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# Zeros of Bessel functions by means of the Trefftz-Fichera orthogonal invariants method through the Schrödinger equation 

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## I. Introduction

To compute the positive zeros of the Bessel functions of the first kind $\mathrm{J}_{n}(x)$ there exists a classical method, going back to Euler and independently developed by Rayleigh, Cayley and others, which is still considered useful [I].

This method, based upon the knowledge of the sums of the even powers of the inverse zeros, can be trivially extended to any entire function, whose zeros are all simple, real and positive, provided the sum of the inverse zeros is a finite quantity.

We will see that this method may be related to the Trefftz-Fichera one for computing upper bounds to the eigenvalues of a positive compact operator acting in a Hilbert space.

For the particular case of the Bessel functions of the first kind, the positive compact operator is explicitly obtained as a Fredholm integral operator, whose kernel is found through the time independent Schrödinger equation with an exponential potential $\mathrm{V}=e^{-b r}, b>0$.

In this case all the orthogonal invariants of the Trefftz-Fichera method are explicitly known or can be obtained through recurrence relations.

To give an idea of the accuracy which can be obtained through these operator techniques, we report a simple numerical application to the above exemple, in order to compute the first two positive zeros of $\mathrm{J}_{1}(x)$ : we get 24 exact figures for the first zero, and 16 exact figures for the second one. Finally it is presented a simple generalization of the Euler method, also included in the Trefftz-Fichera one, where no use of the explicit expression of the integral operator is made.
(*) Pervenuta all'Accademia il 29 agosto 1977.

The paper is organised as follows: in Sect. II we introduce the quantum mechanical problem; in Sect. III we give a short review of the Trefftz-Fichera method: in Sect. IV we apply the considerations of the two former sections to the Bessel functions; in Sect. V we present the numerical computation and finally in Sect. VI we discuss in the most general setting the relationship between the Euler and the Trefftz-Fichera methods.

## II.

Let us consider the one-particle time independent Schrödinger equation for a central potential of exponential type $\overline{\mathrm{V}}=-e^{-b r}, b>0$,

$$
\begin{equation*}
\left(\mathrm{H}_{0}+\bar{g} \overline{\mathrm{~V}}\right) \Psi=\overline{\mathrm{E}} \Psi \tag{1}
\end{equation*}
$$

where $\bar{g}>0, \mathrm{H}_{0}=-\frac{\hbar^{2}}{2 m} \Delta, m$ being the particle mass; $\hbar=\frac{h}{2 \pi}, h$ being the Planck constant.

Eq. (I) is of course an eigenvalue problem for $\Psi \in \mathrm{H}^{2}\left(\mathbf{R}^{3}\right), \mathrm{H}^{2}\left(\mathbf{R}^{3}\right)$ being the common domain of $\mathrm{H}_{0}$ and $\mathrm{H}=\mathrm{H}_{0}+\bar{g} \overline{\mathrm{~V}}$, which is a self-adjoint operator in $L^{2}\left(\mathbf{R}^{3}\right)$ in view of our choice of $\overline{\mathrm{V}}$, as is well known [2].

Since problem (I) is spherically symmetric, looking as usual for spherically symmetric solutions of the form $\Psi=\frac{u(r)}{r}$ we get the following radial Schrödinger equation:

$$
\begin{equation*}
-\frac{\mathrm{d}^{2} u(r)}{\mathrm{d} r^{2}}-2 \frac{m \bar{g}}{\hbar^{2}} e^{-b r} u(r)=2 m \frac{\overline{\mathrm{E}}}{\hbar^{2}} u(r) \tag{2}
\end{equation*}
$$

under the conditions $u \in \mathrm{H}^{2}(0, \infty), u(0)=0$, which clearly represents a singular Sturm-Liouville eigenvalue problem.

Through the scale transformation $r \rightarrow b^{-1} r$ we obtain the new equation:

$$
\begin{equation*}
\left(\mathrm{H}_{0}+g \mathrm{~V}\right) u(r)=\mathrm{E} u(r) \tag{3}
\end{equation*}
$$

with $u \in \mathrm{H}^{2}(\mathrm{o}, \infty), u(0)=0$, and where $g=2 \frac{m \bar{g}}{\hbar^{2} b}$,

$$
\mathrm{E}=2 \frac{m \overline{\mathrm{E}}}{\hbar^{2} b^{2}} \quad, \quad \mathrm{~V}=-e^{-r} \quad, \quad \mathrm{H}_{0}=-\frac{\mathrm{d}^{2}}{\mathrm{~d} r^{2}} .
$$

This last equation can be in turn reduced, as is well known [3], to the Bessel one through a further change of variable: $x=2\left(g e^{-r}\right)^{\frac{1}{2}}$. Substituting in (3) we get:

$$
\begin{equation*}
\frac{\mathrm{d}^{2} \Phi(x)}{\mathrm{d} x^{2}}+\frac{\mathrm{I}}{x} \frac{\mathrm{~d} \Phi(x)}{\mathrm{d} x}+\left(\mathrm{I}-\frac{\nu^{2}}{x^{2}}\right) \Phi(x)=0 \tag{4}
\end{equation*}
$$

where $\quad \Phi(x)=u(r(x)), \nu^{2}=-4 \mathrm{E}$.

For $\mathrm{E}>0$ define $\nu=2 i k, k=\sqrt{\mathrm{E}}$.
It is known (4) that the spectrum of the singular Sturm-Liouville operator (3) consists in an absolutely continuous part covering the whole positive axis and in a finite number of negative eigenvalues with finite multiplicity.

These eigenvalues, which are the only possible bound states of the particle, are also given, as is known [3], by the zeros in the half plane $\operatorname{Im} k<0$ of the Jost function, whose definition we will now recall.

Let $f(r, k)$ be the solution of (3) with the boundary condition at infinity obtained requiring $\lim _{r \rightarrow \infty} f(r, k) e^{i k r}=\mathrm{I}$.

The Jost function is then defined as $f(0, k)$.
In this case, because of (4) and the behavior at zero of $J_{v}(x)$, we have $f(r, k)=g^{-\frac{\nu}{2}} \Gamma(\nu+1) J_{v}(x), x=2\left(g e^{-r}\right)^{\frac{1}{2}}$.

Hence the Jost function is given by $f(0, k)=g^{-\frac{v}{2}} \Gamma(u+1) J_{v}\left(2 g^{\frac{1}{2}}\right)$, since for $r=0$ we have $x=2 g^{\frac{1}{2}}$.

The zeros of $f(0, k)$ in the half plane $\operatorname{Im} k<0$, i.e. $\operatorname{Re} v>0$, give all the eigenvalues of problem (3) through the relation $E=-\frac{v^{2}}{4}$.

In particular the eigenvalues are negative as recalled above and the Jost function has a zero for $v$ positive for any eigenvalue $E$ with $v=2 \sqrt{-E}$.

The number $n_{0}$ of this eigenvalues is finite; more precisely, we report here two upper bounds for $n_{0}$, due to Bargmann [5] and Calogero [6] respectively

$$
n_{0} \leq g \int_{0}^{\infty} r \mathrm{~V} \mathrm{~d} r=g \int_{0}^{\infty} r e^{-r} \mathrm{~d} r=g
$$

$$
\begin{equation*}
n_{0} \leq 2 \frac{g^{\frac{1}{2}}}{\pi} \int_{0}^{\infty} \mathrm{V}^{\frac{1}{2}} \mathrm{~d} r=2 \frac{g^{\frac{1}{2}}}{\pi} \int_{0}^{\infty} e^{-\frac{1}{2} r} \mathrm{~d} r=\frac{4 g^{\frac{3}{2}}}{\pi} \tag{5}
\end{equation*}
$$

We proceed now to obtain the eigenvalues of (I), and hence of (3), through an integral equation according to a general method applicable for a class of potentials whose definition we will now recall.

For a complete treatment of these methods, the reader is referred to Simon [7].

Let R be the set of the measurable functions $f(x), x \in \mathbf{R}^{3}$, such that:

$$
\begin{equation*}
\|f\|_{\mathrm{R}}=\iint \frac{|f(x) \| f(y)|}{|x-y|^{2}} \mathrm{~d} x \mathrm{~d} y<+\infty \tag{6}
\end{equation*}
$$

It can be shown [7] that $R$ is a Banach space under the norm (6), and that if $V \in R$ :
i) The operator $\mathrm{H}=\mathrm{H}_{0}+g V^{T}, \mathrm{H}_{0}=-\frac{\hbar^{2}}{2 m} \Delta, g \in \mathbf{R}$, can be realized as a self-adjoint operator in $L^{2}\left(\mathbf{R}^{3}\right)$
ii) For $\mathrm{E} \notin \sigma\left(\mathrm{H}_{0}\right)$ the operator:

$$
\begin{equation*}
-|\mathrm{V}|^{2}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{2}{2}}} \tag{7}
\end{equation*}
$$

is a Hilbert-Schmidt integral operator in $L^{2}\left(\mathbf{R}^{3}\right)$.
Eingenvalues and eigenvectors of H and of the operator defined by (7), respectively, are related through the following result:

Theorem i. Let $\mathrm{V} \in \mathrm{R}$, and let E belong to the complex half-plane $\operatorname{Re} \mathrm{E}<\mathrm{o}$. Then the eigenvalue equation:

$$
\begin{equation*}
-|\mathrm{V}|^{\frac{1}{2}}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{3}}} w=g^{-1} w, \quad w \in \mathrm{~L}^{2}\left(\mathbf{R}^{3}\right) \tag{8}
\end{equation*}
$$

has a solution if and only if the eigenvalue equation: $\mathrm{H} u=\mathrm{E} u$ has a solution $u \in \mathrm{D}(\mathrm{H})$, and the two solutions are related in the following way:

$$
w=|\mathrm{V}|^{\frac{1}{2}} u \quad, \quad u=\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}} w .
$$

Proof. See Simon [7].
If $\mathrm{V}=-e^{-b r}, b>0$, the conditions of the above theorem are fulfilled, since it is easily seen that $V \in R$.

In particular the equation $-|\mathrm{V}|^{\frac{1}{2}}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}} w=g^{-1} w$, with $\mathrm{H}_{0}=-\frac{\mathrm{d}^{2}}{\mathrm{~d} r^{2}}, \mathrm{~V}=-e^{-r}, w \in \mathrm{~L}^{2}(0, \infty), w(0)=\mathrm{o}$ has a solution if and only if $\left(\mathrm{H}_{0}+g^{\mathrm{V}}\right) u=\mathrm{E} u, u \in \mathrm{H}^{2}(0, \infty), u(0)=0$.

In addition $w=|\mathrm{V}|^{\frac{1}{3}} u, u=\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}} w$.
Let us indicate by $\mathrm{G}(x, y)$ the integral kernel of $\left(\mathrm{H}_{0}-\mathrm{E}\right)^{\mathbf{- 1}}, \mathrm{E}<0$. It is easy to check that $\mathrm{G}(x, y)$ is given by:

$$
G(x, y)= \begin{cases}\frac{2}{\nu} \sinh \left(\frac{\nu}{2} x\right) e^{-\frac{\nu}{2} y} & 0 \leq x \leq y \leq \infty \\ \frac{2}{\nu} \sinh \left(\frac{\nu}{2} y\right) e^{-\frac{\nu}{2} x} & 0 \leq y \leq x \leq \infty\end{cases}
$$

where $\nu=2 \sqrt{-\mathrm{E}}$,
so that the integral kernel $\mathrm{K}(x, y)$ of the operator $-|\mathrm{V}|^{\frac{1}{2}}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}}$ is given by:

$$
\mathrm{K}(x, y)= \begin{cases}f_{1}(x) f_{2}(y) & 0 \leq x \leq y \leq \infty \\ f_{2}(x) f_{1}(y) & 0 \leq y \leq x \leq \infty\end{cases}
$$

wher $f_{1}(x)=\frac{2}{\nu} \sinh \left(\frac{\nu}{2} x\right) e^{-\frac{x}{2}}, f_{2}(x)=e^{-\frac{\nu}{2} x} e^{-\frac{x}{2}}$.

## III.

Let us recall some essential notions of the Trefftz-Fichera orthogonal invariants method, strictly necessary in what follows. The reader is referred to Fichera [8] for a complete treatment.

Let $G$ be a strictly positive compact operator acting on a separable complex Hilbert space X such that $\mathrm{G}^{n}$ belongs to the trace class for some integer $n$.

In this case Fichera has shown that if we represent $X$ by some $L^{2}(A)$ space, A being for example any bounded or unbounded interval on $\mathbf{R}, \mathrm{G}^{n}$ will be a integral operator in $\mathrm{L}^{2}(\mathrm{~A})$

$$
\begin{equation*}
\mathrm{G}^{n} u(x)=\int_{\mathrm{A}} \mathrm{~K}(x, y) u(y) \mathrm{d} y \tag{1}
\end{equation*}
$$

whose kernel $\mathrm{K}(x, y)$ is of the following type:

$$
\begin{equation*}
\mathrm{K}(x, y)=\int_{\mathrm{A}} \mathrm{H}(x, t) \mathrm{H}(t, y) \mathrm{d} t \tag{2}
\end{equation*}
$$

$\mathrm{H}(x, y)$ being a symmetric kernel belonging to $\mathrm{L}^{2}(\mathrm{~A} \times \mathrm{A}, \mathrm{d} x \times \mathrm{d} x)$. Furthermore if we define:

$$
\mathrm{J}_{s}^{n}(\mathrm{G})=\frac{\mathrm{I}}{s!} \int_{\mathrm{A}} \cdots \int_{\mathrm{A}}\left|\begin{array}{l}
\mathrm{K}\left(x_{1}, x_{1}\right) \cdots \mathrm{K}\left(x_{1}, x_{s}\right)  \tag{3}\\
\left.\cdots \cdots \cdots \cdots \cdots \cdots \cdots, x_{s}, x_{s}\right)
\end{array}\right| \mathrm{d} x_{1} \cdots \mathrm{~d} x_{s}
$$

one has:
(4)

$$
\mathrm{J}_{s}^{n}(\mathrm{G})=\sum_{h_{1}<h_{2}<\cdots<h_{s}} \mu_{h_{1}}^{n} \mu_{h_{2}}^{n} \cdots \mu_{h_{s}}^{n}
$$

Here $\left\{\mu_{i}\right\}_{i=1}^{\infty}$ stands for the sequence of the repeated eigenvalues of $G$, arranged in increasing order, and the quantities $\mathrm{J}_{s}^{n}(\mathrm{G}), s=\mathrm{I}, 2, \cdots$, represent a complete set of orthogonal invariants for $G$.

Consider the infinite product:

$$
\begin{equation*}
\prod_{i=1}^{\infty}\left(\mathrm{I}-\mu_{i}^{n} \lambda\right) \tag{5}
\end{equation*}
$$

which converges uniformly on any compact subset of the complex $\lambda$-plane and defines the Fredholm entire function $\Delta(\lambda)$ of $\mathrm{G}^{n}$, whose zeros are given by $\lambda_{i}=\mu_{i}^{-n}, i=1,2, \cdots$.

It is easy to see that $\Delta(\lambda)$ [8] has the following Taylor expansion near $\lambda=0:$

$$
\begin{equation*}
\Delta(\lambda)=\mathrm{r}+\sum_{s=1}^{\infty} \mathrm{J}_{s}^{n}(\mathrm{G})(-\lambda)^{s} \tag{6}
\end{equation*}
$$

Let us notice, for further reference, that taking the logarithmic derivative $\mathrm{R}(\lambda)$ of $\Delta(\lambda)$ we get, for $\lambda \neq \lambda_{i}, i=\mathrm{I}, 2, \cdots$ :

$$
\begin{equation*}
\mathrm{R}(\lambda)=\frac{\Delta^{\prime}(\lambda)}{\Delta(\lambda)}=-\sum_{i=1}^{\infty} \frac{\mu_{i}^{n}}{\left(\mathrm{I}-\mu_{i}^{n} \lambda\right)}=-\sum_{j=0}^{\infty} J_{i}^{(j+1) n}(\mathrm{G}) \lambda^{j} \tag{7}
\end{equation*}
$$

and that the invariants $J_{1}^{s n}(\mathrm{G}), s=1,2, \cdots$, may be determined recursively from the knowledge of the invariants $\mathrm{J}_{s}^{n}(\mathrm{G}), s=1,2$. As a matter of fact, taking into account the identity between entire functions:

$$
\begin{equation*}
\Delta^{\prime}(\lambda)=\Delta(\lambda) R(\lambda) \tag{8}
\end{equation*}
$$

we can impose the equality between their Taylor expansion coefficients, so that:

$$
\begin{equation*}
\mathrm{J}_{s}^{n}(\mathrm{G})=-\frac{\mathrm{I}}{s} \sum_{i=1}^{\infty}(-\mathrm{I})^{i} \mathrm{~J}_{1}^{i n}(\mathrm{G}) \mathrm{J}_{s-i}^{n}(\mathrm{G}) \tag{9}
\end{equation*}
$$

where $J_{0}^{n}(G)=1$, thus recovering a relation between invariants already noticed by Robert [io].

Let us close this section by recalling the Trefftz-Fichera formulas yielding upper bounds on the eigenvalues $\mu_{i}$ in terms of some orthogonal invariant and of the lower bounds given by the Rayleigh-Ritz method [8].

Let $\left\{u_{i}\right\}_{i=1}^{\infty}$ be any orthonormal basis in $\mathrm{X}, \mathrm{X}_{n}$ the $n$-dimensional subspace spanned by the vectors $u_{i}, i=1,2, \cdots, n, \mathrm{P}_{n}$ the orthogonal projector from X onto $\mathrm{X}_{n}$, and $\mathrm{G}_{n}=\mathrm{P}_{n} \mathrm{GP}_{n}$ the compression of G into $\mathrm{X}_{n}$.

As is well known, the Rayleigh-Ritz approximate values for the first $n$ eigenvalues $\mu_{1}, \cdots, \mu_{n}$ are the eigenvalues $\lambda_{1}^{(n)}, \cdots, \lambda_{n}^{(n)}$ of $G_{n}$.

It is also well known that in our conditions $\lambda_{i}^{(n)} \leq \lambda_{i}^{(n+1)} \leq \cdots \leq \mu_{i}$, $\lim _{n \rightarrow \infty} \lambda_{i}^{(n)}=\mu_{i}, i=1,2, \cdots,$.

The Trefftz-Fichera formula yielding the upper bounds we will apply read:

$$
\begin{equation*}
\Lambda_{i, m}^{(n)}=\left(\mathrm{J}_{1}^{m}(\mathrm{G})-\sum_{\substack{j=1 \\ j \neq 1}}^{n}\left(\lambda_{j}^{(n)}\right)^{m}\right)^{\frac{1}{m}}, \quad \quad m=\mathrm{I}, 2, \cdots \tag{io}
\end{equation*}
$$

We have [8]:

$$
\begin{equation*}
\Lambda_{i, m}^{(n)} \geq \Lambda_{i, m}^{(n+1)} \quad, \quad \lim _{n \rightarrow \infty} \Lambda_{i, m}^{(n)}=\mu_{i} \tag{II}
\end{equation*}
$$

To sum up, the Rayleigh-Ritz method yields, for any eigenvalue $\mu_{i}$, a monotonic convergent sequence of lower bounds, and the Trefftz-Fichera one a monotonic convergent sequence of upper bounds.

## IV.

Let us come back to the integral operator:
(I)

$$
\begin{aligned}
& \mathrm{G}_{0}=-|\mathrm{V}|^{\frac{1}{2}}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}}, \quad \mathrm{H}_{0}=-\frac{\mathrm{d}^{2}}{\mathrm{~d} r^{2}}, \mathrm{~V}=-e^{-r}, \\
& \mathrm{D}\left(\mathrm{H}_{0}\right)=\left\{f ; f \in \mathrm{H}^{2}(0, \infty), f(0)=0\right\} \subset \mathrm{L}^{2}(0, \infty), \quad \mathrm{E}<0 .
\end{aligned}
$$

It is easy to see that $\mathrm{G}_{0}$ is not only a Hilbert-Schmidt, but also a trace-class operator, the trace being simply given by:

$$
\begin{align*}
\operatorname{Tr}\left(\mathrm{G}_{0}\right)=\mathrm{J}_{1}^{1}\left(\mathrm{G}_{0}\right) & =\int_{0}^{\infty} \mathrm{K}(x, x) \mathrm{d} x=-\frac{\beta}{\nu^{2}} \int_{0}^{1}\left(\mathrm{I}-z^{-\beta}\right) \mathrm{d} z  \tag{2}\\
& =\frac{\mathrm{I}}{\nu+\mathrm{I}}
\end{align*}
$$

where $\mathrm{K}(x, x)$ is given by [II] of Sect II, $z=e^{-\frac{\nu}{\beta x}}, \beta=\frac{\nu}{(\nu+\mathrm{I})}, \nu=\sqrt{\overline{\mathrm{E}} .}$
We come now to the evaluation of the iterated traces $J_{1}^{n}\left(G_{0}\right)$, i.e. the trace of the operator $\left(G_{0}\right)^{n}$ for any $n>1$.

First of all we notice that in this case it is possible to get an extremely simple expression for the invariants $\mathrm{J}_{s}^{1}\left(\mathrm{G}_{0}\right), s=2,3, \cdots$.

Theorem 2. Let $\Delta_{0}(\lambda)$ be the Fredholm entire function of

$$
\mathrm{G}_{0}=-|\mathrm{V}|^{\frac{1}{2}}\left(\mathrm{H}_{0}-\mathrm{E}\right)^{-1} \frac{\mathrm{~V}}{|\mathrm{~V}|^{\frac{1}{2}}}, \quad \mathrm{E}<0,
$$

$\mathrm{H}_{0}$ and V as in (1). We have:

$$
\begin{equation*}
\Delta_{0}(\lambda)=\lambda^{-\frac{\nu}{2}} \Gamma(\nu+I) J_{\nu}\left(2 \lambda^{\frac{d}{2}}\right) \tag{3}
\end{equation*}
$$

where $\nu=2 \sqrt{-\mathrm{E}}$.
Proof. Let us recall that by the theory of the Jost function (see Sect II), if

$$
\begin{equation*}
f(\mathrm{o}, k) \equiv g^{-\frac{v}{2}} \Gamma(\nu+\mathrm{I}) \mathrm{J}_{\nu}\left(2 g^{\frac{k}{2}}\right)=0, \tag{4}
\end{equation*}
$$

for some $g>0$ and $\nu>0, E=-\frac{\nu^{2}}{4}$ is an eigenvalue of the operator $\mathrm{H}=\mathrm{H}_{0}+g \mathrm{~V}$ and by Theorem $\mathrm{I}, \mathrm{g}^{-1}$ is an eigenvalue of $\mathrm{G}_{0}$ for $\mathrm{E}=-\frac{\nu^{2}}{4}$.

In particular for $v>0$ we have that all the zeros of $f(o, k)$ are obtained for $g=\mu_{n}^{-1}, n=\mathrm{I}, 2, \cdots$, where $\mu_{n}, n=1,2, \cdots$, are the eigenvalues of $G_{0}$ for $E=-\frac{\nu^{2}}{4}$.
5. - RENDICONTI 1977, vol. LXIII, fasc. 1-2.

For $\mathrm{E}<0, \nu=2 \sqrt{-\mathrm{E}}$, as it is well known from the Bessel functions theory ( I$), f(\mathrm{O}, k)=g^{-\frac{\nu}{2}} \Gamma(\nu+\mathrm{I}) \mathrm{J}_{\nu}\left(2 g^{\frac{1}{2}}\right)$ admits an infinite product expansion, and it reads:

$$
\begin{equation*}
\prod_{n=1}^{\infty}\left(\mathrm{I}-\mu_{n} g\right) \tag{5}
\end{equation*}
$$

which is also the definition of $\Delta_{0}(g)$.
Corollary I. The orthogonal invariants $\mathrm{J}_{s}^{1}\left(\mathrm{G}_{0}\right)$ are given by:

$$
\begin{equation*}
\mathrm{J}_{s}^{1}\left(\mathrm{G}_{0}\right)=((\nu+1) \cdots(\nu+s) s!)^{-1}, \quad s=2,3, \cdots \tag{6}
\end{equation*}
$$

Proof. It follows immediately from the power series expansion of the Fredholm function as given by Theorem 2, and from the relation between the coefficients and the invariants (see Sect. III).

Now the invariants $\mathrm{J}_{1}^{s}\left(\mathrm{G}_{0}\right), s=2,3, \cdots$, can be given through recurrence relations that follow from the Robert relations of formula (9) Sect III with $n=1$ and $G=G_{0}$ :

$$
\begin{equation*}
\mathrm{J}_{1}^{k}\left(\mathrm{G}_{0}\right)=-(-\mathrm{I})^{k} k \mathrm{~J}_{k}^{1}\left(\mathrm{G}_{0}\right)-\sum_{i=1}^{k-1}(-\mathrm{I})^{k-i} \mathrm{~J}_{1}^{i}\left(\mathrm{G}_{0}\right) \mathrm{J}_{k-i}^{1}\left(\mathrm{G}_{0}\right) \quad k=2,3, \cdots, s \tag{7}
\end{equation*}
$$

## V.

Let us come to the numerical exemple mentioned in Sect. I. We want to compute the first two positive zeros of $\mathrm{J}_{1}(2 x)$. As we have seen, this is equivalent to computing the first two eigenvalues of the integral operator $G_{0}$.

This will then be accomplished by using the Rayleigh-Ritz and the Trefftz-Fichera method. As for the Rayleigh-Ritz method, let us choose the following orthonormal basis in $\mathrm{L}^{2}(0, \infty)$ :

$$
\begin{equation*}
u_{n}(r)=\left(\frac{\nu}{\beta}\right)^{\frac{1}{2}}((n+\mathrm{I})(n+2))^{-\frac{1}{2}} r^{\prime} \mathrm{L}_{n}^{2}\left(r^{\prime}\right) e^{-\frac{r^{\prime}}{2}}, \quad n=0, \mathrm{I}, \cdots \tag{1}
\end{equation*}
$$

where $r^{\prime}=\frac{\nu}{\beta} r, \mathrm{~L}_{n}^{2}(x)$ being the generalized Laguerre polynomial of order $n$ and index 2 [ IO ].

Such a choice is motivated by the behavior at $r=\infty$ and at $r=0$ of all these functions, which is related to that of the eigensolutions of the Schrödinger equation corresponding to the eigensolutions of $\mathrm{G}_{0}$ (recall that (Sect. II) if $u$ is an eigensolution of the Schrödinger equation, $w=|\mathrm{V}|^{\frac{1}{2}} u$ is an eigensolution of $G_{0}$ ).

We have:

$$
\begin{equation*}
\left(u_{n}, \mathrm{G}_{0} u_{m}\right)=\frac{\mathrm{I}}{\nu}\left(\frac{\beta}{\nu}\right)((n+1)(n+2)(m+1)(m+2))^{-\frac{1}{v}}\left(\mathrm{I}_{n, m}+\mathrm{I}_{m, n}-\mathrm{I}\right) \tag{2}
\end{equation*}
$$

where

$$
\begin{aligned}
& \quad \mathrm{I}_{n, m}=\mathrm{T}_{n, m}^{2}-\mathrm{T}_{n, m-1}^{2}+\sum_{k=0}^{n} \mathrm{~T}_{k, m}^{0}-(n+\mathrm{I}) \mathrm{T}_{n+1, m}^{0}, \\
& \mathrm{~T}_{n, m}^{i}=(n+m+i)!(\mathrm{I}-\beta)^{n+m}\left(n!m!(2-\beta)^{n+m+i+1}\right)^{-1} \\
& \mathrm{~F}\left(-n,-m ;-n-m-i ;-\alpha \frac{(2-\beta)}{(\mathrm{I}-\beta)^{2}}\right), \quad i=0,2,
\end{aligned}
$$

where $\mathrm{F}(a, b ; c ; x)$ is the hypergeometric function.
It is well known that the eigenvalues of the matrices $\left\|\left(u_{m}, \mathrm{G}_{0} u_{k}\right)\right\|_{m, k=1,2 \cdots n}$, $n=\mathrm{I}, 2, \cdots$, are the eigenvalues of the operators $\mathrm{P}_{n} \mathrm{G}_{0} \mathrm{P}_{n}, n=\mathrm{I}, 2, \ldots$ and hence the Rayleigh-Ritz lower bounds to the eigenvalues of $G_{0}$.

Numerical computations have been performed, pushing the RayleighRitz approximation up to $n=58$, by means of the invariant $J_{1}^{16}\left(G_{0}\right)$, obtained from formula (7) of Sect. IV, for $v=\mathrm{I}$. In this way the first positive zeros of the Bessel function $\mathrm{J}_{1}(2 \sqrt{x})$ are obtained.

As an example of the accuracy which can be attained, let us report the results for $\xi_{1,1}$ and $\xi_{1,2}$, where $\xi_{1, n}$ stands for the $n$-th positive zero of $\mathrm{J}_{1}(x)$ :

$$
\begin{align*}
& 3 \cdot 8317059702075123156144359 \leq \xi_{1,1} \leq \\
& 3 \cdot 8317059702075123156144365 \\
& 7 \cdot 01558666981561845  \tag{3}\\
& 7 \cdot 01558666981561875
\end{align*}
$$

Besides the computation of the zeros of the Bessel function $\mathrm{J}_{v}(x)$, the problem can be inverted numerically in order to find for what values of $v$ the Bessel function has to vanish at a given point. This study corresponds to the physical problem of locating the $s$-wave bound states of the one-body quantum mechanical system governed by an exponential potential, and will be treated elsewhere in a wider context.

## VI.

We come now to the relation between the Euler and the Trefftz-Fichera methods.

Let $\Delta(\lambda)$ be an entire function admitting the following representation:

$$
\begin{equation*}
\Delta(\lambda)=\prod_{i=1}^{\infty}\left(\mathrm{I}-\mu_{i} \lambda\right) \tag{1}
\end{equation*}
$$

where $\mu_{i}>0, i=1,2, \cdots, \mu_{1}>\mu_{2}>\cdots$.
Let $\Delta(\lambda)$ be given through its Taylor expansion near $\lambda=0$ :

$$
\begin{equation*}
\Delta(\lambda)=\mathrm{I}+\sum_{s=1}^{\infty}(-\mathrm{I})^{s} \mathrm{~J}_{s}^{1} \lambda^{s} \tag{2}
\end{equation*}
$$

where

$$
J_{s}^{1}=\sum_{h_{1}<h_{2}<\cdots<h_{s}} \mu_{h_{1}} \mu_{h_{2}} \cdots \mu_{h_{s}} .
$$

The logarithmic derivative $\mathrm{R}(\lambda)=\Delta^{\prime}(\lambda) / \Delta(\lambda)$ if $\Delta(\lambda)$ has the following Taylor expansion near $\lambda=0$ :

$$
\begin{equation*}
\mathrm{R}(\lambda)=-\sum_{s=0}^{\infty} \mathrm{J}_{1}^{s+1} \lambda^{s}, \quad \mathrm{~J}_{1}^{i}=\sum_{k=1}^{\infty} \mu_{k}^{i} \tag{3}
\end{equation*}
$$

where the coefficients $J_{1}^{i}, i=2,3, \cdots$, may be computed by recurrence through formula ( 7 ) of Sect IV, with $\mathrm{J}_{k}^{i}\left(\mathrm{G}_{0}\right)$ replaced by $\mathrm{J}_{k}^{i}, i, k=\mathrm{I}, 2, \ldots$

The identity $J_{1}^{s}=\sum_{i=1}^{\infty} \mu_{i}^{s}$ yields the following two-sided estimate for $\mu_{1}$ :

$$
\begin{equation*}
\frac{\mathrm{J}_{1}^{s+1}}{\mathrm{~J}_{1}^{s}} \leq \mu_{1} \leq\left(\mathrm{J}_{1}^{s}\right)^{\frac{1}{s}} \tag{4}
\end{equation*}
$$

Furthermore:

$$
\begin{equation*}
\left(\mathrm{J}_{1}^{s}\right)^{\frac{1}{s}} \geq\left(\mathrm{J}_{1}^{s+1}\right)^{\frac{1}{(s+1)}} \tag{5}
\end{equation*}
$$

and

$$
\lim _{s \rightarrow \infty}\left(J_{1}^{s}\right)^{\frac{1}{s}}=\mu_{1}
$$

$$
\frac{\mathrm{J}_{s}^{1+1}}{\mathrm{~J}_{s}^{1}} \leq \frac{\mathrm{J}_{1}^{s+2}}{\mathrm{~J}_{1}^{s+1}} \quad \text { and } \quad \lim _{s \rightarrow \infty} \frac{\mathrm{~J}_{1}^{s+1}}{\mathrm{~J}_{1}^{s}}=\mu_{1}
$$

For $\mu_{2}$ it is only possible to get a non-increasing sequence of upper bounds:

$$
\begin{equation*}
\mu_{2} \leq\left(\mathrm{J}_{1}^{s}-\left(\frac{\mathrm{J}_{1}^{k+1}}{\mathrm{~J}_{1}^{k}}\right)^{s}\right) \quad k=\mathrm{I}, 2, \cdots \tag{6}
\end{equation*}
$$

This method for estimating the first positive zeros of the entire function (I) has been used by Euler for the Bessel function of the first kind $\mathrm{J}_{0}(x)$, and independently by Rayleigh for the Bessel function $\mathrm{J}_{\nu}(x)$ for $v \geq 0$ (Remember that $x^{-\frac{\nu}{2}} \mathrm{~J}(\nu+\mathrm{I}) \mathrm{J}_{\nu}(2 \sqrt{x})$ has an infinite product expansion of the type (I)).

Rayleigh found the explicit expression of $J_{1}^{s}$, for any $\nu \geq 0$, for $s=1,2, \cdots, 5$, and computed thereby the first positive zero of $\mathrm{J}_{1}(x)$ obtaining:

$$
\begin{equation*}
\xi_{1,1}=3 \cdot 83 \mathrm{I} 706 \tag{7}
\end{equation*}
$$

which is a good upper bound in view of the present results (see formula (3) of Sect. V).

The coefficient $J_{1}^{8}$ was computed by Cayley for any $v \geq 0$, and its expression is still reported on the mathematical tables as an useful quantity for estimating the first positive zeros of the Bessel functions of the first kind [Io].

To find the relationship of this method with the Trefftz-Fichera one, let $G$ be a trace-class positive compact operator acting on some separable
complex Hilbert space $X$, admitting the sequence $\left\{\mu_{i}\right\}_{i=1}^{\infty}$ as the sequence of its eigenvalues, assumed simple. In this case we can identify $\mathrm{J}_{k}^{i}$ with $\mathrm{J}_{k}^{i}(\mathrm{G})$, $i, k=1,2, \ldots$.

The upper bound on $\mu_{1}$ appearing in (5) is clearly of the Trefftz-Fichera type, while it is not evident the Rayleigh-Ritz origin of the lower bound. Anyway, the upper bound on $\mu_{2}$ is also of the Trefftz-Fichera type.

We shall now prove that the lower bound on $\mu_{1}$ is due to a RayleighRitz approximation of the eigenvalues of $G$ which can be performed without the knowledge of an explicit expression of $G$.

At the same time we will prove that the Euler method recalled above can be generalized, in a natural way, in such a way to yield a convergent sequence of upper and lower bounds for any $\mu_{k}$, this method being always contained in the Trefftz-Fichera one as a particular case.

Let $\left\{v_{k}\right\}_{k=1}^{\infty} \in \mathrm{X}$ be the sequence of the (normalized) eigenvectors of G , corresponding to the eigenvalues $\mu_{k}, k=\mathrm{I}, 2, \cdots$.

Let $u_{0}=\sum_{n=1}^{\infty} \frac{\mu_{n}^{\frac{1}{s} s} v_{n}}{\left(\mathrm{~J}_{\mathrm{i}}\right)^{\frac{1}{2}}}$, where $s$ is a positive integral number: $\left\|u_{0}\right\|=\mathrm{I}$ and therefore $u_{0} \in \mathrm{X}$.

Consider in X the vector sequence $u_{i}=\mathrm{G}^{i} u_{0}, i=\mathrm{o}, \mathrm{I}, \cdots$, and let us apply to it the Gram-Schmidt orthogonalization procedute. We have:

$$
\begin{aligned}
& f_{0}=u_{0} \\
& f_{1}=\mathrm{G} f_{0}-a_{0} f_{0} \\
& f_{n+1}=\mathrm{G} f_{n}-a_{n} f_{n}-b_{n}^{2} f_{n-1}, \quad n=1,2, \cdots
\end{aligned}
$$

where $a_{n}=\frac{\left(f_{n}, \mathrm{G} f_{n}\right)}{\left\|f_{n}\right\|^{2},} b_{n}=\frac{\left\|f_{n}\right\|}{\left\|f_{n-1}\right\|}$.
Defining $e_{n}=\frac{f_{n}}{\left\|f_{n}\right\|}$ we get an orthonormal basis sequence $\left\{e_{n}\right\}_{n=0}^{\infty}$. On this basis $G$ takes the following simple form:

$$
\begin{aligned}
& \mathrm{Ge} e_{0}=a_{0} e_{0}+b_{0} e_{1} \\
& \mathrm{G} e_{n}=b_{n-1} e_{n-1}+a_{n} e_{n}+b_{n} e_{n+1}, \quad n=1,2, \cdots
\end{aligned}
$$

Since $\left\{e_{n}\right\}_{n=0}^{\infty}$ is a complete orthonormal basis as $\left\{v_{n}\right\}_{n=1}^{\infty}$ is [II], it can be used for the Rayleigh-Ritz approximations.

Let therefore $\mathrm{X}_{n}$ be the linear hull of the vectors $e_{i}, i=\mathrm{o}, \mathrm{I}, \cdots, n-\mathrm{I}$, $P_{n}$ the projector from $X$ onto $X_{n}$, and $G_{n}=P_{n} G P_{n}$ the compression of $G$ into $\mathrm{X}_{n}$.

The first approximation ( $n=1$ ) yields a single lower approximation $\lambda_{1}^{1} \leq \mu_{1}$, with $\lambda_{1}^{1}=a_{0}=\left(e_{0}, \mathrm{G} e_{0}\right)=\left(u_{0}, \mathrm{G} u_{0}\right)=\frac{\mathrm{J}_{1}^{s+1}}{\mathrm{~J}_{1}^{s}}$ because of the definition of $u_{0}$.

For $s=1,2, \cdots, \lambda_{1}^{1}$ gives exactly the Euler values.
It is easily seen, inductively, that all the $a_{k}$ 's and $b_{k}$ 's depend only on the quantities $c_{i}=\left(u_{0}, \mathrm{G}^{i} u_{0}\right)=\frac{\mathrm{J}_{1}^{s+i}}{\mathrm{~J}_{1}^{s}}$, i.e. on the invariants $J_{1}^{k}$, $k=s, s+1, \cdots$.

Since the non-zero eigenvalues of $\mathrm{G}_{n}$, i.e. the Rayleigh-Ritz approximations, are given by the eigenvalues of the following $n \times n$ symmetric matrix

$$
\left.G_{n}=\| \begin{array}{cccccc}
a_{0} & b_{0} & 0 & \cdots & \cdots & \cdots \\
b_{0} & a_{1} & b_{1} & 0 & \cdots & \cdots
\end{array}\right)
$$

we see that our particular choice of the basis vectors eliminates the need of the explicit knowledge of an expression for $G$.

At the same time we see that Euler's method is included into the TrefftzFichera one as its first approximation.

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[^0]:    Riassunto. - Applicando il metodo degli invarianti ortogonali di Trefftz-Fichera ad un operatore derivato dalla equazione di Schrödinger indipendente dal tempo, si approssimano gli zeri positivi delle funzioni di Bessel di prima specie.

    Come casi particolari si riottengono i classici risultati di Eulero, Rayleigh e Cayley.
    A titolo di esempio si fa un calcolo numerico del primo zero positivo della funzione di Bessel di prima specie $\mathrm{J}_{1}(x)$, ottenendo 24 cifre esatte.

    Si generalizza poi il metodo di Eulero per il calcolo degli zeri di una funzione intera tramite il metodo di Trefftz-Fichera senza far uso dell'espressione esplicita di alcun operatore.

