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More on the Airy averaging method

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The Airy averaging method illustrated in a previous paper [J. Math. Chem. 25 (1999) 93] is a simple and effective procedure for dealing with mathematical expressions/manipulations involving Airy functions. The potentiality of the method is emphasizd through a couple of applications drawn from recent research advances in the field of the discrete variable representation (DVR) basis sets.

KEY WORDS: Airy functions, discrete variable representation, Airy averaging method

1. Introduction

In a recent paper involving two of the present authors [1], the utility of a mathematical procedure, named Airy averaging, has been illustrated by a number of simple applications. The procedure, devised by Schwinger and Englert and specifically exploited by them to bring quantum improvements in the Thomas–Fermi atomic model [2,3], turns out to be an effective, interesting approach that allows dealing with mathematical manipulations involving Airy functions [4].

The important role played by these special functions in various contexts is well documented. Semiclassical scattering theory, molecular photodissociation and predissociation, Raman scattering spectroscopy are only a few examples drawn from the less recent literature [5–10]. More recently, a number of basic developments in the discrete variable representation (DVR) field have been reported [11–14]. In particular, Airy functions have been discussed in depth as a new DVR basis set endowed with advantageous features, for instance to approach the solution of problems in quantum mechanical applications [14].

In this short paper we propose to extend farther our former review of Airy averaging applications [1]. We shall demonstrate, in particular, that some results obtained in [14] follow rather smoothly by our approach, without recourse to lengthy manipulations. Limiting ourselves to summarize only a few essential points of the Airy averaging method, we recall that the pair of linearly independent solutions of the homogeneous

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differential equation (z complex variable)

$$\frac{d^2 y(z)}{dz^2} - zy(z) = 0, \tag{1}$$

denoted $Ai(z)$ and $Bi(z)$, are known as the regular and irregular Airy functions, respectively [4]. The regular Airy function admits the following integral representation,

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \exp\left[-i\left(\frac{y^3}{3} + xy\right)\right], \tag{2}$$

from which one obtains in a straightforward way the Fourier transform

$$\int_{-\infty}^{\infty} dx\, Ai(x) e^{iyx} = \exp\left(-i\frac{y^3}{3}\right). \tag{3}$$

As a special case of equation (3) we have

$$\int_{-\infty}^{\infty} dx\, Ai(x) = 1. \tag{4}$$

This result suggests formally the idea of a normalized Airy distribution. The Airy averaging of a given function $f(x)$ then follows immediately according to the definition

$$\langle f(x) \rangle_{Ai} \equiv \int_{-\infty}^{\infty} dx\; f(x) Ai(x). \tag{5}$$

As a consequence of this definition, the result of equation (3) can be expressed in the form of Airy averaging as

$$\langle \exp(iyx) \rangle_{Ai} = \exp\left(-i\frac{y^3}{3}\right). \tag{6}$$

Equation (6), along with the linear nature of the Airy averaging mapping [1], constitute the basis for the following applications.

2. Applications

As a first example of the formalism just summarized, we shall consider the Airy averaging of the function $f(x) = (x - z)^{-1}$, with z arbitrary complex number,

$$\langle (x - z)^{-1} \rangle_{Ai} \equiv \int_{-\infty}^{\infty} dx\, \frac{Ai(x)}{x - z}. \tag{7}$$

The integrand $Ai(x)(x - z)^{-1}$ plays an important role in recent theoretical work concerning the Airy DVR basis set [14], a specific example in the more general discrete variable representation problematics [12]. For $z = z_n$, with $\{z_n\}$ countable sequence of roots of $Ai(z)$, in fact, the functions $F_n(x) = (-1)^n Ai(x)(x - z_n)^{-1}$ constitute an orthonormal basis, in terms of which, for example, the diagonalization of a given Hamiltonian operator can be set up.

The recourse to the simple exchange of two integration orders (a consequence of the linear nature of the Airy averaging mapping) allows re-expressing equation (7) in the form

$$\langle (x-z)^{-1}\rangle_{Ai} = \mathrm{i}\int_{-\infty}^{0} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}zy}\langle \mathrm{e}^{\mathrm{i}yx}\rangle_{Ai}, \tag{8}$$

valid when $\operatorname{Im} z > 0$. From equation (6), therefore,

$$\langle (x-z)^{-1}\rangle_{Ai} = \mathrm{i}\int_{-\infty}^{0} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}zy}\mathrm{e}^{-\mathrm{i}y^3/3}. \tag{9}$$

Starting from the latter result, it is a very simple exercise to verify that $\langle (x-z)^{-1}\rangle_{Ai}$ satisfies the inhomogeneous Airy equation

$$\frac{\mathrm{d}^2\langle (x-z)^{-1}\rangle_{Ai}}{\mathrm{d}z^2} - z\langle (x-z)^{-1}\rangle_{Ai} = 1. \tag{10}$$

Standard manipulations based on the method of variation of constants lead to the following general solution of equation (10),

$$\langle (x-z)^{-1}\rangle_{Ai} = \left[a - \pi\int_0^z \mathrm{d}t\, Bi(t)\right]Ai(z) + \left[b + \pi\int_0^z \mathrm{d}t\, Ai(t)\right]Bi(z), \tag{11}$$

in terms of the regular and irregular Airy functions, with a, b complex integration constants.

The most obvious way for determining the constants a, b involves the solution of the following linear equation set,

$$\begin{aligned} \left[\langle (x-z)^{-1}\rangle_{Ai}\right]_{z=0} &= aAi(0) + bBi(0), \\ \left[\frac{\mathrm{d}\langle (x-z)^{-1}\rangle_{Ai}}{\mathrm{d}z}\right]_{z=0} &= aAi'(0) + bBi'(0) \end{aligned} \tag{12}$$

(the primed quantity $f'(z)$ denotes first derivative $\mathrm{d}f(z)/\mathrm{d}z$). Here, $Ai(0) = 3^{-3/2}/\Gamma(2/3)$, $Bi(0) = \sqrt{3}Ai(0)$, $Ai'(0) = -3^{-1/3}/\Gamma(1/3)$, $Bi'(0) = -\sqrt{3}Ai'(0)$ (with $\Gamma(z)$ gamma function of argument z) [4] and

$$\begin{aligned} \left[\langle (x-z)^{-1}\rangle_{Ai}\right]_{z=0} &= \mathrm{i}\int_0^{\infty} \mathrm{d}y\, \mathrm{e}^{\mathrm{i}y^3/3}, \\ \left[\frac{\mathrm{d}\langle (x-z)^{-1}\rangle_{Ai}}{\mathrm{d}z}\right]_{z=0} &= -\int_0^{\infty} \mathrm{d}y\, y\mathrm{e}^{\mathrm{i}y^3/3}. \end{aligned} \tag{13}$$

If the exponential figuring in the integrands of equation (13) is interpreted as $\exp(\mathrm{i}y^3/3) = \lim_{\varepsilon\to 0^+} \exp[-(\varepsilon - \mathrm{i}/3)y^3]$, from the general result $\int_0^\infty \mathrm{d}y\, y^{\nu-1} \exp(-\mu y^p) = (1/|p|)\Gamma(\nu/p)/(\mu)^{\nu/p}$ (Re $\nu > 0$) [15], one obtains

$$\left[\left\langle (x-z)^{-1}\right\rangle_{Ai}\right]_{z=0} = 3^{-2/3}\Gamma\left(\frac{1}{3}\right)\exp\left(\frac{2\mathrm{i}\pi}{3}\right),$$
$$\left[\frac{\mathrm{d}\langle (x-z)^{-1}\rangle_{Ai}}{\mathrm{d}z}\right]_{z=0} = -3^{-1/3}\Gamma\left(\frac{2}{3}\right)\exp\left(\frac{\mathrm{i}\pi}{3}\right) \tag{14}$$

and, finally, $a = \pi\mathrm{i}$, $b = -\pi/3$. Therefore,

$$\left\langle (x-z)^{-1}\right\rangle_{Ai} = \pi\mathrm{i}\left\{\left[1 + \mathrm{i}\int_0^z \mathrm{d}t\, Bi(t)\right]Ai(z) + \mathrm{i}\left[\frac{1}{3} - \int_0^z \mathrm{d}t\, Ai(t)\right]Bi(z)\right\}, \tag{15}$$

a result that can be expressed compactly in the alternative form

$$\left\langle (x-z)^{-1}\right\rangle_{Ai} = \pi\mathrm{i}\left[Ai(z) + \mathrm{i}Gi(z)\right], \tag{16}$$

involving the Airy function $Gi(z)$ [4], sometimes referred to as inhomogeneous Airy function [16]. $Gi(z)$ is, in fact, the solution to the inhomogeneous Airy equation

$$\frac{\mathrm{d}^2 Gi(z)}{\mathrm{d}z^2} - zGi(z) = -\pi^{-1}, \tag{17}$$

satisfying the boundary conditions $Gi(0) = Ai(0)/\sqrt{3}$, $Gi'(0) = -Ai'(0)/\sqrt{3}$ [4,16]. The complex variable function $K(z) = Ai(z) + \mathrm{i}Gi(z)$ has already been demonstrated to play a role in theoretical Raman scattering investigations using the reflection approximation [10,16]. To this regard, we point out incidentally that efficient algorithms for evaluating homogeneous and inhomogeneous Airy functions of complex argument are available [16–19].

The second application considered in this paper follows from equation (5) by the choice $f(x) = (x-z)^{-1}Ai(x)$, so that

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \frac{Ai^2(x)}{x-z} = \left\langle (x-z)^{-1}Ai(x)\right\rangle_{Ai}. \tag{18}$$

This integral is basically involved in the demonstration of the orthonormality properties of the Airy DVR basis functions $F_n(x) = (-1)^n(x-z_n)^{-1}Ai(x)$ [14].

The Airy averaging required by equation (18) can be carried out on the basis of the same procedure adopted in the former example. In place of equation (8), we have

$$\left\langle (x-z)^{-1}Ai(x)\right\rangle_{Ai} = \mathrm{i}\int_{-\infty}^{0} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}zy}\left\langle \mathrm{e}^{\mathrm{i}yx}Ai(x)\right\rangle_{Ai}, \tag{19}$$

whose validity is easily verified if Im $z > 0$. From the result [1],

$$\left\langle \mathrm{e}^{\mathrm{i}yx}Ai(x)\right\rangle_{Ai} = (4\pi\mathrm{i}y)^{-1/2}\exp\left(-\frac{\mathrm{i}y^3}{12}\right), \tag{20}$$

we obtain in a straightforward way

$$w(z) \equiv \langle (x-z)^{-1} Ai(x) \rangle_{Ai} = \frac{1}{2}\left(\frac{\mathrm{i}}{\pi}\right)^{1/2} \int_{-\infty}^{0} \mathrm{d}y \, \frac{\mathrm{e}^{-\mathrm{i}y^3/12}\mathrm{e}^{-\mathrm{i}zy}}{y^{1/2}}$$
$$= \frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{\sqrt{\pi}} \int_0^{\infty} \mathrm{d}\xi \, \mathrm{e}^{\mathrm{i}\xi^6/12}\mathrm{e}^{\mathrm{i}z\xi^2}. \tag{21}$$

Simple manipulations on $\mathrm{d}^3 w(z)/\mathrm{d}z^3$ allow demonstrating that $w(z)$ satisfies the following homogeneous differential equation,

$$\frac{\mathrm{d}^3 w(z)}{\mathrm{d}z^3} - 4z\frac{\mathrm{d}w(z)}{\mathrm{d}z} - 2w(z) = 0, \tag{22}$$

that is recognized to be the same satisfied by products of Airy functions, whose linearly independent solutions are $Ai^2(z)$, $Ai(z)Bi(z)$ and $Bi^2(z)$ [4].

The result for the Airy averaging involved, equation (21), can therefore be expressed in the general form

$$w(z) = aAi^2(z) + bAi(z)Bi(z) + cBi^2(z) \tag{23}$$

with a, b, c (complex) constants. The determination of these constants is carried out, as in the former case, by solving the linear set of algebraic equations,

$$\begin{aligned} w(0) &= aAi^2(0) + bAi(0)Bi(0) + cBi^2(0), \\ w'(0) &= 2aAi(0)Ai'(0) + b\big[Ai(0)Bi'(0) + Ai'(0)Bi(0)\big] + 2cBi(0)Bi'(0), \\ w''(0) &= 2a\big[Ai'(0)\big]^2 + 2bAi'(0)Bi'(0) + 2c\big[Bi'(0)\big]^2, \end{aligned} \tag{24}$$

with the primes denoting derivation orders. The nth order derivative $w^{(n)}(z)$ at $z = 0$ is easily calculated starting from equation (21),

$$w^{(n)}(0) = \frac{\mathrm{e}^{\mathrm{i}(\pi/6)(4n-1)}}{\sqrt{\pi}} 2^{2(n-1)/3} \cdot 3^{(2n-5)/6} \Gamma\left(\frac{2n+1}{6}\right) \tag{25}$$

after interpreting $\mathrm{e}^{\mathrm{i}\xi^6/12}$ as $\lim_{\varepsilon \to 0^+} \exp[-(\varepsilon - \mathrm{i}/12)\xi^6]$, in perfect analogy with the procedure leading to equation (14). The solution of the linear equation set (24), with $w(0)$, $w'(0)$, $w''(0)$ provided by equation (25), yields $a = \pi\mathrm{i}$, $b = -\pi$, $c = 0$, so that

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{Ai^2(x)}{x-z} = \langle (x-z)^{-1} Ai(x) \rangle_{Ai} = \pi \mathrm{i} Ai(z)\big[Ai(z) + \mathrm{i}Bi(z)\big]. \tag{26}$$

Equation (26) is a basic equality. The orthonormality of the Airy DVR basis functions $F_n(x) = (-1)^n (x - z_n)^{-1} Ai(x)$ is, in fact, a simple consequence of such result [14].

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