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On the asymptotics of a class of two-dimensional Fourier integrals

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Abstract. We derive the asymptotic expansion of a class of two-dimensional Fourier integrals that typically arise in perturbative treatments of the interaction of the quantized electromagnetic field with atoms and other quantum systems. The principal difficulty that prevents the application of standard methods is the fact that the integrand has a saddle point in the corner of the domain of integration.

1. Introduction

Let $I(\lambda)$ be the two-dimensional integral

$$I(\lambda) = \int_{\mathcal{D}} \frac{yf(x)}{y+1} \cos(\lambda xy) dS \quad (1)$$

where $f(x)$ is well behaved for $0 \leq x \leq 1$ and \mathcal{D} is the half-strip

$$\{(x, y) | 0 \leq x \leq 1, y \geq 0\}.$$

$I(\lambda)$ is typical of the kind of integral that arises when second-order perturbation theory is applied to the interaction of the quantized electromagnetic field with an atom which is not located at the coordinate origin. The variable $y \equiv |k|$ is the modulus of the photon wavevector, the variable $x \equiv \cos \theta$ is the cosine of the angle that the wavevector k forms with the position vector r of the atom with respect to the origin, and $\lambda \equiv 2|r|$. The oscillatory factor $\cos(\lambda xy) \equiv \cos(2k \cdot r)$ comes from the quantization of the electromagnetic field in terms of plane waves, and the denominator $(y+1)$ has its origin in the energy denominator of second-order perturbation theory and reflects the interaction of the photon field with virtual up-transitions in the atom. The function $f(x)$ is specific to the problem under consideration; for instance, when calculating the energy level shifts in an atom placed near a partially reflecting wall, one has

$$f(x) = \frac{x - \sqrt{x^2 + n^2 - 1}}{x + \sqrt{x^2 + n^2 - 1}}$$

where $n > 1$ is the refractive index of the wall (see Wu and Eberlein 1999).

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The problem is to find the asymptotic behaviour of $I(\lambda)$ as $\lambda \rightarrow \infty$. This corresponds to the long-distance approximation which is appropriate when the distance of the atom from the origin is much greater than the typical wavelengths of atomic transitions. It is therefore appropriate for most physical applications.

2. Discussion of the problem

For a general integral of the form

$$\int_{\mathcal{D}'} F(x, y) e^{i\lambda\mathcal{K}(x, y)} dS \quad (2)$$

contributions to the asymptotic expansion come from the boundary of \mathcal{D}' and from stationary points of $\mathcal{K}(x, y)$ (see Wong 1989, ch 8, for example). This can be verified by means of a process that is the two-dimensional equivalent of integration by parts. We have

$$\int_{\mathcal{D}'} F(x, y) e^{i\lambda\mathcal{K}(x, y)} dS = \frac{1}{i\lambda} \int_{\mathcal{D}'} \nabla \cdot (\mathbf{u} e^{i\lambda\mathcal{K}(x, y)}) dS - \frac{1}{i\lambda} \int_{\mathcal{D}'} e^{i\lambda\mathcal{K}(x, y)} \nabla \cdot \mathbf{u} dS \quad (3)$$

where the vector field $\mathbf{u} \equiv (u_1, u_2)$ is chosen so that $\mathbf{u} \cdot \nabla\mathcal{K} = F(x, y)$. A suitable choice is

$$\mathbf{u} = \frac{F(x, y)}{|\nabla\mathcal{K}|^2} \nabla\mathcal{K}.$$

The first of the integrals on the right-hand side of equation (3) can be transformed into a line integral round the boundary of \mathcal{D}' , using Stokes' theorem in the plane (Green's theorem):

$$\int_{\mathcal{D}'} \nabla \cdot (\mathbf{u} e^{i\lambda\mathcal{K}(x, y)}) dS = \oint_{\partial\mathcal{D}'} e^{i\lambda\mathcal{K}(x, y)} (-u_2, u_1) \cdot d\boldsymbol{\ell}.$$

The procedure can be applied again, to the second integral on the right-hand side of equation (3), using a vector field $\tilde{\mathbf{u}}$ such that $\tilde{\mathbf{u}} \cdot \nabla\mathcal{K} = \nabla \cdot \mathbf{u}$. This produces another boundary term and a double integral of order $(i\lambda)^{-2}$. Repeated application produces a series of boundary terms in inverse powers of λ together with a remainder term in the form of a double integral, which one has to estimate in order to demonstrate that the expansion is asymptotic. The method will only fail where \mathbf{u} is badly behaved. If $F(x, y)$ and \mathcal{K} are well behaved, the method only fails at stationary points of \mathcal{K} , where $\nabla\mathcal{K} = 0$. Applying the Riemann–Lebesgue lemma to the boundary integrals shows that the contributions to the asymptotic expansion come from the corner points of \mathcal{D}' (i.e. the end points of each boundary-line integral) and from points on the boundary where $\nabla\mathcal{K} \cdot d\boldsymbol{\ell} = 0$.

There are two standard methods of obtaining asymptotic expansions of integrals of the form (2). One is to use Stokes' theorem as outlined above. The other is to make a change of variable $(x, y) \mapsto (s, t)$, where $t = \mathcal{K}(x, y)$ and s parametrizes the curves of $\mathcal{K}(x, y) = \text{constant}$. The s -integration, which does not involve λ , can then be done, leaving a one-dimensional integral which can, in principle, be tackled by elementary methods.

The particular integral (1) presents difficulties, because:

- convergence problems arise as approximations are attempted;
- \mathcal{K} has a saddle point at the origin ($\nabla\mathcal{K} = \nabla(xy) = (y, x) = 0$) which not only lies on the boundary but is also a corner point;
- two of the boundary curves, namely $x = 0$ and $y = 0$, are also curves of constant $\mathcal{K}(x, y)$: this causes problems because the oscillatory nature of the integrand which gives rise to the asymptotic behaviour is not then present.

In such cases, few general results are known (see e.g., Bleistein 1984); it is best to treat each example individually. Below we show how the asymptotic expansion for integral (1) can be obtained using rigorous methods which may be adapted to deal with other similar integrals.

3. Notation

It is useful to define a function $\mathcal{E}(\lambda)$, for $\lambda > 0$, by

$$\mathcal{E}(\lambda) = \int_0^\infty \frac{e^{iu}}{u + \lambda} du. \tag{4}$$

It is related to standard special functions as follows:

$$\mathcal{E}(\lambda) = e^{-i\lambda} E_1(-i\lambda) = \mathbf{g}(\lambda) + i\mathbf{f}(\lambda) \tag{5}$$

where $E_1(z)$ is the exponential integral $\int_z^\infty t^{-1}e^{-t} dt$, and $\mathbf{g}(z)$ and $\mathbf{f}(z)$ are the auxiliary functions defined, for example, in Abramowitz and Stegun (1970, 5.2.12 and 5.2.13). $\mathcal{E}(z)$ has a simple asymptotic expansion as $|z| \rightarrow \infty$, valid for $|\arg z| < \pi$:

$$\mathcal{E}(z) \sim -\frac{1}{iz} \left(1 + \frac{1}{iz} + \frac{2!}{(iz)^2} + \frac{3!}{(iz)^3} + \dots \right). \tag{6}$$

4. Convergence of the integral

Convergence of the integral (1) is delicate. The obvious problem is that the integrand does not become small as $y \rightarrow \infty$; this limit would be a problem even without the factor of y in the numerator. For fixed x , it is the rapid oscillation of $\cos(\lambda xy)$ that prevents the y -integral from diverging, but this effect is not uniform in x .

In view of these convergence problems, it is necessary to define the integral as a limit of the form

$$I(\lambda) = \lim_{R \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \int_\epsilon^1 \int_0^R \frac{y f(x)}{y + 1} \cos(\lambda xy) dy dx. \tag{7}$$

The order in which the two limits are taken matters. For example, in the case $f(x) = 1$, we can evaluate the integral explicitly. Taking the ϵ limit first gives

$$\lim_{R \rightarrow \infty} \int_0^R \int_0^1 \frac{y}{y + 1} \cos(\lambda xy) dx dy = \int_0^\infty \frac{\sin(\lambda y)}{\lambda(y + 1)} dy = \lambda^{-1} \mathbf{f}(\lambda).$$

Taking the R limit first gives

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \int_\epsilon^1 \int_0^\infty \frac{y}{y + 1} \cos(\lambda xy) dy dx &= \lim_{\epsilon \rightarrow 0} \int_0^\infty \frac{\sin(\lambda y) - \sin(\epsilon \lambda y)}{\lambda(y + 1)} dy \\ &= \lambda^{-1} \mathbf{f}(\lambda) - \lim_{\epsilon \rightarrow 0} \lambda^{-1} \mathbf{f}(\epsilon \lambda) = \lambda^{-1} \mathbf{f}(\lambda) - \frac{\pi}{2\lambda}. \end{aligned}$$

Typically, the difference arising from the order in which the limits are taken is $\pi f(0)/(2\lambda)$. One can see how convergence problems arise in connection with the part of \mathcal{D} close to the y -axis by considering the integral

$$\lim_{R \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \int_\epsilon^1 \int_0^R \frac{y}{y + 1} \sin(\lambda xy) dy dx \tag{8}$$

which fails to converge, whichever limit is taken first.

The correct value of our integral is obtained by taking the ϵ limit first, since the integral arises essentially as an inverse Fourier transform and the Fourier inversion theorem applies in this limit. We have therefore (taking the ϵ limit)

$$I(\lambda) = \lim_{R \rightarrow \infty} \int_0^R \int_0^1 \frac{y f(x)}{y + 1} \cos(\lambda xy) dx dy. \tag{9}$$

We can improve the convergence of $I(\lambda)$ by integrating the x -integral once by parts:

$$\begin{aligned} I(\lambda) &= \lim_{R \rightarrow \infty} \int_0^R f(1) \frac{\sin(\lambda y)}{\lambda(y+1)} dy - \lim_{R \rightarrow \infty} \int_0^R \int_0^1 \frac{f'(x)}{\lambda(y+1)} \sin(\lambda xy) dx dy \\ &\equiv \lambda^{-1} f(1) f(\lambda) - \frac{1}{\lambda} \text{Im } I_1, \end{aligned}$$

where

$$I_1(\lambda) = \int_{\mathcal{D}} \frac{f'(x)}{y+1} e^{i\lambda xy} dS. \quad (10)$$

Further integration by parts is hindered by powers of y emerging in the denominator and preventing the y -integral from converging as $y \rightarrow 0$.

The integral $I_1(\lambda)$ is well defined: we can write

$$I_1(\lambda) = \int_0^1 \int_0^1 \frac{f'(x)}{y+1} e^{i\lambda xy} dx dy + \lim_{R \rightarrow \infty} \int_1^R \int_0^1 \frac{f'(x)}{y+1} e^{i\lambda xy} dx dy. \quad (11)$$

The first of these integrals is clearly Riemann integrable, while the second can be integrated by parts with respect to x giving an integrand which tends to zero as $y \rightarrow \infty$ fast enough for the modulus to be Riemann integrable.

The integral (10) can be evaluated explicitly in certain cases. The y -integral can be expressed in terms of $\mathcal{E}(\lambda x)$. The resulting x -integral can then be evaluated by repeated integration by parts if, for example, $f(x)$ is a polynomial or of the form $\cos(n\pi x)$ (see Prudnikov *et al* 1990, 1.4.2.2 and 1.4.3.3). Although general asymptotic formulae can then be obtained using Taylor series or Fourier series with estimates of the error terms, it is interesting and important to investigate the asymptotic behaviour directly.

5. Asymptotics

The obstruction to further integration of $I_1(\lambda)$ by parts is the behaviour at the origin and the way round this is to subtract off the troublesome term. For a general integral of this form, we write

$$\int_{\mathcal{D}} F(x, y) e^{i\lambda xy} dS = \int_{\mathcal{D}} (F(x, y) - F(0, y)) e^{i\lambda xy} dS + \int_{\mathcal{D}} F(0, y) e^{i\lambda xy} dS.$$

The first of these integrals is sufficiently well behaved at $x = 0$ to allow integration by parts of the y -integral. For $I_1(\lambda)$, this would increase the power of $(y+1)$ in the denominator. This corresponds to taking the vector field \mathbf{u} in equation (3) to be $(0, F)$. Alternatively, we could integrate the x -integral by parts, which would generate higher derivatives of $f(x)$ in the numerator; this corresponds to taking $\mathbf{u} = (F, 0)$. More generally, we could choose \mathbf{u} to be unaligned with either of the axes.

For $I_1(\lambda)$, we are forced to work on the x -integral because the convergence as $y \rightarrow \infty$ is not good enough to allow integration by parts of the y -integral. We have

$$\begin{aligned} I_1(\lambda) &= \int_{\mathcal{D}} \frac{xh(x)}{y+1} e^{i\lambda xy} dS + \int_{\mathcal{D}} \frac{f'(0)}{y+1} e^{i\lambda xy} dS \\ &= \frac{1}{i\lambda} \int_{\mathcal{D}} \nabla \cdot [(0, h(x)/(y+1)) e^{i\lambda xy}] dS \\ &\quad + \frac{1}{i\lambda} \int_{\mathcal{D}} \frac{h(x)}{(y+1)^2} e^{i\lambda xy} dS + \frac{f'(0)}{i\lambda} \int_0^{\infty} \frac{e^{i\lambda y} - 1}{(y+1)y} dy \\ &= -\frac{1}{i\lambda} \int_0^1 h(x) dx + \frac{1}{i\lambda} I_2(\lambda) + \frac{f'(0)}{i\lambda} \int_0^{\infty} \frac{e^{i\lambda y} - 1}{(y+1)y} dy \end{aligned} \quad (12)$$

where

$$h(x) = \frac{f'(x) - f'(0)}{x}$$

and

$$I_2(\lambda) = \int_{\mathcal{D}} \frac{h(x)}{(y+1)^2} e^{i\lambda xy} dS. \tag{13}$$

The last integral in equation (12) can be written in terms of $\mathcal{E}(\lambda)$:

$$\begin{aligned} \int_0^\infty \frac{e^{i\lambda y} - 1}{(y+1)y} dy &= \int_0^\infty \frac{i \sin \lambda y}{y} dy - \int_0^\infty \frac{e^{i\lambda y}}{y+1} dy \\ &+ \int_0^\infty (\cos \lambda y - \cos y) \frac{dy}{y} + \int_0^\infty \left(\cos y - \frac{1}{1+y} \right) \frac{dy}{y} \\ &= i\pi/2 - \mathcal{E}(\lambda) - \ln \lambda - \gamma. \end{aligned} \tag{14}$$

The standard integrals are given by Gradshteyn and Ryzhik (1994, 3.781(2) and 3.784(1)).

It is not hard to estimate that the integral $I_2(\lambda)$ is $o(\lambda^{-1})$ as $\lambda \rightarrow \infty$ so the expansion (12) is asymptotic to order λ^{-1} .

So far, the method has been fairly general. The procedure could be repeated on the integral I_2 in order to obtain the next term in the expansion and a new integral I_3 and the whole series could be developed in this way. However, because of the specific form of the integrand of $I_2(\lambda)$, it is possible to obtain a neater reduction formula which does not require the calculation of new integrals. From the definition (13) follows

$$I_2(\lambda) = \int_{\mathcal{D}} \frac{h(x)e^{i\lambda xy}}{y+1} dS - \int_{\mathcal{D}} \frac{yh(x)e^{i\lambda xy}}{(y+1)^2} dS. \tag{15}$$

The first of these integrals can be transformed using the method of equation (12):

$$\begin{aligned} \int_{\mathcal{D}} \frac{h(x)e^{i\lambda xy}}{(y+1)} dS &= -\frac{1}{i\lambda} \int_0^1 \frac{h(x) - h(0)}{x} dx + \frac{1}{i\lambda} \int_{\mathcal{D}} \frac{h(x) - h(0)}{x} \frac{e^{i\lambda xy}}{(y+1)^2} dS \\ &+ \frac{h(0)}{i\lambda} (i\pi/2 - \mathcal{E}(\lambda) - \ln \lambda - \gamma). \end{aligned} \tag{16}$$

The second of the integrals in equation (15) can be transformed by integration by parts of the x -integral:

$$\begin{aligned} - \int_{\mathcal{D}} \frac{yh(x)e^{i\lambda xy}}{(y+1)^2} dS &= \frac{1}{i\lambda} \int_0^\infty \frac{h(0)}{(y+1)^2} dy - \frac{1}{i\lambda} \int_0^\infty \frac{h(1)e^{i\lambda y}}{(y+1)^2} dy + \frac{1}{i\lambda} \int_{\mathcal{D}} \frac{h'(x)e^{i\lambda xy}}{(y+1)^2} dS \\ &= \frac{h(0)}{i\lambda} - \frac{h(1)}{i\lambda} - h(1)\mathcal{E}(\lambda) + \frac{1}{i\lambda} \int_{\mathcal{D}} \frac{h'(x)e^{i\lambda xy}}{(y+1)^2} dS. \end{aligned}$$

Adding gives

$$I_2(\lambda) = \frac{h(0)}{i\lambda} (i\pi/2 - \mathcal{E}(\lambda) - \ln \lambda - \gamma) - h(1)\mathcal{E}(\lambda) - \frac{1}{i\lambda} \int_0^1 h_1(x) dx + \frac{1}{i\lambda} \mathcal{L}_1(\lambda)$$

where

$$h_1(x) = \frac{xh'(x) + h(x) - h(0)}{x} \equiv \frac{f''(x) - f''(0)}{x}$$

and

$$\mathcal{L}_1(\lambda) = \int_{\mathcal{D}} \frac{h_1(x)}{(y+1)^2} e^{i\lambda xy} dS.$$

Note that $\mathcal{L}_1(\lambda)$ has exactly the same form as $I_2(\lambda)$, so we can repeat the process to obtain the full asymptotic expansion for $I_2(\lambda)$:

$$I_2(\lambda) \sim \sum_{n=0}^{\infty} \frac{h_n(0)}{(i\lambda)^{n+1}} (i\pi/2 - \mathcal{E}(\lambda) - \ln \lambda - \gamma) - \sum_{n=0}^{\infty} \frac{h_n(1)}{(i\lambda)^n} \mathcal{E}(\lambda) - \sum_{n=1}^{\infty} \frac{1}{(i\lambda)^n} \int_0^1 h_n(x) dx$$

where $xh_{n+1}(x) = xh'_n(x) + h_n(x) - h_n(0) \equiv f^{(n+2)}(x) - f^{(n+2)}(0)$, $h_0(x) = h(x)$ and $h_n(0) = f^{(n+2)}(0)$. Re-expressing in terms of $f(x)$ and tidying up gives

$$I_2(\lambda) \sim \sum_{n=0}^{\infty} \frac{f^{(n+2)}(0)}{(i\lambda)^{n+1}} (i\pi/2 - \ln \lambda - \gamma) + \mathcal{E}(\lambda) \left(f'(0) - \sum_{n=0}^{\infty} \frac{f^{(n+1)}(1)}{(i\lambda)^n} \right) - \sum_{n=1}^{\infty} \frac{1}{(i\lambda)^n} \int_0^1 \frac{f^{(n+1)}(x) - f^{(n+1)}(0)}{x} dx. \quad (17)$$

Again, the asymptotic nature of the expansion is easily established by approximating the remainder term, which is essentially the integral

$$\mathcal{L}_n(\lambda) = \int_D \frac{h_n(x)}{(y+1)^2} e^{i\lambda xy} dS. \quad (18)$$

Note that the expression (17) depends on λ only through powers of $i\lambda$ and through the combination $-\ln \lambda + i\pi/2 \equiv -\ln(-i\lambda)$, which is expected, since $I_2^*(-\lambda) = I_2(\lambda)$.

Finally, we have the asymptotic expansion for $I(\lambda)$:

$$I(\lambda) \sim \text{Re} \left\{ \left(\ln \lambda + \gamma - \frac{i\pi}{2} \right) \sum_{n=1}^{\infty} \frac{f^{(n)}(0)}{(i\lambda)^{n+1}} + \mathcal{E}(\lambda) \sum_{n=0}^{\infty} \frac{f^{(n)}(1)}{(i\lambda)^{n+1}} + \sum_{n=1}^{\infty} \frac{1}{(i\lambda)^{n+1}} \int_0^1 \frac{f^{(n)}(x) - f^{(n)}(0)}{x} dx \right\}. \quad (19)$$

We remark that \mathcal{L}_n , defined by (18), vanishes if $f(x)$ is a polynomial of degree n or less, in which case the expansion is exact.

The coefficient of λ^{-n-1} , taking into account the asymptotic expansion (6), is

$$(-1)^{(n+1)/2} \left[(\ln \lambda + \gamma) f^{(n)}(0) - \sum_{m=0}^{n-1} (n-m-1)! f^{(m)}(1) + \int_0^1 \frac{f^{(n)}(x) - f^{(n)}(0)}{x} dx \right]$$

for odd n , and

$$-(-1)^{n/2} \frac{\pi}{2} f^{(n)}(0)$$

for $n = 2, 4, \dots$

There are alternative ways of expressing this coefficient: any of quantities $f^{(n)}(x)$ (in the integral), $f^{(n)}(1)$ or $f^{(n)}(0)$ can be written in Taylor series about zero or about one. This means that there may be some amount of ambiguity in answers to physical questions. For the example of an atom outside a partially reflecting wall one cannot *a priori* decide whether the energy level shifts are primarily caused by perpendicularly reflected photons at $x \equiv \cos \theta = 1$, as one would assume intuitively, or whether they are also substantially influenced by photons travelling parallel to the surface of the wall at the grazing angle $x \equiv \cos \theta = 0$. A simple and unambiguous answer to this question can be given only for the idealized limit of a perfectly reflecting wall, when $f(x) = -1$ so that only the second term in equation (19) contributes anything at all and $I(\lambda) = -\text{Re} \mathcal{E}(\lambda) = -\text{g}(\lambda)$ exactly; then the effect is dominated by virtual photons travelling on the shortest path to the wall and getting reflected back to the atom. For non-ideal reflectors the physics involved is too complex to picture the situation in such a simple way.

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