = \left[[E - vg(v)]g'^2 + \frac{\hbar g'''}{2g'} - \frac{3\hbar^2}{4} \left(\frac{g''}{g'} \right)^2 \right] = P_{cr}^2(y). \tag{3.6}$$

Under these transformations, the quantum action variable integral is

$$J_r = \frac{1}{2\pi} \int_{C_r} P(y) dy \tag{3.7}$$

where the contour $C_{y_r}(y)$ encloses the two physical turning points of $P_{cr}(y)$. These transformed equations are easier to solve than the original equations, for a wide range of potentials.

Before leaving this section, let us consider the boundary conditions on the transformed quantum momentum function $P(y)$ with respect to the new variable y . In variable y (2.2) becomes

$$u = \exp\left(\frac{i}{\hbar} \int P(y) dy + \frac{1}{2} \ln g' \right). \tag{3.8}$$

Then the boundary conditions on transformed QMF P becomes

$$\frac{i}{\hbar} \int P(y) dy + \frac{1}{2} \ln g' \rightarrow -\infty \tag{3.9}$$

as $y \rightarrow \infty$ or $y \rightarrow$ any pole of $p_c(y)$. In three dimensions, the boundary conditions on the transformed radial QMF are

$$\frac{i}{\hbar} \int P(y) dy + \frac{1}{2} \ln g' \rightarrow -\infty \tag{3.10}$$

as $y \rightarrow \infty$, $y \rightarrow 0$, or $y \rightarrow$ any pole of $P_{cr}(y)$. In the next section we show how these transformations and boundary conditions are used to evaluate quantum action variable and hence get the bound-state energy eigenvalues for a range of potentials.

4. Illustrations: one dimension

The ‘barrier oscillator’ potential is defined as $v(x) = a^2/x^2 + x^2$. This system has four turning points and can be solved by using its symmetric properties [2]. As for the first illustration we solve this system by the transformed QMF equation (3.4). Under the transformation $x = g(y) = \sqrt{y}$, the transformed quantum momentum function for the barrier oscillator becomes

$$\frac{\hbar}{i} \left(\frac{dP(y)}{dy} \right) + P^2(y) = P_c^2(y) \tag{4.1}$$

where

$$P_c^2(y) = \frac{E}{4y} - \frac{a^2}{4y^2} - \frac{1}{4} + \frac{3\hbar^2}{16y^2}. \tag{4.2}$$

The new classical momentum function $P_c(y)$ now has two real turning points unlike the original system which had four turning points. The oscillatory theorems in the appendix can be used to prove that there are no poles of $P(y)$ present in the complex y plane except at $y = 0, y = \infty$ (fixed poles), and on the real axis between two turning points (moving poles).

J has the value $n\hbar$ which corresponds to the contour C enclosing n moving poles of $P(y)$ ($n = 0, 1, 2, \dots$). As in [1], we evaluate the contour integral for J by distorting the contour C to enclose poles at $y = 0$ and $y = \infty$. Let J_0 and J_∞ be the contributions from poles at $y = 0$ and $y = \infty$ respectively. J_0 is calculated by expanding $P(y)$ near the origin. Let

$$P(y) = a_{-1}y^{-1} + a_0 + \dots \tag{4.3}$$

Substituting (4.3) in (4.1) and equating coefficient of y^{-2} , we get

$$a_{-1} = \frac{\hbar}{2i} \pm \frac{1}{2i} \sqrt{a^2 + \hbar^2/4}.$$

The boundary condition (3.9) is satisfied only by

$$a_{-1} = \frac{\hbar}{2i} + \frac{1}{2i} \sqrt{a^2 + \hbar^2/4}. \tag{4.4}$$

Since the distorted contour encloses the point $y = 0$ in the clockwise direction, $J_0 = -ia_{-1}$ and hence

$$J_0 = \frac{-\hbar}{2} - \frac{1}{2} \sqrt{a^2 + \hbar^2/4}. \tag{4.5}$$

J_∞ is calculated by making the transformation $s = 1/r$. Under this transformation (4.1) becomes

$$\frac{-\hbar}{i} \left(\frac{dP(s)}{ds} \right) + \frac{P^2(s)}{s^2} = \frac{P_c^2(1/s)}{s^2} \tag{4.6}$$

where

$$P_c^2(1/s) = \frac{Es}{4} - \frac{a^2s^2}{4} - \frac{1}{4} + \frac{3\hbar^2s^2}{16}. \tag{4.7}$$

Now we expand $P(s)$ near $s=0$ as

$$P(s) = a_0 + a_1s + \dots \tag{4.8}$$

Substituting (4.8) in (4.7) and equating the coefficient of s^{-2} , we get $a_0 = \pm i/2$ and $a_1 = E/8a_0$. The boundary condition (3.9) is satisfied only by $a_0 = i/2$. Therefore

$$J_\infty = \frac{E}{4} \tag{4.9}$$

Summing J_0 and J_∞ gives

$$J = \frac{E}{4} - \frac{\hbar}{2} - \frac{1}{2} \sqrt{a^2 + \hbar^2/4} \tag{4.10}$$

Since J is also $n\hbar$, equating two forms of J gives the bound-state energy

$$E = 2(2n + 1)\hbar + 2\sqrt{a^2 + \hbar^2/4} \tag{4.11}$$

The second illustration is the one-dimensional Pöschl-Teller potential hole

$$v(x) = \frac{a}{\sin^2 \alpha x} + \frac{b}{\cos^2 \alpha x} \tag{4.12}$$

where a and b are positive real constants. The $p_c(x)$ has an infinite number of turning points. The number of turning points is reduced to two by the transformation $x = g(y) = \alpha^{-1} \sin^{-1} \sqrt{y}$. The transformed QMF equation for this potential is (4.1) with

$$P_c^2 = \frac{E}{4\alpha^2 y(1-y)} - \frac{a}{4\alpha^2 y^2(1-y)} - \frac{b}{4\alpha^2 y(1-y)^2} - \frac{\hbar^2}{4y(1-y)} + \frac{3\hbar^2}{16y^2}.$$

This system has three fixed poles of P at $y=0$, $y=1$, and $y=\infty$ and moving poles between two turning points. Thus $J = J_0 + J_1 + J_\infty$ where J_0 , J_1 , and J_∞ are the contribution from poles of $P(y)$ at $y=0$, $y=1$ and $y=\infty$ respectively. Following the same procedure used in the first illustration we get

$$J_0 = -\frac{\hbar}{2} - \frac{\sqrt{a + \hbar^2 \alpha^2/4}}{2\alpha} \tag{4.13}$$

$$J_1 = -\frac{\hbar}{2} - \frac{\sqrt{b + \hbar^2 \alpha^2/4}}{2\alpha} \tag{4.14}$$

and

$$J_\infty = \frac{\hbar}{2} + \frac{\sqrt{E}}{2\alpha} \tag{4.15}$$

Hence the quantum action variable J is

$$J = \frac{\hbar}{2} + \frac{\sqrt{E}}{2\alpha} - \frac{\hbar}{2} - \frac{\sqrt{a + \hbar^2 \alpha^2/4}}{2\alpha} - \frac{\hbar}{2} - \frac{\sqrt{b + \hbar^2 \alpha^2/4}}{2\alpha} \tag{4.16}$$

For convenience take $a = \hbar^2 \alpha^2 \beta(\beta - 1)$ and $b = \hbar^2 \alpha^2 \lambda(\lambda - 1)$. Thus we have

$$J = \frac{\hbar}{2} + \frac{\sqrt{E}}{2\alpha} - \frac{\hbar(\lambda + \beta)}{2} \tag{4.17}$$

Since $J = n\hbar$, we obtain the boundstate energy E as

$$E = \hbar^2 \alpha^2 (2n + \lambda + \beta)^2 \tag{4.18}$$

where $n = 0, 1, 2, \dots$

The last one-dimensional illustration is the ‘cosh’ potential [3]. This system also has an infinite number of complex turning points. Consider the transformation $x = g(y) = \alpha^{-1} \cosh^{-1} \sqrt{y}$, where the transformed QMF equation is (4.1) with

$$P_c^2(y) = \frac{E}{4\alpha^2 y(1-y)} - \frac{\hbar^2 \lambda(\lambda-1)}{4y^2(1-y)} - \frac{\hbar^2}{4y(1-y)} + \frac{3\hbar^2}{16y^2}. \tag{4.19}$$

As in the two previous systems, this system has two real turning points. The $P(y)$ has three poles at $y = 0$, $y = 1$, and $y = \infty$ as in the previous illustration. Thus $J = J_0 + J_1 + J_\infty$ and J_0 , J_1 , and J_∞ are evaluated as before. The result is

$$J_0 = -\frac{3\hbar}{4} + \frac{\hbar\lambda}{2} \tag{4.20}$$

$$J_1 = \frac{-\hbar}{4} \text{ or } \frac{-3\hbar}{4} \tag{4.21}$$

and

$$J_\infty = \frac{\hbar}{2} - \frac{\kappa\alpha}{2} \tag{4.22}$$

where $\kappa = +\sqrt{-E}$. J_1 has two possible values and both of these values agree with the boundary condition (3.3). Therefore

$$J = \frac{-\hbar}{2} + \frac{\hbar\lambda}{2} - \frac{\kappa\alpha}{2} \tag{4.23}$$

or

$$J = -\hbar + \frac{\hbar\lambda}{2} - \frac{\kappa\alpha}{2}. \tag{4.24}$$

The bound-state energies are found by combining (4.22), (4.23) and $J = n\hbar$.

$$E = -\alpha^2 \hbar^2 (\lambda - 1 - n) \tag{4.25}$$

with $\lambda - 1 \geq n$. Note that the condition $\lambda - 1 \geq n$ is obtained by using the fact that $\kappa \geq 0$.

5. Illustrations: three dimensions

Two illustrations are given in this section to show how to use the transformed radial QMF equation to evaluate the contour integral for J_r . Both systems are solved for S states ($l = 0$).

The first 3D illustration is the Morse potential. The potential is

$$v(r) = D \left\{ \exp \left[-2\alpha \left(\frac{r-r_0}{r_0} \right) \right] - 2 \exp \left[-\alpha \left(\frac{r-r_0}{r_0} \right) \right] \right\}. \tag{5.1}$$

Consider the transformation $r = g(y) = r_0 - \alpha^{-1} r_0 \ln(y)$. The transformed radial QMF equation is

$$\frac{\hbar}{i} \left(\frac{dP_r(y)}{dr} \right) + P_r^2(y) = P_{rc}^2(y) \tag{5.2}$$

where

$$P_{rc}^2(y) = \frac{\lambda E}{y^2} - D\lambda + \frac{2D\lambda}{y} + \frac{\hbar^2}{4y^2}$$

and $\lambda = r_0^2/\alpha^2$.

This system has two real turning points and the method of evaluating quantum action variable J_r is same as in the 1D case. This system has two fixed poles at $y = 0$ and $y = \infty$. Thus $J = J_0 + J_\infty$. Expanding $P_r(y)$ at $y = 0$ and $y = \infty$ and applying boundary conditions (3.10), we get

$$J_0 = \frac{-\hbar}{2} - \kappa\sqrt{\lambda} \tag{5.3}$$

and

$$J_\infty = -\sqrt{D\lambda} \tag{5.4}$$

where $\kappa = \sqrt{-E}$. Thus

$$J = \frac{-\hbar}{2} - \kappa\sqrt{\lambda} + \sqrt{D\lambda}. \tag{5.5}$$

J is also $n\hbar$ where $n = 0, 1, 2, \dots$. Bound-state energies are given by

$$E = -D + 2(n + \frac{1}{2})\hbar\sqrt{\frac{D}{\lambda}} - \frac{(n + \frac{1}{2})^2\hbar^2}{\lambda}. \tag{5.6}$$

For convenience, we introduce ω , β , and ξ (see [3])

$$\omega^2 = \frac{4D\alpha^2}{r_0^2} \quad \beta^2 = \frac{Er_0^2}{\hbar^2} \quad \gamma = \frac{Dr_0}{\hbar^2} \quad \xi = \frac{2\gamma}{\alpha}.$$

E in these parameters is

$$E = -D + \hbar\omega \left[(n + \frac{1}{2}) - \frac{1}{\xi} (n + \frac{1}{2})^2 \right]. \tag{5.7}$$

The last illustration is the Hulthén potential

$$v(r) = -y_0 \frac{e^{-r/a}}{1 - e^{-r/a}} \tag{5.8}$$

The suitable transformation is $r = g(y) = -a \ln(y)$. The transformed radial QMF equation is (5.2) with

$$P_c^2(y) = \frac{Ea^2}{y^2} + \frac{v_0 a^2}{y(1-y)} + \frac{\hbar^2}{4y^2}.$$

This system has two turning points; one is at

$$y = \left(\frac{4Ea^2 + \hbar^2}{4Ea^2 - 4v_0} \right)$$

and the other is at ∞ . $P_r(y)$ has three fixed poles at $y=0$, $y=1$, and $y=\infty$, where $J = J_0 + J_1 + J_\infty$ and J_0 , J_1 , and J_∞ are calculated as before. The result is

$$J_0 = \frac{-\hbar}{2} - \kappa a \tag{5.9}$$

$$J_1 = -\hbar \tag{5.10}$$

and

$$J_\infty = \frac{\hbar}{2} + a\sqrt{\kappa^2 + v_0} \tag{5.11}$$

where $\kappa = \sqrt{-E}$. Thus the quantum action variable is

$$J_r = -\kappa a - \hbar + a\sqrt{\kappa^2 + v_0}. \tag{5.12}$$

For convenience we introduce a new parameter β where $\beta = v_0 a^2 / \hbar^2$. The bound-state energy is found in terms of β

$$E = -\frac{v_0[\beta^2 - (n-1)^2]^2}{2\beta(n+1)^2}. \tag{5.13}$$

6. Conclusions

In this paper, a new form of boundary conditions is introduced to the QMF. These conditions are extended to deal with the transformed QMF equation. Illustrations given in the last two sections show how the transformed QMF equation can be used to evaluate the quantum action variable J for a wide range of potentials, most of which cannot be solved by the direct method ([1] and [2]).

For certain potentials one cannot find a suitable transformation to make the system exactly solvable. However in most of these cases the transformed quantum momentum function equation combined with the quantum action variable perturbation theory [4] can be used to find the approximate bound-state energy eigenvalues.

Appendix

The following theorems on the zeros of second-order differential equations are useful in determining the distribution of poles of the quantum momentum function [5, 6]. To apply these theorems one uses the relation $p(x) = (\hbar/i)u'(x)/u(x)$ where $p(x)$ is the QMF and u is the solution of the second-order Schrödinger equation.

Theorem 1. Consider the equation

$$\frac{d^2u(x)}{dx^2} + J(x)u(x) = 0.$$

Suppose J is continuous and bounded in the interval $a \leq x \leq b$ and let g be the upper bound of J in this interval. A sufficient condition that the solution of the above equation should have at least m zeros in (a, b) is that

$$g \geq m^2 \pi^2 / (b - a)^2.$$

Consider the differential equation

$$\frac{d^2 u(z)}{dz^2} + J(z)u(z) = 0. \quad (\text{A1})$$

Theorem 2. If throughout the interval (a, b) [on the $\text{Re } z$ axis], either $\text{Re } J(z) \leq 0$ or $\text{Im } J(z)$ does not change the sign, then there can be at most one zero of $w \, dw/dz$ in that interval.

Theorem 3. If $w(z)$ is a solution which is real on a segment (a, b) of the real axis; if, further, T is a region symmetrically situated with respect to the real axis, and such that every line perpendicular to the real axis which cuts the region cuts its boundary in two points and meets (a, b) in an interior point; and if finally $\text{Re } J(z) \geq 0$ throughout T , then $w(z)$ can have no complex zero or extremum in T .

Theorem 4. Let the region T be as before, and let $w(z)$ be a solution, real on the segment (a, b) and such that in (a, b) $w \, dw/dz$ has a fixed sign; let $\text{Im } J(z)$ have this sign throughout that part of the region T which lays above the real axis, then $w(z)$ can have no complex zero or extremum in T .

Theorem 5. If $J(z)$ is analytic in a domain D bounded by an analytic Jordan curve Γ , and if

$$\int_{\Gamma} |J(z)| \, dz < \infty$$

then equation (A1) is non-oscillatory in D . In [2], illustrations are given to show how some of these theorems may be employed to find the distribution of poles of the QMF.

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