The method of Airy averaging and some useful applications

G.P. Arrighini [a], N. Durante [b] and C. Guidotti [a]

[a] *Dipartimento di Chimica e Chimica Industriale dell'Università, Via Risorgimento 35, 56126 Pisa, Italy*
[b] *Istituto di Chimica Quantistica ed Energetica Molecolare del CNR, Via Risorgimento 35, 56126 Pisa, Italy*

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An interesting approach named Airy averaging, introduced some years ago by Englert and Schwinger, is brought to the attention of a broader audience as a simple and powerful mathematical tool for applications involving Airy functions.

1. Introduction

The pair of linearly independent solutions *Ai*(z) and *Bi*(z) of the differential equation

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

are known as Airy functions [1].

Although such functions have found applications in the study of phenomena as different as rainbows [3] and earthquakes [15], their most familiar use is probably in quantum mechanics, for example, in the context of the WKB connection problem [8, 16,35] and the solution of the one-dimensional Schrödinger equation of a particle subjected to a constant force [26] (these two topics are actually closely related to each other). To remain in the quantum-mechanical context, we should remember the role of the Airy functions in some approaches addressed to improve the statistical-atom model beyond the Thomas–Fermi approximation [13].

Much experience concerning these special functions has been gained thanks to work carried out by chemical research groups in various fields. Semiclassical theory of scattering [9], molecular photodissociation and photofragmentation [21], Raman scattering spectroscopy [28] are a few of them. It is also a remarkable fact that the study of the analytical properties of the Airy functions has gone along with the development of efficient methods for their calculation to high accuracy [19,27].

The time-independent one-dimensional Schrödinger equations for a particle (mass m) acted by a constant force F,

$$\frac{\mathrm{d}^2\phi(x;E)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E + Fx)\phi(x;E) = 0, \tag{2}$$

has the well-known solution

$$\phi(x;E) = \beta F^{1/2} Ai\big[-\beta(E+Fx)\big], \quad \beta = \left(\frac{2m}{\hbar^2 F^2}\right)^{1/3}, \tag{3}$$

which satisfies the boundary condition $\phi(-\infty;E) = 0$. The eigenvalue spectrum supported by the problem on issue is continuous and spans the infinite range $(-\infty,+\infty)$.

The recourse to the integral representation of the Airy function,

$$Ai(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}x \exp\left[-\mathrm{i}\left(\frac{x^3}{3} + yx\right)\right], \tag{4}$$

allows one to verify easily the two following properties:

$$\begin{aligned} &\text{(i)} \quad \int_{-\infty}^{\infty} \mathrm{d}x\, \phi^*(x;E)\phi(x;E') = \delta(E-E') \quad \text{(orthonormality)},\\ &\text{(ii)} \quad \int_{-\infty}^{\infty} \mathrm{d}E\, \phi^*(x;E)\phi(x';E) = \delta(x-x') \quad \text{(completeness)}. \end{aligned} \tag{5}$$

Property (ii) is particularly important, because it warrants the existence of a rigorous basis-set representation for both scattering and bound states in one-dimensional quantum systems. Airy functions $Ai(z)$ have actually been employed in this perspective, for instance, for studies of collision-induced dissociation processes [22,23]. A nice feature of the use of such functions lies in the simple mathematical structure of the (continuum) matrix elements encountered in the calculations.

A number of useful (and elegant) results for mathematical quantities related to the Airy functions $Ai(z)$ have been obtained in [13]. Therein, in particular, a remarkable procedure called "Airy averaging" is introduced, which proves to be a versatile tool for manipulating conveniently mathematical expressions involving Airy functions. In the present paper, we propose to review this ingenious procedure, so as to make it better known in view of its utility and simplicity. Some applications will then be discussed to illustrate concretely such virtues.

2. Airy averaging

The integral representation of the Airy function $Ai(y)$, equation (4), allows one to obtain readily the following result:

$$\int_{-\infty}^{\infty} \mathrm{d}y\, Ai(y)\mathrm{e}^{\mathrm{i}xy} = \exp\left(-\mathrm{i}\frac{x^3}{3}\right), \tag{6}$$

interpretable as the Fourier transform of $Ai(y)$ itself. As a special case of equation (6), we have

$$\int_{-\infty}^{\infty} \mathrm{d}y\, Ai(y) = 1. \tag{7}$$

The validity of the last result suggests immediately the idea of a (normalized) "Airy distribution". The "Airy averaging" of an arbitrary function $f(y)$ then follows in a straightforward way according to the definition

$$\langle f(y)\rangle_{Ai} \equiv \int_{-\infty}^{\infty} \mathrm{d}y\, f(y) Ai(y). \tag{8}$$

It is soon realized that the "Airy averaging" operation is a linear mapping. In particular, with $f(y) = \int_a^b \mathrm{d}t\, K(t, y)$,

$$\left\langle \int_a^b \mathrm{d}t\, K(t, y) \right\rangle_{Ai} = \int_a^b \mathrm{d}t\, \langle K(t, y)\rangle_{Ai}, \tag{9}$$

as one recognizes after simply exchanging two integration orders.

The following result is a trivial consequence stemming from the comparison of equations (6) and (8):

$$\langle \exp(\mathrm{i}xy)\rangle_{Ai} = \exp\left(-\mathrm{i}\frac{x^3}{3}\right). \tag{10}$$

Everything found in this section derives from [13]. Despite its brevity, it is enough for our purposes. In the next section, we start by presenting a few mathematical results which descend from the utilization of the procedure just described. Emphasis will be placed on the evaluation of certain integrals involving Airy functions $Ai(z)$.

3. Airy averaging: some mathematical applications

As a first (and direct) consequence of the procedure outlined in the previous section, we consider the evaluation of the following type of integrals:

$$I_n \equiv \int_{-\infty}^{\infty} \mathrm{d}y\, y^n Ai(y) = \langle y^n\rangle_{Ai}, \tag{11}$$

which can be regarded as defining the nth order moment of the "Airy distribution". If we set, in equation (8), $f(y) = y^n \mathrm{e}^{\mathrm{i}xy}$ (with n positive or null integer), it is easily verified that

$$I_n = \mathrm{i}^{-n}\left[\frac{\partial^n}{\partial x^n}\langle \exp(\mathrm{i}xy)\rangle_{Ai}\right]_{x=0} = \mathrm{i}^{-n}\left[\frac{\partial^n}{\partial x^n}\mathrm{e}^{-\mathrm{i}x^3/3}\right]_{x=0}. \tag{12}$$

The non-zero "Airy distribution" moments I_n are therefore only those with $n = 3k$ ($k = 0, 1, 2, \ldots$). The general result $I_{3k} = (3k)!/(k!3^k)$ which follows from equation (12) had been obtained previously by Gislason on the basis of a different analytical procedure [18].

A second application is offered by the evaluation of the following family of two-parameter integrals involving Airy functions:

$$I(\alpha,\beta) \equiv \int_{-\infty}^{\infty} \mathrm{d}y\ \exp(\mathrm{i}\alpha y) Ai(y) Ai(y+\beta), \tag{13}$$

which can be interpreted as the Fourier transform of the product of two Airy functions with shifted arguments. The solution of a (one-dimensional) quantum problem in terms of a continuum basis set of Airy functions leads to matrix elements which can be reduced immediately to a form involving integrals containing products of Airy functions with shifted arguments.

Taking into account equation (8), we have

$$I(\alpha,\beta) = \left\langle \mathrm{e}^{\mathrm{i}\alpha y} Ai(y+\beta) \right\rangle_{Ai}. \tag{14}$$

The integral representation of the Airy function, equation (4), combined with the linear nature of the Airy averaging allows to cast equation (14) into the form

$$I(\alpha,\beta) = \frac{\mathrm{e}^{-\mathrm{i}\alpha^3/3}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x \exp\left[-\mathrm{i}\alpha\left(x^2 - \frac{\alpha^2-\beta}{\alpha} x\right)\right], \tag{15}$$

which involves a simple Gaussian integral. The final result,

$$I(\alpha,\beta) = \frac{1}{2(\mathrm{i}\pi\alpha)^{1/2}} \exp\left[-\frac{\mathrm{i}}{2}\left(\frac{\alpha^3}{6} + \alpha\beta - \frac{\beta^2}{2\alpha}\right)\right], \tag{16}$$

should be compared with that obtained previously by Lee and Light [29] through a procedure based on the representation of the one-dimensional quantum propagator of a particle subjected to a uniform field in terms of the continuum eigenstates of the problem, equation (4).

A corollary of the preceding result is

$$I(0,\beta) = \delta(\beta), \tag{17}$$

clearly a consequence of the completeness condition of the Airy functions, equation (5) (ii). The result just derived is a particular case of the family of integrals

$$J_n(\beta) \equiv \int_{-\infty}^{\infty} \mathrm{d}y\, y^n Ai(y) Ai(y+\beta), \tag{18}$$

which can be evaluated from equation (16) according to the simple rule

$$J_n(\beta) = \mathrm{i}^{-n} \left[\frac{\partial^n I(\alpha,\beta)}{\partial\alpha^n}\right]_{\alpha=0}. \tag{19}$$

Continuum matrix elements of the type of relation (18) between Airy functions have been employed in the study of collision-induced processes [22,23].

As a further example of the instrumental use of the Airy averaging for mathematical manipulations, we propose to deduce a useful integral representation of $[Ai(x)]^2$, the square of the Airy function $Ai(x)$. Such a quantity is encountered in semiclassical $\mathcal{S}$-matrix theory of inelastic collisions [31] and has been found of utility in the quantum-mechanical study of the electron photodetachment from negative ions in the presence of a static electric field [12,17,20]. From the obvious identity

$$\left[Ai(x)\right]^2 = \left\langle Ai(y)\delta(y-x)\right\rangle_{Ai}, \tag{20}$$

the simple recourse to the Fourier representation of the Dirac delta function and equation (9) yield

$$\left[Ai(x)\right]^2 = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}tx}\left\langle Ai(y)\mathrm{e}^{\mathrm{i}ty}\right\rangle_{Ai}. \tag{21}$$

From equations (14) and (16), the equality

$$\left\langle Ai(y)\mathrm{e}^{\mathrm{i}ty}\right\rangle_{Ai} \equiv I(t,0)$$

is soon recognized, so that

$$\left[Ai(x)\right]^2 = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} \mathrm{d}t \left(\frac{\pi}{\mathrm{i}t}\right)^{1/2} \exp\left[-\mathrm{i}\left(\frac{t^3}{12} + xt\right)\right], \tag{22}$$

an integral representation already known [29], obtained here in a very simple and admittedly elegant way.

The result just derived can be cast into a form which proves to be useful for some developments considered in the next section. The change of variable $z = 2^{-2/3}t$ and the recourse to equation (10) allow one to re-express equation (22) as follows:

$$\left[Ai(x)\right]^2 = \frac{2^{4/3}\pi^{1/2}}{(2\pi)^2}\,\mathrm{Re}\int_{0}^{\infty} \mathrm{d}z\, \frac{\exp(-\mathrm{i}2^{2/3}xz)}{(\mathrm{i}z)^{1/2}}\left\langle \mathrm{e}^{\mathrm{i}zx}\right\rangle_{Ai}. \tag{23}$$

A further change of variable, $z = s^2$, then leads to a Gaussian integral that is easily evaluated. After a few additional manipulations, one attains the following alternative expression for $[Ai(x)]^2$:

$$\left[Ai(x)\right]^2 = \frac{1}{2\pi}\,\mathrm{Re}\left\langle\left(2^{-2/3}y - x\right)^{-1/2}\right\rangle_{Ai}. \tag{24}$$

According to equation (24), $[Ai(x)]^2$ is proportional to the real part of the Airy averaging of the function $(2^{-2/3}y - x)^{-1/2}$. Essentially the same result as equation (23) has been put forward by Englert and Schwinger [13] in a nice paper aimed at introducing quantum corrections to the statistical atom beyond the Thomas–Fermi approximation.

An asymptotic expansion of $[Ai(x)]^2$ for $x < 0$, $|x| \gg 1$, according to equation (24) (see the appendix) will be extremely useful for developing a physical application presented in the next section.

As a final example of the potentiality of procedures founded on the Airy averaging, we shall derive an interesting representation of the Airy function in the form of a series involving Dirac delta function and its derivatives. The integral representation of the Airy function, equation (4), by use of equation (10), can be cast into the following form:

$$Ai(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \, \mathrm{e}^{-\mathrm{i}ky} \langle \mathrm{e}^{\mathrm{i}kx} \rangle_{Ai}.$$

If we now expand $\mathrm{e}^{\mathrm{i}kx}$ in power series, from equation (12) it follows that

$$\langle \mathrm{e}^{\mathrm{i}kx} \rangle_{Ai} = \sum_{n=0}^{\infty} \frac{(\mathrm{i}k)^{3n}}{3^n n!}$$

and, after simple manipulations,

$$Ai(y) = \delta(y) + \sum_{n=1}^{\infty} \frac{(-1)^n \, \mathrm{d}^{3n}}{3^n n! \, \mathrm{d}y^{3n}} \delta(y), \tag{25}$$

the searched representation. A truncated form of equation (25) has been used by Heller in a paper [21] addressing to introduce quantum corrections to classical molecular photodissociation models, so as to overcome the “reflection” approximation [11,36]. Further applications of equation (25) to discuss semiclassical expansions in the context of Franck–Condon transitions are found in a very recent paper [24].

4. The response of confined charged particles to a d.c. electric field

Electric polarizability and hyperpolarizabilities are well-known microscopic response functions which play a basic role in characterizing the linear and non-linear optical behaviour of molecules subjected to electromagnetic fields. In particular, thanks to recent technological progress, one is nowadays allowed to produce very smooth nanostructure semiconducting systems based on quantum-well concepts [14,25], endowed with peculiar response properties compared to those of bulk matter. Systems of this sort can be mimicked usefully by recourse to schematic models. Here we shall consider one of these models, a single carrier (effective mass m and electric charge $-e$) acted on by a d.c. electric field and confined to a parallelepiped box with impenetrable walls, a quantum-mechanical system revisited many times, mostly for pedagogic reasons [6,7,30,32].

Assuming the electric field to be oriented along one of the box edges (x-axis), the quantum stationary states of the carrier in the (y, z)-plane are those of a particle bouncing freely within a two-dimensional closed “court” delimited by infinitely high walls, an elementary model treated in introductory textbooks of quantum mechanics, and thus the problem is reduced to getting the solutions of the one-dimensional Schrödinger equation in the presence of a constant field, equation (2), with the boundary conditions $\phi(0; E) = \phi(L; E) = 0$ (the two relevant walls of the box being placed at $x = 0$ and $x = L$, respectively).

The searched solution to equation (2) can be expressed as follows:

$$\phi(x; E) = NAi\big[-\beta(E + Fx)\big] + MBi\big[-\beta(E + Fx)\big], \tag{26}$$

Bi(y) being the irregular Airy function of the argument indicated. The impenetrable-box boundary conditions $\phi(0;E) = \phi(L;E) = 0$ yield the secular equation

$$\begin{vmatrix} Ai[-\beta E] & Bi[-\beta E] \\ Ai[-\beta(E+FL)] & Bi[-\beta(E+FL)] \end{vmatrix} = 0, \tag{27}$$

whose solution provides the allowed eigenvalues E_n of the problem. The implementation of a procedure leading to exact eigenvalues rigorously dressed by the field is not a trivial matter (for a suggested graphical approach, see, for example, [10]); for our present purposes, however, we are exempted from such task. For any eigenvalue E_n, the ratio M_n/N_n between the coefficients of equation (26) must satisfy the conditions

$$\frac{M_n}{N_n} = -\frac{Ai[-\beta E_n]}{Bi[-\beta E_n]} = -\frac{Ai[-\beta(E_n+FL)]}{Bi[-\beta(E_n+FL)]}. \tag{28}$$

Equation (26) for the eigenfunction $\phi(x;E_n)$ is then usefully expressed in the form

$$\phi(x;E_n) = N_n\left\{Ai\big[-\beta(E_n+Fx)\big] + \frac{M_n}{N_n}Bi\big[-\beta(E_n+Fx)\big]\right\}, \tag{29}$$

to be used in conjunction with equation (28).

The centroid of the carrier distribution in the presence of field, i.e., the expectation value $\langle x\rangle$ of its position in a given energy eigenstate, $\langle x\rangle = \int_0^L \mathrm{d}x\, x|\phi(x;E)|^2$, can be cast into the form

$$\langle x\rangle = \frac{N^2}{3\pi^2(\beta F)^2}\left[\frac{2\beta E}{Bi^2[-\beta E]} - \frac{\beta(2E-FL)}{Bi^2[-\beta(E+FL)]}\right], \tag{30}$$

where, for the sake of simplicity, any label related to the specific state considered has been deleted. Equation (30) follows after some rather direct manipulations where known exact results for indefinite integrals involving products of Airy functions *Ai*(x) and/or *Bi*(x) and powers have been used [4], along with the conditions expressed by equation (28) and the Wronskian property $W[Ai,Bi] = \pi^{-1}$ [1].

A procedure entirely equivalent to that just described allows to express the squared normalization constant N^2 as

$$N^2 = \pi^2\beta F\left[\frac{1}{Bi^2[-\beta(E+FL)]} - \frac{1}{Bi^2[-\beta E]}\right]^{-1}. \tag{31}$$

At the cost of some additional labor, the centroid of the carrier distribution in a given energy eigenstate can be cast into the following final form:

$$\langle x\rangle(F) = \frac{L}{3\big[1 - \big(\frac{Ai[-\beta(E(F)+FL)]}{Ai[-\beta E(F)]}\big)^2\big]} - \frac{2}{3}\frac{E(F)}{F}, \tag{32}$$

which involves the ratio between squared Airy functions *Ai*(y) with shifted arguments.

In equation (32), the F-dependence of the various quantities has been emphasized. The carrier-distribution centroid $\langle x\rangle(F)$ depends on the electric force strength F in a surely complicated way, considering that F appears not only explicitly, but also implicitly, through the F-dependence of the energy eigenvalue $E(F)$. All of this, however, is hardly surprising, inasmuch as the result derived, equation (32), is a rigorous one, without restrictions posed, for example, by perturbation-theory validity arguments.

The departure of $\langle x\rangle(F)$ from its value $L/2$ in the absence of the external field is essentially a measure of the response of the charged-carrier distribution, confined within the box, to the applied electric field $\mathcal{E} = F/(-e)$. For relatively weak fields, a perturbation-theory description truncated at a proper order appears to be a sensible way of proceeding. Thus, according to the usual approaches, we set

$$E(F) = E(0) - \mu_{\mathrm{p}}\mathcal{E} - \frac{1}{2!}\alpha\mathcal{E}^2 - \frac{1}{3!}\beta\mathcal{E}^3 - \frac{1}{4!}\gamma\mathcal{E}^4 + \cdots, \tag{33}$$

an (asymptotic) series in powers of the field. The quantities on the right-hand side of equation (33) are soon identified as the permanent dipole moment (μ_{p}), the static electric dipole polarizability (α) and the various electric dipole hyperpolarizabilities ($\beta, \gamma, \ldots$) [33]. The truncation of equation (31) after the fourth power of the field corresponds to considering a nonlinear electric response which is adequate to most realistic situations.

From equation (33), application of the Hellmann–Feynman theorem [5], $\partial E(F)/\partial\mathcal{E} = e\langle x\rangle(F) = -\mu(\mathcal{E})$, yields

$$\mu(\mathcal{E}) = \mu_{\mathrm{p}} + \alpha\mathcal{E} + \frac{1}{2!}\beta\mathcal{E}^2 + \frac{1}{3!}\gamma\mathcal{E}^3 + \cdots, \tag{34}$$

so that the extraction from equation (33) of the response functions $\alpha, \beta, \gamma, \ldots$ leads to consider the equation

$$\begin{aligned} \mu_{\mathrm{p}} + 2\alpha\mathcal{E} + \frac{7}{6}\beta\mathcal{E}^2 + \frac{5}{12}\gamma\mathcal{E}^3 + \cdots &= -\left[\frac{eL}{v(\mathcal{E})} + \frac{2E(0)}{\mathcal{E}}\right], \\ v(\mathcal{E}) &\equiv 1 - \left\{\frac{Ai[-\beta(E(F) - e\mathcal{E}L)]}{Ai[-\beta E(F)]}\right\}^2, \end{aligned} \tag{35}$$

with $E(F)$ expressed by equation (33). The most obvious way of proceeding involves an expansion of the right-hand side of equation (35) in powers of the field $\mathcal{E}$. It is then straightforward to verify the following expressions for $\mu_{\mathrm{p}}, \alpha, \beta, \gamma, \ldots$:

$$\begin{aligned} &\mu_{\mathrm{p}} = -\lim_{\mathcal{E}\to 0}\left[\frac{2E(0)}{\mathcal{E}} + \frac{eL}{v(\mathcal{E})}\right], \\ &\alpha = \lim_{\mathcal{E}\to 0}\left[\frac{E(0)}{\mathcal{E}^2} - \frac{eL}{2}\frac{\partial}{\partial\mathcal{E}}\left(\frac{1}{v(\mathcal{E})}\right)\right], \qquad \beta = -\lim_{\mathcal{E}\to 0}\left[\frac{12}{7}\frac{E(0)}{\mathcal{E}^3} + \frac{3eL}{7}\frac{\partial^2}{\partial\mathcal{E}^2}\left(\frac{1}{v(\mathcal{E})}\right)\right], \\ &\gamma = \lim_{\mathcal{E}\to 0}\left[\frac{24}{5}\frac{E(0)}{\mathcal{E}^4} - \frac{2eL}{5}\frac{\partial^3}{\partial\mathcal{E}^3}\left(\frac{1}{v(\mathcal{E})}\right)\right], \qquad \ldots. \end{aligned} \tag{36}$$

Considering the form of equations (36), in particular the requested limit $\mathcal{E} \to 0$ and the expression of $v(\mathcal{E})$, equation (35), one becomes soon convinced that the needed developments for obtaining $\alpha, \beta, \gamma, \ldots$ by necessity require manipulations involving the asymptotic behaviour of $[Ai(-|y|)]^2$ ($|y| \gg 1$). Such asymptotic behaviour in the form of expansion in inverse powers of $|y|$ is derived in the appendix starting from equation (24), a consequence of the Airy averaging trick.

At the cost of much paper and very annoying algebra, a procedure bristling with noticeable error occurrence leads to the following results for linear and non-linear dipole polarizabilities in the case of a carrier in the field-free energy level $E_n(0) = \pi^2\hbar^2 n^2/(2mL^2)$ ($n = 1, 2, \ldots$):

$$\alpha = \frac{e^2 L^2}{8E_n(0)}\left[-\frac{1}{3} + \frac{5\hbar^2}{2mL^2 E_n(0)}\right], \qquad \beta = 0,$$
$$\gamma = \frac{e^4 L^4}{32E_n^3(0)}\left[-\frac{1}{3} + \frac{35\hbar^2}{mL^2 E_n(0)} - \frac{165\hbar^4}{m^2 L^4 E_n^2(0)}\right]. \tag{37}$$

The expressions just derived agree perfectly with those obtained by Rustagi and Ducuing [34] through a straightforward perturbation-theory treatment. They have been used for rough estimates of the electric response of systems involving delocalized electrons, for example, organic molecules such as polyenes and cyanines. The linear response α of the model on issue has been evaluated many times [2,6,7,10,32], with results not always agreeing with each other.

Appendix

The result for the square of the Airy function $Ai(y)$, equation (24), can be expressed as follows:

$$2\pi\left[Ai(y)\right]^2 = \mathrm{Re}\left[\int_{-\infty}^{2^{2/3}y} \mathrm{d}x\,\frac{Ai(x)}{(2^{-2/3}x - y)^{1/2}} + \int_{2^{2/3}y}^{\infty} \mathrm{d}x\,\frac{Ai(x)}{(2^{-2/3}x - y)^{1/2}}\right], \tag{A.1}$$

so that

$$2\pi\left[Ai(y)\right]^2 = \int_{2^{2/3}y}^{\infty} \mathrm{d}x\,\frac{Ai(x)}{(2^{-2/3}x - y)^{1/2}}. \tag{A.2}$$

We shall be particularly interested in the case $y < 0$, with $|y| \gg 1$. Under such conditions, the neglect of the contribution to the integral from the interval $(2^{2/3}|y|, \infty)$ leads to the result

$$2\pi\left[Ai(-|y|)\right]^2 \cong |y|^{-1/2} \int_{-2^{2/3}|y|}^{2^{2/3}|y|} \mathrm{d}x\, Ai(x)\left[1 + \frac{2^{-2/3}x}{|y|}\right]^{-1/2}. \tag{A.3}$$

After expanding the quantity $(1+2^{-2/3}x/|y|)^{-1/2}$ in powers of $2^{-2/3}x/|y|$ and restoring the integration limits to $\pm\infty$, we obtain readily the following asymptotic expansion for $[Ai(-|y|)]^2$:

$$\left[Ai\left(-|y|\right)\right]^2 \cong \frac{|y|^{-1/2}}{2\pi}\left[1+\sum_{n=1}^{\infty}\frac{(-1)^n 2^{-2n/3}}{2^n n!|y|^n}\left\langle x^n\right\rangle_{Ai}\right]. \tag{A.4}$$

Use of the results for the Airy averaging $\langle x^n\rangle_{Ai}$ found in section 2 (see equation (12)) leads to the final result

$$\left[Ai\left(-|y|\right)\right]^2 \cong \frac{|y|^{-1/2}}{2\pi}\left[1+\sum_{k=1}^{\infty}\frac{(-1)^k(6k-1)!!}{(96)^k k!|y|^{3k}}\right]. \tag{A.5}$$

As remarked elsewhere [13], we could have attained the result expressed by equation (A.5) starting from the known asymptotic behaviour of the Airy function $Ai(y)$ for $-y \gg 1$ [1]. Such a procedure would be surely much more troublesome, because of the presence of oscillatory factors in the usual Airy function asymptotic behaviour for $-y \gg 1$, and the necessity of having recourse to some averaging over oscillations.

References

[1] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
[2] V.C. Aguilera-Navarro, H. Iwamoto, E. Ley-Koo and A.H. Zimerman, Am. J. Phys. 49 (1981) 648.
[3] G.B. Airy, Trans. Cambridge Philos. Soc. 6 (1838) 397.
[4] J.R. Albright, J. Phys. A 10 (1977) 485.
[5] P.W. Atkins, *Molecular Quantum Mechanics*, 2nd ed. (Oxford University Press, Oxford, 1983).
[6] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures I* (Les Editions de Physique, Paris, 198).
[7] W.L. Bloss, Superlact. Microstr. 6 (1989) 129.
[8] M. Brack and R.K. Bhaduri, *Semiclassical Physics* (Addison-Wesley, Reading, 1997).
[9] M.S. Child, ed., *Semiclassical Methods in Molecular Scattering and Spectroscopy* (Reidel, Dordrecht, 1980).
[10] J.N. Churchill and F.O. Arntz, Am. J. Phys. 37 (1969) 693.
[11] E.U. Condon, Phys. Rev. 32 (1928) 858.
[12] M.L. Du and J.B. Delos, Phys. Rev. A 38 (1988) 5609.
[13] B.G. Englert and J. Schwinger, Phys. Rev. A 29 (1984) 2339.
[14] L. Esaki, in: *Recent Topics in Semiconductor Physics*, eds. H. Kamimura and Y. Toyozawa (World Scientific, Singapore, 1983).
[15] W.H. Ewing, W.S. Jardetzky and F. Press, *Elastic Waves in Layered Media* (McGraw-Hill, New York, 1957).
[16] A. Galindo and P. Pascual, *Quantum Mechanics II* (Springer, Berlin, 1991).
[17] N.D. Gibson, B.J. Davies and D.J. Larson, Phys. Rev. A 48 (1993) 310.
[18] E.A. Gislason, J. Chem. Phys. 58 (1973) 3702.
[19] R.G. Gordon, J. Chem. Phys. 51 (1969) 14.
[20] N.A. Guschina and V.K. Nikulin, Chem. Phys. 10 (1975) 23.
[21] E.J. Heller, J. Chem. Phys. 68 (1978) 2066.
[22] P.M. Hunt, Mol. Phys. 44 (1981) 653.
[23] P.M. Hunt and S. Sridharan, J. Chem. Phys. 77 (1982) 4022.

[24] B. Hüpper and B. Eckardt, Phys. Rev. A 57 (1998) 1536.
[25] C.F. Klingshirn, *Semiconductor Optics* (Springer, Berlin, 1997).
[26] L. Landau and E. Lifchitz, *Mécanique Quantique, Théorie non Relativiste* (Mir, Moscou, 1974).
[27] S.-Y. Lee, J. Chem. Phys. 72 (1980) 332.
[28] S.-Y. Lee and E.J. Heller, J. Chem. Phys. 71 (1979) 4777.
[29] S.-Y. Lee and J.C. Light, J. Chem. Phys. 63 (1975) 5274.
[30] M. Matsuura and T. Kamizato, Phys. Rev. A 33 (1986) 8385.
[31] W.H. Miller, J. Chem. Phys. 48 (1968) 464; 53 (1970) 3578.
[32] D. Nguyen and T. Odagaki, Am. J. Phys. 55 (1987) 466.
[33] P.N. Prasad and D.J. Williams, *Introduction to Nonlinear Optical Effects in Molecules and Polymers* (Wiley, New York, 1991).
[34] K.C. Rustagi and J. Ducuing, Opt. Comm. 10 (1974) 258.
[35] F. Schwabl, *Quantum Mechanics* (Springer, Berlin, 1992).
[36] E.C.G. Stuckelberg, Phys. Rev. 42 (1932) 518.