PHOT 301: Quantum Photonics

Homework: Probability & definite integrals

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Integrals

Here we will give some exercises on doing the typical integrals required to calculate probability, and expection values for given probability density functions $\rho(x) = |\psi(x)|^2$.

Please read the very brief description of statistics of discrete and continuous variables which is given in the first Chapter of Griffith's (our textbook). Further, use the formula sheet for the definition of the basic integrals.

Substitution rule

Doing integration by substitution works similar to the *inverse of the chain rule*. For an anti-derivative, i.e. indefinite integral, try to put it in following form:

$$\int f(g(x))g'(x)dx = \int f(u)du, \qquad \text{with} \quad u = g(x)$$

As an example take $\int x\cos(-x^2)$:

$$\begin{aligned}\int \cos(x^2)x dx &= \frac{1}{2}\int \cos(x^2)d(x^2) \\ &= \frac{1}{2}\sin(x^2) + C\end{aligned}$$

When you have a **definite integral** then the limits change as well:

$$\int_a^b f(g(x))g'(x)dx = \int_{g(a)}^{g(b)} f(u)du, \qquad \text{with} \quad u = g(x)$$

Remark: a **condition** is that both g' and f need to be continuous over $x \in [a, b]$. Let's take the same example integral again:

$$\begin{aligned}\int_0^{\sqrt{\pi/2}} \cos(x^2) x dx &= \frac{1}{2}\int_0^{\pi/2} \cos(u) d(u) \\ &= \frac{1}{2}\left[\sin(u)\right]\Big|_0^{\pi/2} \\ &= \frac{1}{2}\left[\sin(\pi/2) - \sin(0)\right] = \frac{1}{2}\end{aligned}$$

Exercises on substitution:

$$\int (x-1)^5 dx, \qquad \int_0^1 (x-1)^3 dx$$

$$\int_0^1 [(x-1)^2 - 1] dx, \qquad \int_0^{+\infty} \frac{1}{(x+5)^2}$$

$$\int_{-1}^1 [(x+1)(x-1)^2 + 3] dx, \qquad \int_{-1}^1 \sqrt{x+1} dx$$

$$\int_0^1 \sin^2\left(\frac{23x}{5}\right) dx, \qquad \int_0^1 \sin x \, \cos^2 x dx$$

$$\int_0^\infty e^{-3x} dx, \qquad \int_{-\infty}^\infty e^{-3|x|}$$

Partial integration

Partial integration can help to solve certain integrals when we can write the integrand in the specific form:

$$\int f(x) g'(x)\, dx = f(x)\, g(x) - \int g(x) f'(x)\, dx$$

Exercises on partial integration:

$$\int x \cos x \, dx, \qquad \int_0^\pi x^2 \cos x \, dx$$

$$\int x e^{3x}\, dx, \qquad \int (4x^3 - 9x^2 + 7x + 3) e^{-x} x \, dx$$

Gaussian integrals

An often encountered probability distribution is the Gaussian probability density function. In quantum mechanics we find this distribution appearing for the free particle and the ground state of the harmonic oscillator. Unfortunately the anti-derivative (indefinite integral) cannot be expressed in closed-form, however we can calculate the definite integrals $G = \int_{-\infty}^{\infty} e^{-x^2}\, dx$.

We will first show a **trick to calculate Gaussian integrals**: $G \equiv \int_{-\infty}^{\infty} e^{-x^2}\,dx$, by converting to an integral over the 2D plane in polar coordinates.

$$
\begin{aligned}
G^2 = \left[\int_{-\infty}^{\infty} e^{-x^2}\,dx\right]^2 &= \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy = \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dxdy = \int_{0}^{\infty}\int_{0}^{2\pi} e^{-r^2}\,r\,d\phi dr = 2\pi \int_{0}^{\infty} e^{-r^2}\,r\,dr \\
&= 2\pi\,\frac{1}{2}\int_{-\infty}^{0} e^{s}\,ds \qquad \text{with} \quad s=-r^2, \quad dr=-\frac{1}{2}ds \\
&= \pi\,[e^s]\big|_{-\infty}^{0} = \pi
\end{aligned}
$$

Therefore $G = \int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}$.

Exercises on Gaussian integrals: First show the following equalities (*hint*: use substitution):

$$
\begin{aligned}
G(\mu,a) &= \int_{-\infty}^{\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}} \\
G(\mu,a) &= \int_{-\infty}^{\infty} e^{-a(x-\mu)^2}\,dx = \sqrt{\frac{\pi}{a}} \\
G(a,b,c) &= \int_{-\infty}^{\infty} e^{-(ax^2+bx+c)}\,dx = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}-c}
\end{aligned}
$$

Leibniz rule: differentiation under the integral sign

Leibniz rule for differentiation under the integral sign, i.e. Feynman's trick to calculate the integral:

$$
\frac{\partial}{\partial\nu}\left[\int f(x;\nu)\,dx\right] = \int \frac{\partial f(x;\nu)}{\partial\nu}\,dx
$$

Let's apply this to find the Gaussian integral times a polynomial term x^n. For x ($n=1$), we know the result from above via substituation. Let's start with x^2:

$$
\begin{aligned}
&\int_{-\infty}^{\infty} \frac{\partial}{\partial a}\left[e^{-ax^2}\right]\,dx = \int_{-\infty}^{\infty}(-x^2)e^{-ax^2}\,dx = -\frac{1}{2}\sqrt{\frac{\pi}{a^3}} \\
\Rightarrow \quad &\int_{-\infty}^{\infty} x^2\,e^{-ax^2}\,dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}
\end{aligned}
$$

Now let's take the second derivative:

$$\int_{-\infty}^{\infty} \frac{\partial^2}{\partial a^2}\left[e^{-ax^2}\right] dx = \int_{-\infty}^{\infty} (-x^2)^2 e^{-ax^2}\, dx = \frac{1}{2}\frac{3}{2}\frac{1}{a^2}\sqrt{\frac{\pi}{a}}$$
$$\Rightarrow \quad \int_{-\infty}^{\infty} x^2\, e^{-ax^2}\, dx = \frac{1\cdot 3}{(2a)^2}\sqrt{\frac{\pi}{a}}$$

Doing the derivative n times gives

$$\int_{-\infty}^{\infty} \frac{\partial^n}{\partial a^n}\left[e^{-ax^2}\right] dx = \int_{-\infty}^{\infty} (-x^2)^n e^{-ax^2}\, dx = \left[\frac{1}{2}\frac{3}{2}\cdots\frac{2n-1}{2}\right]\frac{1}{a^n}\sqrt{\frac{\pi}{a}}$$
$$\Rightarrow \quad \int_{-\infty}^{\infty} x^{2n}\, e^{-ax^2}\, dx = \frac{1\cdot 3\cdots(2n-1)}{(2a)^n}\sqrt{\frac{\pi}{a}}$$

Exercises on probability density functions:

Most of the time you start off with the (time-independent solution of the) wavefunction $\Psi(x,t=0)=\psi(x)$ and you first need to calculate the probability density function $\rho(x)=|\psi(x)|^2$ and fill it in in the integral with correct limits. In the following exercises, **calculate** $\rho(x)=|\psi(x)|^2$ and **write down the integral** (you don't need to calculate the resulting integral). In the following $A\neq 0$ is a normalization constant.

$$\begin{aligned}
\psi(x) &= Axe^{-x} && \text{with } x\in[0,+\infty[\\
\psi(x) &= A\sin(x)e^{-ix} && \text{with } x\in[0,\pi]\\
\psi(x) &= A\frac{1}{x+i} && \text{with } x\in]-\infty,+\infty[\\
\psi(x) &= A\sin(x)\sin(\pi-x) && \text{with } x\in[0,\pi]\\
\psi(x) &= A\sin(4\pi x) && \text{with } x\in[0,1]
\end{aligned}$$

It is always good to sketch the function $\rho(x)=|\psi(x)|^2$ as well, so you can verify whether the probability density function $\rho(x)$ leads to a total probability of one, i.e. the wave function is normalized (this requires $\rho(x)$ to go to zero at infinity).