Exponential Integrals for Quantum and Statistical Mechanics

Symbols of primary interest:

Γ(n): the Gamma Function

G(n): the Family of Gaussian Integrals

Sinc(x) = $^{\sin(x)}/_{x}$ and ($^{\sin(x)}/_{x}$)^2 Integrals

Definitions

$$\Gamma(s+1) = \int_0^\infty x^s\, e^{-x}\, dx \quad G(n) = \int_0^\infty x^n\, e^{-x^2}\, dx = (\tfrac{1}{2})\,\Gamma(\tfrac{n+1}{2})$$

Tools of the Trade

Parameter Calculus to extend integral results

Γ(x): Table and Plot for 1 < x < 2

Regularizing Functions to promote convergence - $^{\sin(x)}/_{x}$

Quantum Harmonic Oscillator integrals

Appendix

The Stirling Approximation $n! \approx n^n\, e^{-x} \sqrt{2\pi n}\,(1 + \tfrac{1}{12n})$

Integrals of exponentials arise in statistical physics and in quantum calculations involving the hydrogen atom and harmonic oscillators. The definitions and a few properties of two special exponential integrals are presented next section, and then some results directly applicable to the hydrogen atom problem and to harmonic oscillators are provided. There are more powerful methods for evaluating integrals in quantum mechanics that are based on the concepts of complete sets of orthogonal functions and recursion relations. Make the extra effort to embrace these methods when you encounter them. The final two integrals to be presented are of the {*sink*} function sinc(x) and its square. These integrals appear in the treatment of time-dependent perturbation and transitions in quantum mechanics.

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A extended table of integrals can be found later in this handout just before the problems.

Table of Integrals

$$\Gamma(s+1) = \int_0^\infty u^s\, e^{-u}\, du \qquad \Gamma(s+1) = s\,\Gamma(s) \qquad \Gamma(n+1) = n!$$

$$G(n) = \int_0^\infty u^n\, e^{-u^2}\, du = (\tfrac{1}{2})\,\Gamma(\tfrac{n+1}{2}) \qquad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \qquad \Gamma(1) = 0! = 1$$

Some specialized results appear in the extended integral table

$$\int_0^{\pi/2} [\cos\theta]^{2\mu-1}\, [\sin\theta]^{2\nu-1}\, d\theta = \frac{\Gamma(\mu)\Gamma(\nu)}{2\,\Gamma(\mu+\nu)} \quad \ldots\ \mu,\ \nu > 0$$

$$\int_{-\infty}^{\infty} \frac{\sin(x)}{x}\, dx = \pi \qquad \int_{-\infty}^{\infty} \left[\frac{\sin(x)}{x}\right]^2 dx = \pi$$

$$\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = \int_{-\infty}^{\infty} e^{-\left(ax - b/2a\right)^2}\, e^{-b^2/4a^2}\, dx = \sqrt{\pi}/a\ \ e^{-b^2/4a^2}$$

The Gamma Function: $\Gamma(s + 1)$ is defined as:

$$\Gamma(s+1) = \int_0^\infty x^s\, e^{-x}\, dx$$

and the Gaussian integral is defined as:

$$G(n) = \int_0^\infty x^n\, e^{-x^2}\, dx$$

Using integration by parts,

$$\Gamma(s+1) = \int_0^\infty x^s\, e^{-x}\, dx = -x^s\, e^{-x}\Big|_0^\infty + \int_0^\infty s\, x^{s-1}\, e^{-x}\, dx = s\,\Gamma(s)\ \ (\text{for } s > 0)$$

It follows that $\Gamma(0) = 1$, that $\Gamma(1) = 1$ and that the Gamma Function obeys the recursive relation:

$$\Gamma(s + 1) = s\,\Gamma(s) \quad (\text{for } s > 0)$$

For the special case that n is a non-negative integer, and recalling that $\Gamma(1) = 1$.

$$\Gamma(n + 1) = n\,!$$

Using the change of variable ($u = x^2$; $du = 2x\,dx$), the Gaussian integrals can be expressed in terms of the Gamma Function. For example:

$$G(0) = \int_0^\infty e^{-x^2}\,dx = \tfrac{1}{2}\int_0^\infty u^{-1/2}\,e^{-u}\,du = \tfrac{1}{2}\Gamma(\tfrac{1}{2})$$

$$G(n) = \int_0^\infty x^n\,e^{-x^2}\,dx = \tfrac{1}{2}\int_0^\infty u^{\left(\frac{n-1}{2}\right)}\,e^{-u}\,du = \tfrac{1}{2}\Gamma(\tfrac{n+1}{2})$$

The value $\Gamma(1/2)$ can be found by evaluating the square of $G(0)$.

$$\left[G(0)\right]^2 = \int_0^\infty e^{-x^2}\,dx \int_0^\infty e^{-y^2}\,dy = \int_0^\infty \int_0^{\pi/2} e^{-r^2}\,r\,dr\,d\theta = \tfrac{\pi}{4}\Gamma(1) = \left[\tfrac{1}{2}\Gamma(\tfrac{1}{2})\right]^2$$

In the first two integrals, x and y are dummy variables and so any label may be chosen for them. The choice of x and y suggests that the product of the integrals be represented as the integral of e^{-r^2} over the first quadrant of the x-y plane where $r^2 = x^2 + y^2$. The angular integration yields a factor of $\pi/2$, and the radial integral is just G(1) which is $1/2\,\Gamma(1)$ by the rule above. Finally, $G(0) = \sqrt{\pi}/2$ so $\Gamma(1/2) = \sqrt{\pi}$.

Important Exercise: Consider the integral $\int_{-\infty}^{\infty} x^n\,e^{-x^2}\,dx$. Sketch the integrand for n = 0, 1, 2 and 3. Review the definition of $G(n)$ carefully. Express $I(n) = \int_{-\infty}^{\infty} x^n\,e^{-x^2}\,dx$ in terms of gamma functions for n odd and for n even.

Applications of $G(n)$ and $\Gamma(s)$:

Expectation value integrals for the hydrogen atom problem involve angular integrations followed by radial integrals of the form:

$$\int_0^\infty r^n\,e^{-\alpha r}\,e^{-\beta r}\,dr = \frac{1}{\left[\alpha+\beta\right]^{n+1}}\,\Gamma(n+1) = \frac{n!}{\left[\alpha+\beta\right]^{n+1}}$$

The Boltzmann distribution function from statistical physics is a Gaussian leading to integrals of the form:

$$\int_0^\infty x^n\, e^{-a^2x^2}\, dx = \frac{G(n)}{a^{n+1}} = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\, a^{n+1}} = \left[\frac{n-1}{2}\right]\left(\frac{\Gamma\left(\frac{n-1}{2}\right)}{2\, a^{n+1}}\right) = \ \ldots$$

where the recursion relation is used repeatedly until $\Gamma(1) = 1$ or $\Gamma(\tfrac{1}{2}) = \sqrt{\pi}$ is reached.

For odd powers, $\int_0^\infty x^{2n+1}\, e^{-a^2x^2}\, dx = \frac{G(2n+1)}{a^{2n+2}} = \frac{\Gamma(n+1)}{2\, a^{2n+2}} == \frac{n!}{2\, a^{2n+2}}$. The harmonic oscillator problems involve integrals from -∞ to ∞ so that only the integrals with even powers of x survive.

$$\int_0^\infty x^{2n}\, e^{-a^2x^2}\, dx = \frac{G(2n)}{a^{2n+1}} = \frac{\Gamma(n+\tfrac{1}{2})}{2\, a^{2n+1}}$$
$$= \frac{1}{2\, a^{2n+1}}\left[n-1+\tfrac{1}{2}\right]\ldots\left[\tfrac{1}{2}\right]\Gamma\left(\tfrac{1}{2}\right) = \frac{\sqrt{\pi}}{2\, a^{2n+1}}\left[n-1+\tfrac{1}{2}\right]\ldots\left[\tfrac{1}{2}\right]$$

The factor $\left[n-1+\tfrac{1}{2}\right]\ldots\left[\tfrac{1}{2}\right]$ indicates that the recursion relation for the Gamma Function is to be used repeatedly until the factor $^1/_2$ is reached. If n = 0 or 1, the results are:

$$\int_0^\infty e^{-a^2x^2}\, dx = \frac{G(0)}{a} = \frac{\sqrt{\pi}}{2\, a} \qquad \int_0^\infty x^2\, e^{-a^2x^2}\, dx = \frac{G(2)}{a^3} = \frac{\Gamma(1+\tfrac{1}{2})}{2\, a^3} = \frac{\sqrt{\pi}}{4a^3}$$

$$\int_0^\infty e^{-x^2}\, dx = \sqrt{\pi}/2 \quad ; \quad \int_0^\infty x^{2n}\, e^{-x^2}\, dx = \left(\sqrt{\pi}/2\right)\left(n-\tfrac{1}{2}\right)\left(n-\tfrac{3}{2}\right)\ldots\left(\tfrac{1}{2}\right)$$

Recommendation: Each of the sample applications has lead to an integral specialized to certain application. The recommended method to attack exponential integrals is to use ***change of variable*** to convert the integral of interest to one of the *bare* forms:

$$\Gamma(s+1) = \int_0^\infty u^s\, e^{-u}\, du \qquad G(n) = \int_0^\infty u^n\, e^{-u^2}\, du = (\tfrac{1}{2})\,\Gamma(\tfrac{n+1}{2})$$

In the process, all the dimensioned constants will be factored out of the integral leaving the integral itself dimensionless. Always do follow this approach. Do not use pre-digested integrals like: $\int_0^\infty r^n\, e^{-\alpha r}\, e^{-\beta r}\, dr = \frac{n!}{[\alpha+\beta]^{n+1}}$.

Gaussian integral change of variable example:

The goal is to transform the integral into standard Gaussian $G(n)$ forms.

The nut to crack: $\int_{-\infty}^{\infty} x^2\, e^{-\lambda[x-a]^2}\, dx$. Clearly, $u = \lambda^{1/2}\,[x - a]$. $x = \lambda^{-1/2}\, u + a$; $dx = \lambda^{-1/2}\, du$

$$\int_{-\infty}^{\infty} x^2 e^{-\lambda[x-a]^2}\, dx = \lambda^{-½}\int_{-\infty}^{\infty}[\lambda^{-½}u+a]^2 e^{-u^2}\, du = \lambda^{-½}\int_{-\infty}^{\infty}[\lambda^{-1}u^2+2\lambda^{-½}ua+a^2]e^{-u^2}\, du$$

$$= \lambda^{-½}\int_{-\infty}^{\infty}[\lambda^{-1}u^2]e^{-u^2}\, du + \lambda^{-½}\int_{-\infty}^{\infty}[2\lambda^{-½}au]e^{-u^2}\, du + \lambda^{-½}\int_{-\infty}^{\infty}[a^2]e^{-u^2}\, du$$

$$= \lambda^{-3/2}\, 2G(2) + 0 + \lambda^{-1/2}a^2\, 2G(0) = \lambda^{-3/2}\,\Gamma(3/2) + 0 + \lambda^{-1/2}a^2\,\Gamma(1/2)$$

$$= \left[½\Gamma(1/2)\,\lambda^{-3/2} + 0 + \lambda^{-1/2}a^2\,\Gamma(1/2)\right] = \left[½\lambda^{-3/2} + 0 + \lambda^{-1/2}a^2\right]\Gamma(1/2)$$

$$\int_{-\infty}^{\infty} x^2 e^{-\lambda[x-a]^2}\, dx = \left[½\lambda^{-3/2} + 0 + \lambda^{-1/2}a^2\right]\sqrt{\pi}$$

Exercise: Why does $\int_{-\infty}^{\infty} u\, e^{-u^2}\, du$ vanish? How is the relation $\Gamma(n+1) = n\,\Gamma(n)$ used?

Gaussian Integrals and Completing the Square:

Consider the integral: $\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = \int_{-\infty}^{\infty} e^{-\left(ax-b/2a\right)^2} e^{-b^2/4a^2} dx$. The exponent has been rewritten by completing the square. Define: $u = a\,x - {}^{b}/_{2a}$. After changing variables,

$$\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = \int_{-\infty}^{\infty} e^{-u^2}\, e^{-b^2/4a^2}\, a^{-1} du = 2\, e^{-b^2/4a^2}\, a^{-1}\int_0^{\infty} e^{-u^2}\, du\,.$$

$$\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = 2\, e^{-b^2/4a^2}\, a^{-1}\int_0^{\infty} e^{-u^2}\, du = {}^{\sqrt{\pi}}/_{a}\; e^{-b^2/4a^2}$$

This technique is used for a quantum mechanics problem about the time development of wave packets.

Tools of the Trade

PARAMETER CALCULUS & REGULARIZING FUNCTIONS

THE GAMMA FUNCTION RECURSION RELATION

THE GAMMA FUNCTION AND FACTORIAL

THE INTEGRAL OF THE SINC FUNCTION

THE INTEGRAL OF SINC-SQUARED

MIXING METHODS $\int_0^{\infty} \frac{x^3\, dx}{e^x - 1} = \frac{\pi^4}{90}$

The integral of an even function over an even range is twice the integral over the positive half. The integral of an odd function over an even range is zero.

$$\int_{-\infty}^{\infty} x^n\, e^{-x^2}\, dx = \int_{-\infty}^{0} x^n\, e^{-x^2}\, dx + \int_{0}^{\infty} x^n\, e^{-x^2}\, dx \quad \text{Use } u = -x$$

$$\int_{-\infty}^{\infty} x^n\, e^{-x^2}\, dx = \int_{\infty}^{0} (-1)^n\, u^n\, e^{-x^2}\, du + \int_{0}^{\infty} x^n\, e^{-x^2}\, dx = \left[1 + (-1)^{n)}\right] \int_{0}^{\infty} x^n\, e^{-x^2}\, dx$$

$$\int_{-L}^{L} [\, f_{odd}(x) + f_{even}(x)]\, dx = \int_{-L}^{0} [\, f_{odd}(x) + f_{even}(x)]\, dx + \int_{0}^{L} [\, f_{odd}(x) + f_{even}(x)]\, dx$$

$$\int_{-L}^{L} [\, f_{odd}(x) + f_{even}(x)]\, dx = \int_{L}^{0} [\, f_{odd}(-u) + f_{even}(-u)](-du) + \int_{0}^{L} [\, f_{odd}(x) + f_{even}(x)]\, dx$$

$$= \int_{0}^{L} [\big(\, f_{odd}(x) + f_{odd}(-x)\big) + \big(\, f_{even}(x) + f_{even}(-x)\big)]\, dx = 2\int_{0}^{L} [\, f_{even}(x)]\, dx$$

THE GAMMA FUNCTION RECURSION RELATION

An alternative approach to developing the recursion relation for the Gamma function $\Gamma(n)$ is to insert a parameter into the defining integral and then to differentiate (and sometimes integrate) with respect to it.

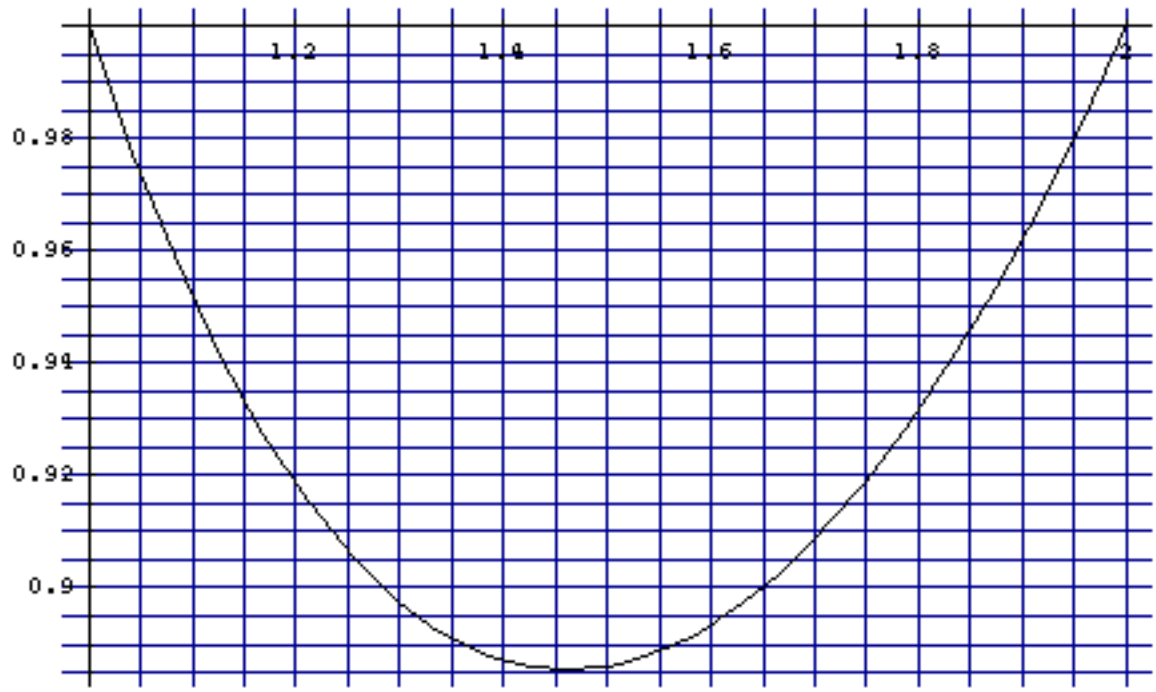
$$\Gamma(s,a) = \int_{0}^{\infty} x^{s-1}\, e^{-ax}\, dx = \frac{1}{a^s} \int_{0}^{\infty} u^{s-1}\, e^{-u}\, du = \frac{1}{a^s}\, \Gamma(s)$$

Compute the negative of the derivative with respect to the parameter a.

$$-\frac{d}{da}\big(\Gamma(s,a)\big) = -\frac{d}{da}\left(\int_{0}^{\infty} x^{s-1}\, e^{-ax}\, dx\right) = \int_{0}^{\infty} x^{s}\, e^{-ax}\, dx = \frac{1}{a^{s+1}}\, \Gamma(s+1)$$

$$-\frac{d}{da}\left[\frac{1}{a^s} \int_{0}^{\infty} u^{s-1}\, e^{-u}\, du\right] = -\frac{d}{da}\left(\frac{1}{a^s}\, \Gamma(s)\right) = \frac{s}{a^{s+1}} \Gamma(s)$$

Comparing for $a = 1$, the recursion relation follows: $\Gamma(s+1) = s\, \Gamma(s)$. The evaluation is anchored by noting that $\Gamma(1) = 1$. Hence $\Gamma(n+1) = n!$ for n an integer. The recursion relation was derived without assuming that s was an integer so it can be used to make unit steps between non-integer values. The process is anchored by picking values of $\Gamma(s)$ for $1 \le s \le 2$ from a plot, from the table or by numerically evaluating the integral.

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Plot[Gamma[s],{s,1,2}, GridLines ->
{Table[.95+i*.05,{i,21}],Table[.88+j*.005,{j,25}]}]
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Tabulated Values for Γ(*x*)

$\Gamma(1.0) = 1.0000$	$\Gamma(1.1) = .9514$	$\Gamma(1.2) = .9182$	$\Gamma(1.3) = .8975$	$\Gamma(1.4) = .8873$
$\Gamma(1.5) = \sqrt{\pi}/2$	$\Gamma(1.6) = .8935$	$\Gamma(1.7) = .9086$	$\Gamma(1.8) = .9314$	$\Gamma(1.9) = .9618$

Relation of Γ(z) for positive and negative arguments: $\Gamma(-z) = \dfrac{-\pi}{z\,\Gamma(z)\sin(\pi z)}$

Note that $\Gamma(z)$ is undefined for non-positive integer arguments. These points are designated as poles of the Gamma.

THE GAMMA FUNCTION AND FACTORIAL

If $\Gamma(s,a) = \int_0^\infty x^{s-1}\, e^{-ax}\, dx = \frac{1}{a^s}\int_0^\infty u^{s-1}\, e^{-u}\, du = \frac{1}{a^s}\,\Gamma(s)$ then $\Gamma(1,a) = \int_0^\infty e^{-ax}\, dx = \frac{1}{a}$. Taking a few derivatives $\Gamma(n+1,a) = \int_0^\infty x^s\, e^{-ax}\, dx = \frac{d^n}{da^n}\big(\Gamma(1,a)\big) = \frac{d^n}{da^n}\left(\frac{1}{a}\right) = \frac{n!}{a^{n+1}}$. Note that *n* is now

restricted to integer values as it counts the times that the derivative operation has been applied. Setting a = 1 and with n restricted to positive integers, it follows that $\Gamma(n+1) = n!$. The value is $\Gamma(1) = 1$ is used to extend the definition of factorial by setting $\Gamma(1) = 0! = 1$.

$$\Gamma(s+1) = s\,\Gamma(s)\ \forall\, s$$
$$\Gamma(n+1) = n!\ \forall\, n \in \text{integers}$$

(*Note the recursion relation was developed without restriction and that s can be non-integer.*)

Large Argument Limits: Stirling's Formula: $x! \approx x^x e^{-x}\sqrt{2\pi x}\,(1+1/12x)$

$$\ln(n!) \approx n\ln(n) - n$$

$$\Gamma(z) \approx \sqrt{\frac{2\pi}{z}}\left(\frac{z}{e}\sqrt{z\sinh\left(1/z\right)+\frac{1}{810\,z^6}}\right)^z$$

REGULARIZATION AND THE INTEGRAL OF THE SINC FUNCTION

The rather simple definite integral $\int_0^\infty \cos(kx)\,dx$ is undefined.

$$\int_0^\infty \cos(kx)\,dx = \left.\frac{\sin(kx)}{k}\right|_{x=\infty}$$

One can attempt to regulate the integral by inserting a factor that slowly decays to render a convergent integral.

$$\int_0^\infty \cos(kx)\,e^{-ax}\,dx = \left(1/2\right)\int_0^\infty\left[e^{ikx-ax}+e^{-ikx-ax}\right]dx = \frac{a}{k^2+a^2}$$

The result for $\int_0^\infty \cos(kx)\,dx$ should be the limit of the expression above as a approaches zero if it is to make any sense at all. The limit yields $\int_0^\infty \cos(kx)\,dx = 0$. This result may seem reasonable, but the correct answer remains: the integral fails to converge, and the value is *undefined*. Nonetheless, the integral above provides the basis for evaluating two integrals of interest using *regularization* and *integration with respect to a parameter*.

Consider $\int_0^\infty \frac{\sin(kx)}{x}\,dx$. A trick using integration with respect to a parameter follows by noting that $\int_0^1 \cos(kx)\,dk = \frac{\sin(kx)}{x}$ and that

$$\int_0^1\left[\int_0^\infty \cos(kx)\,e^{-ax}\,dx\right]dk = \int_0^\infty \frac{\sin(kx)}{x}\,e^{-ax}\,dx = \int_0^1\left[\frac{a}{k^2+a^2}\right]dk$$

The last integral is actually rather familiar. Setting $u = k/a$,

$$\int_0^\infty \frac{\sin(kx)}{x}\,e^{-ax}\,dx = \int_0^1\left[\frac{a}{k^2+a^2}\right]dk = \int_0^{1/a}\left[\frac{1}{1+u^2}\right]du = \tan^{-1}(1/a)$$

Now, the limit a approaches zero is well-defined.

$$\int_0^\infty \frac{\sin(kx)}{x}\,dx = \underset{a\to 0^+}{Limit}\left[\tan^{-1}(1/a)\right] = \tan^{-1}(\infty) = \pi/2$$

The trick is to generate the inverse power of x by integrating with respect to a parameter. Can this method be extended?

THE INTEGRAL OF SINC-SQUARED

Consider $\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 dx$. One guesses that integration twice with respect to k is in order. To find the starting point try differentiated $[\sin(kx)]^2$ twice with respect to k.

$$\frac{d}{dk}\left(\left[\sin(kx)\right]^2\right) = 2\,k\sin(kx)\cos(kx) = k\sin(2kx)$$

$$\frac{d^2}{dk^2}\left(\left[\sin(kx)\right]^2\right) = \frac{d}{dk}\left(k\sin(2kx)\right) = 2\,k^2\cos(2kx)$$

In order to reverse the process, nested parameter integrations are needed.

$$\int_0^1\left[\int_0^k \cos(2k'x)\,dk'\right]dk = \int_0^1\left[\frac{\sin(2kx)}{2x}\right]dk = \left.\frac{-\cos(2kx)}{4x^2}\right|_0^1 = \frac{1-\cos(2x)}{4x^2} = \frac{\sin^2(x)}{2x^2}$$

Note that this value is one-half the desired integrand, and pay attention to the nesting and use of dummy integration variables.

Starting point:

$$2\int_0^\infty \cos(2kx)\,e^{-ax}\,dx = \int_0^\infty \left[e^{i2kx-ax} + e^{-i2kx-ax}\right]dx = \left[\frac{1}{a-2ik} + \frac{1}{a+2ik}\right] = 2\left[\frac{a}{4k^2+a^2}\right]$$

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 e^{-ax}\,dx = 2\int_0^\infty \left[\int_0^1 \left[\int_0^k \cos(2k'x)\,e^{-ax}\,dk'\right]dk\right]^2 e^{-ax}\,dx = 2\int_0^1 \left[\int_0^k \frac{a}{a^2+(4k')^2}\,dk'\right]dk$$

This first integration is just another inverse tangent. Use $u = 2k'/a$.

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 e^{-ax}\,dx = \int_0^1 \left[\int_0^{2k/a} \frac{1}{1+(u)^2}\,du\right]dk = \int_0^1 \left[\tan^{-1}(2k/a)\right]dk = \left(a/2\right)\int_0^{2/a} \left[\tan^{-1}(u)\right]du$$

What is the integral of $\tan^{-1}(u)$? Let's work through this one. Clearly, one could begin with

$$\frac{d}{du}\left(u\tan^{-1}(u)\right) = \tan^{-1}(u) + u\frac{d}{du}\left(\tan^{-1}(u)\right) = \tan^{-1}(u) + \frac{u}{1+u^2}$$

Next, the last term must be eliminated. We get one over *something* when we take the derivative of ln(*something*).

$$\frac{d}{du}\left(\ln\left[1+u^2\right]\right) = \frac{2u}{1+u^2}$$

The path to contentment is now clear.

$$\frac{d}{du}\left(u\tan^{-1}(u) - (1/2)\,\ln[1+u^2]\right) = \tan^{-1}(u)$$

This final integration becomes:

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 e^{-ax}\,dx = \left(a/2\right)\int_0^{2/a} \left[\tan^{-1}(u)\right]du = \left(a/2\right)\left[u\tan^{-1}(u) - (1/2)\ln[1+u^2]\right]_0^{2/a}$$

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 e^{-ax}\,dx = \left(a/2\right)\int_0^{2/a} \left[\tan^{-1}(u)\right]du = (a/2)\left[(2/a)\tan^{-1}(2/a) - (1/2)\ln[1+(4/a^2)]\right]$$

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 dx = \underset{a\to 0^+}{Limit}\left[\tan^{-1}(2/a) - (a/4)\ln[1+(4/a^2)]\right] = \tan^{-1}(\infty) = \pi/2$$

$$\int_0^\infty \left[\frac{\sin(kx)}{x}\right]^2 dx = \pi/2$$

In the interest of full disclosure, the limiting form of the log term is to be examined.

$$\underset{a\to 0}{Limit}\left[\,(a)\ln[1+(4/a^2)]\right] = \underset{a\to 0}{Limit}\left[\frac{\ln[1+(4/a^2)]}{a^{-1}}\right] \underset{L'Hospital}{\rightarrow}$$

$$= \underset{a\to 0}{Limit}\left[\frac{\frac{1}{1+(4/a^2)}\left(-2/a^3\right)}{-a^{-2}}\right] = \underset{a\to 0}{Limit}\left[\frac{a}{2+a^2/2}\right] = 0$$

The techniques of regularization and parameter calculus have been demonstrated and have provided the values of some useful definite integrals. The effort required was significant, but the rewards will justify that effort. The exponential integrals are the keys to many calculations that arise in quantum mechanics. The sinc(x) integrals are used for representations of the Dirac delta function, and they appear in the treatment of time dependent perturbation theory. The theory permits one to calculate transition rates between quantum states.

Table II: Extended Integral Table

Table of Integrals including some special cases

$$\Gamma(s+1) = \int_0^\infty u^s\, e^{-u}\, du \qquad \Gamma(s+1) = s\,\Gamma(s) \qquad \Gamma(n+1) = n!$$

$$G(n) = \int_0^\infty u^n\, e^{-u^2}\, du = (1/2)\,\Gamma(\tfrac{n+1}{2}) \qquad \Gamma(1/2) = \sqrt{\pi} \qquad \Gamma(1) = 0! = 1$$

$$\int_0^\infty r^n\, e^{-\alpha r}\, e^{-\beta r}\, dr = \frac{1}{\left[\alpha+\beta\right]^{n+1}}\,\Gamma(n+1) = \frac{n!}{\left[\alpha+\beta\right]^{n+1}}$$

$$\int_0^\infty x^n\, e^{-a^2x^2}\, dx = \frac{G(n)}{a^{n+1}} = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\,a^{n+1}} = \left[\frac{n-1}{2}\right]\left(\frac{\Gamma\left(\frac{n-1}{2}\right)}{2\,a^{n+1}}\right) = \ldots$$

$$\int_0^\infty x^{2n}\, e^{-a^2x^2}\, dx = \frac{G(2n)}{a^{2n+1}} = \frac{\Gamma(n+1/2)}{2\,a^{2n+1}}$$

$$\int_0^\infty x^{2n+1}\, e^{-a^2x^2}\, dx = \frac{G(2n+1)}{a^{2n+2}} = \frac{\Gamma(n+1)}{2\,a^{2n+2}} = \frac{n!}{2\,a^{2n+2}}$$

$$\int_0^{\pi/2}\left[\cos\theta\right]^{2\mu-1}\left[\sin\theta\right]^{2\nu-1} d\theta = \frac{\Gamma(\mu)\,\Gamma(\nu)}{2\,\Gamma(\mu+\nu)} \quad \ldots\ \mu,\ \nu > 0$$

$$\int_{-\infty}^{\infty} \frac{\sin(x)}{x}\, dx = \pi \qquad\qquad \int_{-\infty}^{\infty} \left[\frac{\sin(x)}{x}\right]^2 dx = \pi$$

$$\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = \int_{-\infty}^{\infty} e^{-\left(ax-b/2a\right)^2} e^{-b^2/4a^2}\, dx = \sqrt{\pi}/a \;\; e^{-b^2/4a^2}$$

$$\int_0^{\pi/2} \left[\cos\theta\right]^k\, d\theta = \int_0^{\pi/2} \left[\sin\theta\right]^k\, d\theta = \frac{\Gamma(\frac{k+1}{2})\Gamma(\frac{1}{2})}{2\,\Gamma(\frac{k}{2}+1)} = \frac{\sqrt{\pi}\;\Gamma(\frac{k+1}{2})}{k\,\Gamma(\frac{k}{2})} \quad for\;\; k > -1$$

$$\int_0^1 x^{n-1}(1-x)^{m-1}\, dx = \int_0^{\pi/2} \left[\cos\theta\right]^{2m-1} \left[\cos\theta\right]^{2n-1} d\theta = \frac{\Gamma(m)\Gamma(n)}{2\,\Gamma(m+n)} \quad \ldots\; m,n > 0$$

$$\int_0^t e^{rt'}\, \sin(bt')\, dt' = \frac{e^{rt}\left\{r\sin(bt) - b\cos(bt)\right\} + b}{r^2+b^2}$$

$$\int_0^t e^{rt'}\, \cos(bt')\, dt' = \frac{e^{rt}\left\{r\cos(bt) + b\sin(bt)\right\} - r}{r^2+b^2}$$

Riemann Zeta Function

$$\zeta(s) = \sum_{k=1}^{\infty} k^{-s} = \frac{1}{\Gamma(s)} \int_0^{\infty} \left(\sum_{k=1}^{\infty} e^{-ks}\right) x^{s-1}\, dx = \frac{1}{\Gamma(s)} \int_0^{\infty} \left(\frac{e^{-x}}{1-e^{-x}}\right) x^{s-1}\, dx$$

Error Function and Complementary Error Function

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2}\, du = 1 - erfc(x)$$

$$\int_0^{\pi} \frac{d\theta}{a + b\cos\theta} = \frac{\pi}{\sqrt{a^2-b^2}} \quad \text{for } (a > b \geq 0)$$

$$\int_0^{\pi/2} \frac{d\theta}{a^2\sin^2\theta + b^2\cos^2\theta} = \frac{\pi}{|ab|}$$

Complete Elliptic Integral of the First Kind (*small k*)

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = \frac{\pi}{2}\left[1 + \left(\frac{1}{2}\right)^2 k^2 + \left(\frac{1*3}{2*4}\right)^2 k^4 + \ldots\right]$$

Complete Elliptic Integral of the Second Kind (*small k*)

$$E(k) = \int_0^{\pi/2} \sqrt{1-k^2\sin^2\theta}\;\; d\theta = \frac{\pi}{2}\left[1 - \frac{1}{4}k^2 - \frac{3}{64}k^4 + \ldots\right]$$

Mixing Methods: Consider the integral $\int_0^{\infty} \frac{x^3\, dx}{e^x - 1} = \frac{\pi^4}{90}$

Rewriting: $\int_0^\infty \frac{x^3\,dx}{e^x-1} = \int_0^\infty \frac{x^3\,e^{-x}dx}{1-e^{-x}} = \int_0^\infty x^3\,e^{-x}\,\left[1-e^{-x}\right]^{-1}\,dx$

Expanding:

$$\int_0^\infty x^3\,e^{-x}\,\left[1-e^{-x}\right]^{-1}\,dx = \int_0^\infty x^3\,e^{-x}\,\left(\sum_{n=0}^{\infty} e^{-nx}\right)\,dx$$

$$= \sum_{n=1}^{\infty}\int_0^\infty x^3\,e^{-nx}\,dx = \sum_{n=1}^{\infty}\frac{1}{n^4}\int_0^\infty u^3\,e^{-u}\,du$$

Make identifications: $\sum_{n=1}^{\infty}\frac{1}{n^4} = \zeta(4)$; $\Gamma(4) = \int_0^\infty u^3\,e^{-u}\,du = 3!$

The symbol $\zeta(4)$ is the Riemann zeta of 4. Our most basic tool for evaluating sums is to use Fourier series. Given: $f(x) = x\,(\pi - x)$ for the interval $[0, \pi]$, $x\,(\pi - x) = \frac{\pi^2}{6} - \sum_{m=1}^{\infty}\frac{\cos(2\,m\,x)}{m^2}$. Using the Parseval relation:

$$\frac{1}{\pi}\int_0^\pi \left[x(\pi-x)\right]^2\,dx = \frac{\pi^4}{36} + \left(\tfrac{1}{2}\right)\sum_{m=1}^{\infty}\frac{1}{m^4} = \frac{\pi^4}{30}$$

Solving for the factor of interest: $\zeta(4) = \sum_{m=1}^{\infty}\frac{1}{m^4} = \frac{\pi^4}{90}$ leading to $\int_0^\infty \frac{x^3\,dx}{e^x-1} = \frac{\pi^4}{90}$.

Quantum Integrals: Sample Calculations

Normalization Integrals for the Quantum Harmonic Oscillator: Checking the normalization of the second excited state of a quantum harmonics oscillator.

$$u_2(x) = \alpha^{1/2}\big/(8^{1/2}\,\pi^{1/4})\,(4\alpha^2\,x^2 - 2)\,e^{-\alpha^2 x^2/2}$$

Normalization Condition: Show that: $\int_{-\infty}^{\infty} u_n^*(x)\,u_n(x)\,dx = 1$

$$\int_{-\infty}^{\infty} u_2^*(x)\,u_2(x)\,dx = \alpha\big/(8\sqrt{\pi})\int_{-\infty}^{\infty}(4\alpha^2\,x^2-2)^2\,e^{-\alpha^2 x^2}\,dx$$

Note that x has the dimensions of *length* so α has the dimension of *inverse-length*. Choose the dimensionless variable $w = \alpha x$.

$$dw = \alpha\,dx \quad \text{or } dx = \alpha^{-1}\,d\omega$$

$$\tfrac{1}{(8\sqrt{\pi})}\int_{-\infty}^{\infty}(4w^2-2)^2\,e^{-\alpha^2 w^2}\,dw=\tfrac{1}{(\sqrt{\pi})}\int_{-\infty}^{\infty}(2w^4e^{-w^2}-2w^2e^{-w^2}+\tfrac{1}{2}e^{-w^2})dw$$

Use: $\int_{-\infty}^{\infty} w^{2m}e^{-w^2}dw=2\int_0^{\infty} w^{2m}e^{-w^2}dw=2G(2m)=\Gamma(\frac{2m+1}{2})$

$$\begin{aligned}\int_{-\infty}^{\infty}u_2^*(x)u_2(x)\,dx&=\tfrac{1}{(\sqrt{\pi})}\int_{-\infty}^{\infty}(2w^4e^{-w^2}-2w^2e^{-w^2}+\tfrac{1}{2}e^{-w^2})dw\\&=\tfrac{1}{(\sqrt{\pi})}\left[2\Gamma(\tfrac{5}{2})-2\Gamma(\tfrac{3}{2})+\tfrac{1}{2}\Gamma(\tfrac{1}{2})\right]\\&=\tfrac{1}{(\sqrt{\pi})}\left[2(\tfrac{3}{2})(\tfrac{1}{2})\Gamma(\tfrac{1}{2})-2(\tfrac{1}{2})\Gamma(\tfrac{1}{2})+\tfrac{1}{2}\Gamma(\tfrac{1}{2})\right]=\frac{\Gamma(\tfrac{1}{2})}{\sqrt{\pi}}\equiv 1\end{aligned}$$

Used: $\Gamma(x+1)=x\,\Gamma(x)$ and $\Gamma(\tfrac{1}{2})=\sqrt{\pi}$ so: $\Gamma(^3/_2)=\Gamma(1+\tfrac{1}{2})=\tfrac{1}{2}\Gamma(\tfrac{1}{2})=\tfrac{1}{2}\sqrt{\pi}$

Find the expectation value of x^2 in the first excited state of a quantum harmonics oscillator. $u_1(x)=\alpha^{1/2}/(2^{1/2}\pi^{1/4})\,(2\alpha x)e^{-\alpha^2x^2/2}$

$$\begin{aligned}\langle 1|x^2|1\rangle&=\int_{-\infty}^{\infty}u_1^*(x)(x^2)u_1(x)\,dx\\&=\alpha/(2\sqrt{\pi})\int_{-\infty}^{\infty}(2\alpha x)e^{-\alpha^2x^2/2}\,x^2\,(2\alpha x)e^{-\alpha^2x^2/2}dx\end{aligned}$$

This integral can be completed using the same methods that crushed the normalization integral above. Just to add spice, it is assumed that the wavefunction has not been properly normalized or $u_1(x)=Axe^{-\alpha^2x^2/2}$. In this case, one must divide by the normalization integral.

$$\langle 1|x^2|1\rangle=\frac{\int_{-\infty}^{\infty}u_1^*(x)(x^2)u_1(x)\,dx}{\int_{-\infty}^{\infty}u_1^*(x)\,u_1(x)\,dx}=\frac{|A|^2\int_{-\infty}^{\infty}x^4\,e^{-\alpha^2x^2}\,dx}{|A|^2\int_{-\infty}^{\infty}x^2\,e^{-\alpha^2x^2}\,dx}$$

Choose the dimensionless variable $w=\alpha x$ to reach the form for $G(n)$.

$$dw=\alpha\,dx\quad\text{or } dx=\alpha^{-1}\,d\omega$$

$$\langle 1|x^2|1\rangle=\frac{\alpha^{-5}\int_{-\infty}^{\infty}x^4\,e^{-\alpha^2x^2}\,dx}{\alpha^{-3}\int_{-\infty}^{\infty}x^2\,e^{-\alpha^2x^2}\,dx}=\alpha^{-2}\frac{\int_{-\infty}^{\infty}w^4\,e^{-w^2}\,dw}{\int_{-\infty}^{\infty}w^2\,e^{-w^2}\,dw}$$

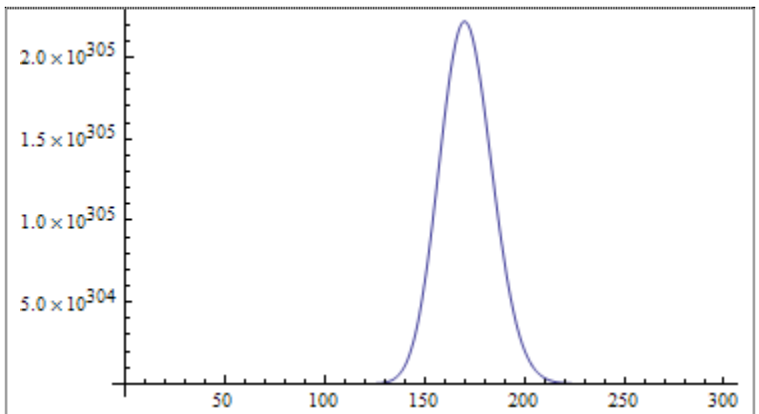
$$\langle 1|x^2|1\rangle=\alpha^{-2}\frac{2G(4)}{2G(2)}=\alpha^{-2}\frac{\Gamma(\frac{4+1}{2})}{\Gamma(\frac{2+1}{2})}=\alpha^{-2}\frac{\frac{3}{2}\Gamma(\frac{3}{2})}{\Gamma(\frac{3}{2})}=\frac{3}{2}\alpha^{-2}$$

It is almost easier to compute the answer without normalizing the wavefunction than it is to do it using the normalized form. The constant α has dimensions of *inverse-length* so the answer has the dimensions of $(\textit{length})^2$ as expected.

Appendix:

The Stirling Approximation:

Integration by parts identifies $\int_0^\infty t^n e^{-t}\, dt$ as $n!$. We will study $\int_0^\infty t^z e^{-t}\, dt$ just to emphasize that z is treated as a continuous variable. The plot shows that the integrand is very large in a small region with the peak value occurring for $t = z$. The integral is re-written as:



n =170; Plot[t^n Exp[-t],{t,0,300}, PlotRange → All]

$$z! = \int_0^\infty e^{-(t - z\ln(t))}\, dt = \int_0^\infty e^{-f(t)}\, dt$$

The function $f(t)$ has its maximum at $t = z$ and can be expanded in a Taylor's series about that value.

$$f(t) = z - z\ln(z) + {}^1/_{2z}\,(t-z)^2 - {}^1/_{3z^2}\,(t-z)^3 + {}^1/_{4z^3}\,(t-z)^4 - \ldots$$

Proceeding in small steps, a new variable is defined, $\tau = z^{-½}\,(t - z)$.

$$f(t) \to g(\tau) = z - z\ln(z) + {}^1/_2\,\tau^2 - {}^1/_3\,z^{-½}\,\tau^3 + {}^1/_4\,z^{-1}\,\tau^4 - \ldots$$

With this change of variable, the limits are $-z$ to $+\infty$, and $dt \to z^{½}\, d\tau$.

$$z! \approx \int_{-z}^\infty e^{-g(\tau)}\, z^{½} d\tau = \int_{-z}^\infty e^{-\{z - z\ln(z) + ½\tau^2 - \ldots\}}\, z^{½} d\tau = z^{z+½}\, e^{-z} \int_{-z}^\infty e^{-\{+½\tau^2 - \ldots\}}\, d\tau$$

As the integrand is sharply peaked about $\tau = 0$, the lower limit can be set to $-\infty$ without harm. A *final* change of variable $u = 2^{-½}\,\tau$ is made so $d\tau = 2^{½}\, du$.

$$z! \approx z^{z+½}\, e^{-z} \sqrt{2} \int_{-\infty}^\infty e^{-u^2}\, \{ e^{⅓ z^{-½} (\sqrt{2}u)^3}\, e^{-¼ z^{-1} (\sqrt{2}u)^4} \}\, du$$

The large z limit is desired. In this limit the small argument expansions of the exponential factors in braces can be used. Expanding to consistently to order z^{-1},

$$z! \approx z^{z+½}\, e^{-z} \sqrt{2} \int_{-\infty}^{\infty} e^{-u^2} [1 + ⅓\, z^{-½} (\sqrt{2}u)^3 + ⅛\, z^{-1} (\sqrt{2}u)^6][1 - ¼\, z^{-1} (\sqrt{2}u)^4]\, du$$

$$z! \approx z^{z+½}\, e^{-z} \int_{-\infty}^{\infty} e^{-u^2} [\sqrt{2} + z^{-½}\, \{⅔\, u^3\} + \sqrt{2}\; z^{-1} \{⅔\, u^6 - u^4]\, du$$

We use our standard exponential integral relations:

$$\Gamma(s+1) = \int_0^{\infty} u^s\, e^{-u}\, du \qquad \Gamma(s+1) = s\,\Gamma(s) \qquad \Gamma(n+1) = n! \qquad \Gamma(½) = \sqrt{\pi}$$

$$G(n) = \int_0^{\infty} u^n\, e^{-u^2}\, du = (½)\,\Gamma(\tfrac{n+1}{2}) \qquad \int_{-\infty}^{\infty} u^n\, e^{-u^2}\, du = \begin{cases} \Gamma(\tfrac{n+1}{2}) & \text{for } n \text{ even} \\ 0 & \text{for } n \text{ odd} \end{cases}$$

$$z! \approx z^{z+½}\, e^{-z} \left(\sqrt{2}\; \Gamma(½) + \sqrt{2} z^{-1} \{⅔\, \Gamma(⅞) - \Gamma(⅝) \right)$$

$$= z^{z+½}\, e^{-z}\; \sqrt{2}\; \Gamma(½) \left(1 + z^{-1} \{⅔\, ⅝\, ⅜\, ½ - ⅜\, ½ \right)$$

$$z! \approx z^{z+½}\, e^{-z}\; \sqrt{2\pi}\; \left(1 + ⅟_{12z} \right)$$

$$\boxed{z! \approx z^{z}\, e^{-z}\; \sqrt{2\pi z}\; \left(1 + ⅟_{12z} \right)} \qquad \text{(for large } z\text{)}$$

Problems

1.) Compute the values of Γ(2.5), Γ(0.5), Γ(5) and Γ(3.8). Use the tabulated values as necessary.

2.) The spatial parts of the hydrogen atom wave functions have the form:

$$u_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\; Y_{\ell m}(\theta,\phi)$$

The full time-dependent eigenfunction is $\Psi(\vec{r},t) = u_{n\ell m}(r,\theta,\phi)\, e^{-i\omega_n t}$. The $Y_{\ell m}(\theta,\phi)$ are the spherical harmonics, the QM eigenfunctions of angular momentum. They satisfy the orthogonality relation:

$$\int_0^{\pi}\int_0^{2\pi}\left[Y_{\ell' m'}(\theta,\phi)\right]^* Y_{\ell m}(\theta,\phi)\sin\theta\, d\theta\, d\phi = \delta_{\ell\ell'}\ \delta_{mm'}$$

$$\delta_{mn} = \begin{cases} 1 & if \quad m = n \\ 0 & if \quad m \neq n \end{cases}$$ ***The Kronecker Delta Notation***

Compute the expectation value of the potential energy for the hydrogen atom 1s ground state u_{100} and for the $2p_0$ state u_{210}. What to values or concepts are represented by the symbol e in this problem? What does a_0 represent?

The expectation value of V: $\langle V(r)\rangle_{nlm} = \int_{all\ space} u^*_{nlm}(\vec{r})\, V(r)\, u_{nlm}(\vec{r})\ dV$

$$V(r) = \frac{-e^2}{4\pi\,\varepsilon_0\, r}\ ;\ u_{100}(r,\theta,\phi) = \frac{1}{\pi^{1/2}\ a_0^{3/2}}\ e^{-r/a_0} = \frac{2}{a_0^{3/2}}\ e^{-r/a_0}\ \frac{1}{\sqrt{4\pi}} = \frac{2}{a_0^{3/2}}\ e^{-r/a_0}\ Y_{00}(\theta,\phi)$$

$$u_{210}(r,\theta,\phi) = \frac{1}{(32\pi)^{1/2}\ a_0^{3/2}}\left(\frac{r}{a_0}\right) e^{-r/2a_0}\cos\theta = \frac{1}{(24)^{1/2}\ a_0^{3/2}}\left(\frac{r}{a_0}\right) e^{-r/2a_0}\ Y_{10}(\theta,\phi)$$

Note that $\dfrac{e^2}{4\pi\,\varepsilon_0\, a_0} = 27.2\ electron\ volts$. V_{100} = -27.2 eV and V_{210} = - 6.8 eV

3.) Compute: $\int_{-\infty}^{\infty}\left[\pi^{\pi}\ x + \left(2/81\right)x^2 + \left(4/729\right)x^4\right] e^{-x^2/9}\, dx$

4.) The lowest three states for a quantum harmonic oscillator have the spatial wavefunctions: $u_0(x) = \alpha^{1/2}/\pi^{1/4}\ e^{-\alpha^2 x^2/2}$; $u_1(x) = \alpha^{1/2}/(2^{1/2}\pi^{1/4})\ (2\alpha\, x)\, e^{-\alpha^2 x^2/2}$ and $u_2(x) = \alpha^{1/2}/(8^{1/2}\pi^{1/4})\ (4\alpha^2 x^2 - 2)\, e^{-\alpha^2 x^2/2}$. Show that these wavefunctions are normalized. Show that u_0 and u_2 are orthogonal.

Normalized: $\int_{-\infty}^{\infty} u_n^*(x)\, u_n(x)\, dx = 1$

Orthogonal: $\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = 0$ for $m \neq n$

The operator for a coordinate q is just that coordinate q. The operator for the momentum conjugate to the coordinate is: $\hat{p}_q = -i\hbar\, \partial/\partial q$. $\langle S\rangle$ represents the expectation

value of S computed as $\langle S\rangle_n = \int u_n^*(x)\ \hat{S}(x, -i\hbar\,\partial/\partial x)\, u_n(x)\ dx = \langle n|S|n\rangle$

5.) Compute $<x>$, $<p>$, $<x^2>$, $<p^2>$, $<\Delta x>$, $<\Delta p>$and $<(\Delta x)^2>$ $<(\Delta p)^2>$ for each state in problem 5. Show that: $<(\Delta x)^2> = <x^2> - <x>^2$ given $\Delta x = x - <x>$.

6.) Calculate $\langle u_2|\hat{x}|u_0\rangle$ and $\langle u_2|\hat{p}|u_0\rangle$ using the harmonic oscillator states in problem 4.

7.) Calculate $\langle\psi\ |\hat{x}|\psi\ \rangle$ and $\langle\psi|\hat{p}|\psi\rangle$ for the states $\psi_A(x,t) = \frac{1}{\sqrt{2}}\left[\psi_0(x,t) + \psi_1(x,t)\right]$ and $\psi_B(x,t) = \frac{1}{\sqrt{2}}\left[\psi_0(x,t) + i\ \psi_1(x,t)\right]$ based on the time dependent harmonic oscillator states $\psi_n(x,t) \quad = u_n(x)e^{-i[n+\frac{1}{2}]\omega_0 t}$. At what frequency do these *matrix elements* oscillate?

8.) Calculate $\langle\psi\ |\hat{x}|\psi\ \rangle$ and $\langle\psi|\hat{p}|\psi\rangle$ for the states $\psi_C(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x,t) + \psi_2(x,t)\right]$ and $\psi_D(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x,t) + i\ \psi_2(x,t)\right]$ based on the time dependent harmonic oscillator states $\psi_n(x,t) \quad = u_n(x)e^{-i[n+\frac{1}{2}]\omega_0 t}$. At what frequency do these *matrix elements* oscillate? Compare the results of this problem to those of the previous problem.

9.) The spatial parts of the hydrogen atom wave functions have the form:

$$u_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\ Y_{\ell m}(\theta,\phi)$$

The $Y_{\ell m}(\theta,\phi)$ are the spherical harmonics, the QM eigenfunctions of angular momentum. They satisfy the orthogonality relation:

$$\int_0^{\pi}\ \int_0^{2\pi}\left[Y_{\ell' m'}(\theta,\phi)\right]^*\ Y_{\ell m}(\theta,\phi)\sin\theta\, d\theta\, d\phi = \delta_{\ell\ell'}\ \delta_{mm'}$$

Compute the expectation value of r for the hydrogen atom ground state u_{100} and for the $2p_0$ state u_{210}.

$$u_{100}(r,\theta,\phi) = \frac{1}{\pi^{1/2}\ a_0^{3/2}}\ e^{-r/a_0} = \frac{2}{a_0^{3/2}}\ e^{-r/a_0}\ \frac{1}{\sqrt{4\pi}} = \frac{2}{a_0^{3/2}}\ e^{-r/a_0}\ Y_{00}(\theta,\phi)$$

$$u_{210}(r,\theta,\phi) = \frac{1}{(32\pi)^{1/2}\ a_0^{3/2}}\left(\frac{r}{a_0}\right) e^{-r/2a_0}\cos\theta = \frac{1}{(24)^{1/2}\ a_0^{3/2}}\left(\frac{r}{a_0}\right) e^{-r/2a_0}\ Y_{10}(\theta,\phi)$$

10.) It happens that the functions below are a Fourier transform pair.

$$U_a(t) = \begin{cases} 0 & for\ t<0 \\ e^{-at} & for\ t>0 \end{cases} \qquad \tilde{U}_a(\omega) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{a+i\omega}\right) = \frac{1}{\sqrt{2\pi}}\left(\frac{a-i\omega}{a^2+\omega^2}\right)$$

Show that: $\frac{1}{a-i\omega} = \frac{a+i\omega}{a^2+\omega^2}$. Take the inverse Fourier transform to show that:

$$U_a(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{a\ \cos(\omega t)}{a^2+\omega^2}d\omega + \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\omega\ \sin(\omega t)}{a^2+\omega^2}d\omega$$

Setting $z = \omega/a$ and using symmetry to reset the limits.

$$U_a(t) = \frac{1}{\pi}\int_0^{\infty}\frac{\cos(a\,z\,t)}{1^2+z^2}dz + \frac{1}{\pi}\int_0^{\infty}\frac{\omega\ \sin(\omega t)}{a^2+\omega^2}d\omega$$

Taking the limit that a vanishes:

$$U_{a=0}(t) = \frac{1}{\pi}\int_0^{\infty}\frac{1}{1^2+z^2}dz + \frac{1}{\pi}\int_0^{\infty}\frac{\sin(\omega t)}{\omega}d\omega = \frac{1}{2} + \frac{1}{\pi}\int_0^{\infty}\frac{\sin(\omega t)}{\omega}d\omega$$

Use $U_{a=0}(1) = \frac{1}{2} + \frac{1}{\pi}\int_0^{\infty}\frac{\sin(x)}{x}dx$ to evaluate $\int_0^{\infty}\frac{\sin(x)}{x}dx$.

11.) The technique used to compute $G(0)$ can be generalized to show that:

$$\int_0^{\pi/2}[\cos\theta]^{2\mu-1}\ [\sin\theta]^{2\nu-1}\ d\theta = \frac{\Gamma(\mu)\Gamma(\nu)}{2\ \Gamma(\mu+\nu)} \quad \ldots\ \mu,\ \nu > 0$$

Show that $\Gamma(m) = \int_0^{\infty} 2\,x^{2m-1}\,e^{-x^2}dx$. Study the product: $\int_0^{\infty} 2\,x^{2m-1}\,e^{-x^2}dx\ \int_0^{\infty} 2\,y^{2n-1}\,e^{-y^2}dy$.

Convert the product to a double integral in polar coordinates.

12.) Use the result above to evaluate: $\int_0^{\pi/2}[\cos\theta]^k\ d\theta$ and $\int_0^{\pi/2}[\sin\theta]^k\ d\theta$.

Show that $\int_0^{\pi/2}[\cos\theta]^2\ d\theta = ½\int_0^{\pi/2}[1+\cos 2\theta]\ d\theta = \pi/4$. Using

$\int_0^{\pi/2}[\cos\theta]^{2m-1}\ [\sin\theta]^{2n-1}\ d\theta = \dfrac{\Gamma(m)\,\Gamma(n)}{2\ \Gamma(m+n)}$, $\int_0^{\pi/2}[\cos\theta]^2\ d\theta = \dfrac{\Gamma(3/2)\,\Gamma(1/2)}{2\ \Gamma(2)} = \dfrac{½\,\Gamma(½)\,\Gamma(½)}{2\ (1!)} = \dfrac{\pi}{4}$.

Conclude that it just works as long as $m,n > 0$.

13.) Evaluate the integral $\int_0^t e^{rt'}\ \sin(bt')\,dt'$ by expressing the sin in terms of complex exponentials. *Answer*: $\int_0^t e^{rt'}\ \sin(bt')\,dt' = \dfrac{e^{rt}\left\{r\sin(bt) - b\cos(bt)\right\} + b}{r^2+b^2}$

14.) Evaluate the integral $\int_0^t e^{rt'}\ \sin(bt')\,dt'$ by integrating by parts twice. Set the trig function to *du* each time. Solve the final relation to find $\int_0^t e^{rt'}\ \sin(bt')\,dt'$.

15.) Show that $\int_0^{\pi} e^{2x}\ \sin(4x)\,dx = -\dfrac{e^{2\pi}-1}{5} = -\frac{2}{5}\ e^{\pi}\ \sinh(\pi) \approx -106.9$.

16.) Use $\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\,dx = \int_{-\infty}^{\infty} e^{-\left(ax-b/2a\right)^2}\ e^{-b^2/4a^2}dx = \sqrt{\pi}/a\ \ e^{-b^2/4a^2}$ to solve the wave packet problem.

a.) The wavefunction $\psi(x) = N\,e^{ik_0x}\ e^{-a^2(x-x_0)^2}$. Find the magnitude of the normalization constant N by requiring that: $\int_{-\infty}^{\infty}\psi^*(x)\ \psi(x)\,dx = 1$.

b.) Compute the Fourier transform: $(2\pi)^{-1}\int_{-\infty}^{\infty}\psi(x)\,e^{-ikx}\ dx = \phi(k)$.

Recall that different powers of 2π appear in the various forms of the Fourier transform.

c.) Use $\psi(x)$ to compute $\langle x\rangle$, $\langle x^2\rangle$ and $\langle(\Delta x)^2\rangle$.

d.) Use $\phi(k)$ to compute $\langle k\rangle$, $\langle k^2\rangle$ and $\langle(\Delta k)^2\rangle$. Note that you may need to divide by the normalization integral as the Fourier transform may not be designed to deliver a unity normalized $\phi(k)$.

$$\langle k \rangle = \left\{ \int_{-\infty}^{\infty} \phi^*(k) \quad k \quad \phi(k)\, dk \right\} * \left[\int_{-\infty}^{\infty} \phi^*(k)\ \phi(k)\, dk \right]^{-1}$$

e.) What is the uncertainty product $\Delta k\ \Delta x$ for the function $\psi(x)$?

Answers: $|N| = \left(\sqrt{\frac{\pi}{2\,a^2}}\right)^{-1/2}$, $\phi(k) = \frac{1}{2\pi}\left(\frac{2\pi}{a^2}\right)^{1/4} e^{-[(k-k_o)^2/(4a^2)]}\ e^{-i(k-k_o)x_o}$, $\left\{x_o, x_o^2 + \frac{1}{4a^2}, \frac{1}{4a^2}\right\}$,

$\left\{k_o, k_o^2 + a^2, a^2\right\}$, $\Delta k\ \Delta x = {}^1/_2$. ***!!! not checked !!!***

17.) **Blackbody Radiation**: The following integral arises in the study of blackbody radiation.

$$\int_0^{\infty} \frac{q^3\, dq}{e^q - 1} = \int_0^{\infty} q^3\, dq\, e^{-q}\left[1 - e^{-q}\right]^{-1} =$$

$$= \int_0^{\infty} q^3\, dq\, e^{-q}\left[1 + e^{-q} + e^{-2q} + e^{-3q} + \ldots\right] = \int_0^{\infty} q^3\, dq \sum_{n=1}^{\infty} e^{-nq}$$

Show that this integral is equal to $6!\sum_{n=1}^{\infty} n^{-4}$. This sum can be evaluated using Parseval's equality as introduced in the Fourier series handout.

18.) a.) Use Stirling's Formula: $x! \approx x^x\, e^{-x}\sqrt{2\pi x}\,(1 + \frac{1}{12x})$ to increase the accuracy of the approximation $\ln(n!) \approx n\ln(n) - n$ to the order $\ln(n!) \approx n\ln(n) - n + c\ln(n)$. That is: Determine the value of the constant c. b.) Complete the table below.

n	$n!$	$\ln(n!)$	$n\ln(n) - n$	$n\ln(n) - n + c\ln(n)$
6	720	6.57925		
15	1.307_ x 10^{12}	27.8993		
40	8.159_ x 10^{47}		107.555	
100	9.33_ x 10^{157}			363.739

18.) Assuming the relations

$$\Gamma(n+1) = \int_0^{\infty} x^n\, e^{-x}\, dx = n! \qquad \Gamma(n+1) = n\,\Gamma(n)$$

$$G(n) = \int_0^\infty x^n e^{-x^2}\, dx = (\tfrac{1}{2})\,\Gamma(\tfrac{n+1}{2}) \qquad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \qquad \Gamma(1) = 1$$

show that:

$$\int_0^\infty x^{2n} e^{-x^2/a^2}\, dx = \sqrt{\pi}\,\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1} \qquad \text{and} \qquad \int_0^\infty x^{2n+1} e^{-x^2/a^2}\, dx = \frac{n!}{2}\, a^{2n+2}$$

19.) Show that: $\int_0^\pi \int_0^{2\pi} (\vec{A}\cdot\hat{r})(\vec{B}\cdot\hat{r}) \sin\theta\, d\theta\, d\phi = \frac{4\pi}{3}(\vec{A}\cdot\vec{B})$.

Hint: Use $\hat{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}$

20.) It has been shown that: $\int_{-\infty}^{\infty} e^{-a^2x^2+bx}\, dx = \sqrt{\pi}/a\; e^{-b^2/4a^2}$. Make a similar evaluation of

$\int_{-\infty}^{\infty} x^2 e^{-\lambda[x-a]^2}\, dx$.

Complete Elliptic Integral of the First Kind (*small k*)

21.) Show that Complete Elliptic Integral of the First Kind,

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = \frac{\pi}{2}\left[1 + \left(\frac{1}{2}\right)^2 k^2 + \left(\frac{1*3}{2*4}\right)^2 k^4 + \ldots\right] \text{ for small } k.$$

As a first step, use the result $\int_0^{\pi/2} [\sin\theta]^k\, d\theta = \frac{\sqrt{\pi}\;\Gamma(\frac{k+1}{2})}{k\,\Gamma(\frac{k}{2})}$ *for* $k > -1$ to compute

$$\int_0^{\pi/2} [\sin\theta]^{2m}\, d\theta = \frac{\sqrt{\pi}\;\Gamma(m+\tfrac{1}{2})}{2m\,\Gamma(m)} = \frac{\sqrt{\pi}\,(2m-1)!!\;\Gamma(\tfrac{1}{2})}{2\,(m!)\;\;2^m} = \frac{\pi\,(2m-1)!!}{2\,(m!)\;\;2^m}$$

$$\int_0^{\pi/2} [\sin\theta]^{2}\, d\theta = \frac{\sqrt{\pi}\;\Gamma(1+\tfrac{1}{2})}{2\,\Gamma(1)} = \frac{\sqrt{\pi}\,(1)\;\Gamma(\tfrac{1}{2})}{2(1!)\;\;2^1} = \frac{\pi}{4}$$

$$\int_0^{\pi/2} [\sin\theta]^{4}\, d\theta = \frac{\sqrt{\pi}\;\Gamma(2+\tfrac{1}{2})}{2(2)\,\Gamma(2)} = \frac{\sqrt{\pi}\,(4-1)!!\;\Gamma(\tfrac{1}{2})}{2\,(2!)\;\;2^2} = \frac{3\pi}{16}$$

$$K(k) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = \frac{\pi}{2}\left[1 + \sum_{m=1}^{\infty}\left(\frac{[2m-1]!!}{[2m]!!}\right)^2 k^{2m}\right] \text{ could be OK}$$

22.) Show that Complete Elliptic Integral of the Second Kind,

$$E(k)=\int_0^{\pi/2}\sqrt{1-k^2\sin^2\theta}\;\;d\theta=\frac{\pi}{2}\left[1-\frac{1}{4}k^2-\frac{3}{64}k^4+...\right]$$ for small k.

You may use the result $\int_0^{\pi/2}[\sin\theta]^k\;\;d\theta=\frac{\sqrt{\pi}\;\;\Gamma(\frac{k+1}{2})}{k\,\Gamma(\frac{k}{2})}\quad for\;\;k>-1$. See the previous problem.

$$E(k)=\int_0^{\pi/2}\sqrt{1-k^2\sin^2\theta}\;\;d\theta=\frac{\pi}{2}\left[1-\sum_{m=1}^{\infty}\left(\frac{[2m-1]!!}{[2m]!!}\right)^2\frac{k^{2m}}{(2m-1)}\right]$$

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