DALHOUSIE UNIVERSITY

PHYC 3640 Quantum Physics I: Tutorial 2

Volume Integration

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Volume Integration

Problem 1

Even and Odd Functions

Problem 2

Problem 3

Useful Integrals

Problem 4

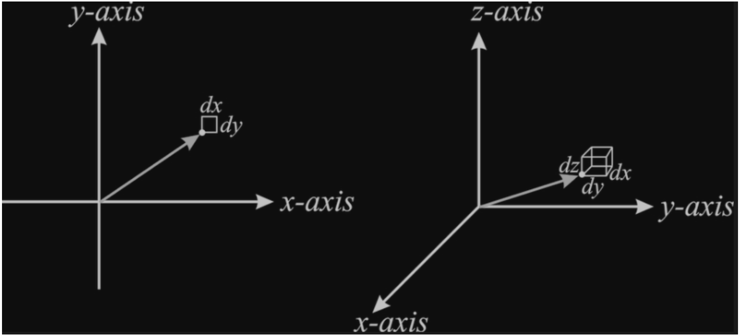
Types of Volume Integrals

- Cartesian (x, y, z)
- Spherical (r, θ, ϕ)
- Cylindrical (ρ, ϕ, z)
- Elliptical (λ, μ, ϕ)

This URL will save your life:

https://en.wikipedia.org/wiki/Del_in_cylindrical_and_spherical_coordinates

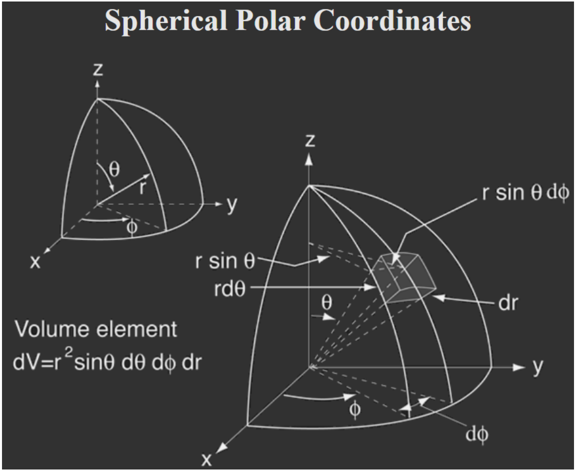
Cartesian



$$d\tau = dx\,dy\,dz$$

https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Book%3A_Mathematical_Methods_in_Chemistry_(Levitus)/10%3A_Plane_Polar_and_Spherical_Coordinates/10.02%3A_Area_and_Volume_Elements

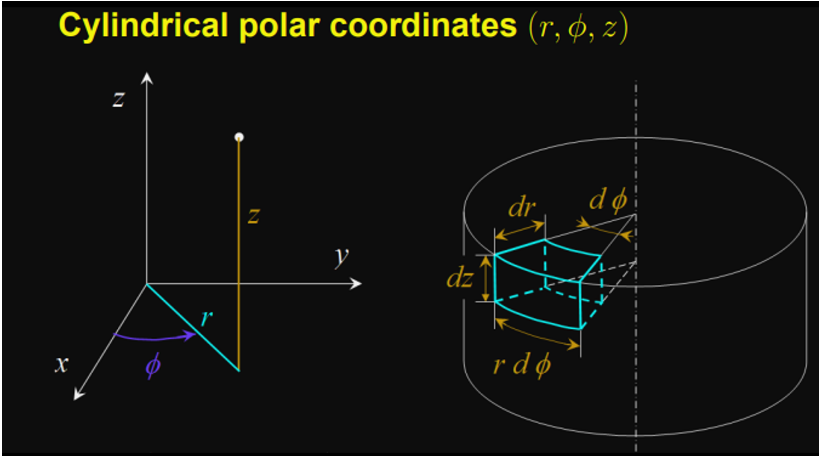
Spherical



$$d\tau = r^2 \sin(\theta)\, dr\, d\theta\, d\phi$$

http://hyperphysics.phy-astr.gsu.edu/hbase/sphc.html

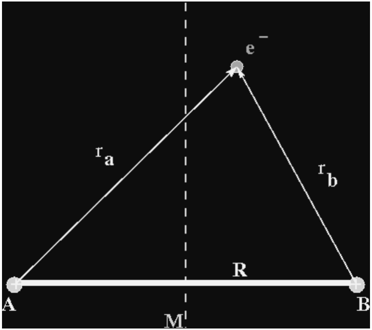
Cylindrical

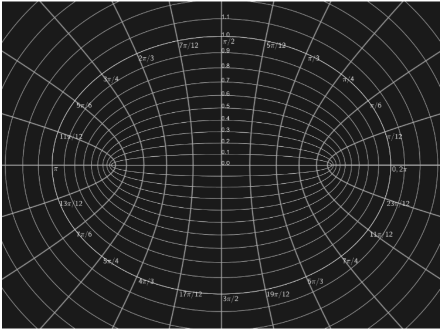


$$d\tau = r\,dr\,d\phi\,dz$$

https://s2629002012.files.wordpress.com/2012/10/cylincricalsphericalcoordinates.pdf

Elliptical





$$\lambda = \frac{r_a + r_b}{R} \qquad \mu = \frac{r_a - r_b}{R}$$

$$d\tau = \frac{R^3}{8}\left(\lambda^2 - \mu^2\right) d\lambda \, d\mu \, d\phi$$

https://opencommons.uconn.edu/cgi/viewcontent.cgi?article=1004&context=chem_educ
https://chem.libretexts.org/Courses/BethuneCookman_University/B-CU%3ACH-331_Physical_Chemistry_I/CH-331_Text/CH-331_Text/09%3A_The_Chemical_Bond%3A_Diatomic_Molecules/09.3B%3A_Evaluating_the_Overlap_Integral

Problem 1

1) We have all heard that $\int e^{x^2} dx$ is impossible to integrate. However, it is possible to show that

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

Show this.

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Show this.

Solution

Odd Functions

A particularly useful property is that the integral of an odd function, (i.e. $g(-x) = -g(x)$) over a symmetric interval (i.e. from $-a$ to a) is zero. This makes intuitive sense, since half of the area is negative and half positive. This result can be proved as follows:

$$I = \int_{-a}^{a} g(x)dx = \int_{-a}^{0} g(x)dx + \int_{0}^{a} g(x)dx$$

Reversing the limits on the first integral

$$I = \int_{0}^{-a} -g(x)dx + \int_{0}^{a} g(x)dx = \int_{0}^{-a} g(-x)dx + \int_{0}^{a} g(x)dx$$

and making the change of variable $u = -x$, $du = -dx$, we have

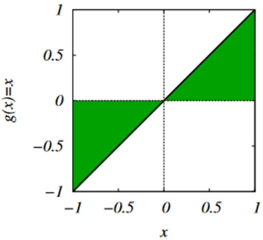
$$I = \int_{0}^{a} -g(u)du + \int_{0}^{a} g(x)dx = 0$$

As an example, consider

$$I = \int_{-1}^{1} xdx$$

this is an integral of an odd function over a symmetric interval, so we can say that it is zero by inspection. To show this

$$I = \int_{-1}^{1} xdx = \frac{1}{2}x^2\Big|_{-1}^{1} = \frac{1}{2}(1^2 - (-1)^2) = 0$$



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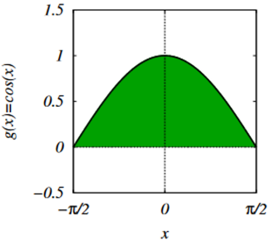
Even Functions

Also, the integral of an even function (i.e. $g(-x) = g(x)$) over a symmetric interval is

$$\int_{-a}^{a} g(x)dx = 2\int_{0}^{a} g(x)dx$$

As an example, consider

$$\begin{aligned} I &= \int_{\pi/2}^{\pi/2} \cos(x)dx \\ &= \sin(x)\Big|_{-\pi/2}^{\pi/2} \\ &= \sin(\pi/2) - \sin(-\pi/2) \\ &= 1 - (-1) \\ &= 2 \end{aligned}$$



which is equivalent to

$$\begin{aligned} I &= 2\int_{0}^{\pi/2} \cos(x)dx \\ &= 2\sin(x)\Big|_{0}^{\pi/2} \\ &= 2\sin(\pi/2) - \sin(0) \\ &= 2(1 - 0) \\ &= 2 \end{aligned}$$

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Problem 2

List whether the following composite functions are even, odd, or neither

a) $x\sin(x)\cos(x)$

b) $|x|\sin^2(x)\tan(x)$

c) $\sin(x)\cos(x)\mathrm{e}^{x^2}\tan(x)$

d) $\dfrac{x}{x^2-1}$

e) $\mathrm{e}^{1/x}\sin\left(x^2\right)$

f) $\tan\left(x^2-1\right)$

g) $\mathrm{e}^{x^2-1}\sinh\left(x^2+1\right)$

h) $\sin(x)\left[x+x^3\right]$

i) $\cos(x)+i\sin(x)$

Problem 2

List whether the following composite functions are even, odd, or neither

a) $x\sin(x)\cos(x)$	even
b) $\lvert x\rvert \sin^2(x)\tan(x)$	odd
c) $\sin(x)\cos(x)e^{x^2}\tan(x)$	even
d) $\dfrac{x}{x^2-1}$	odd
e) $e^{1/x}\sin\left(x^2\right)$	neither
f) $\tan\left(x^2-1\right)$	even
g) $e^{x^2-1}\sinh\left(x^2+1\right)$	even
h) $\sin(x)\left[x+x^3\right]$	even
i) $\cos(x)+i\sin(x)$	neither

Problem 3

2) Using the results from problems 1 and 2, where

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

Consider a wavefunction given by

$$\psi(r) = A\mathrm{e}^{-r^2}\,,$$

Determine the normalization constant for this wavefunction. i.e., Determine the value of A such that $\int \psi(r)^* \psi(r) d\mathbf{r} = 1\,.$

Problem 3: Solution

$$\int \psi(r)^* \psi(r) d\mathbf{r} = \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} A\mathrm{e}^{-r^2} A\mathrm{e}^{-r^2} r^2 \sin(\theta) dr\, d\theta\, d\phi$$
$$= 4\pi A^2 \int_{r=0}^{\infty} r^2 \mathrm{e}^{-2r^2} dr\,.$$

Let $u = r$ and $dv = r\mathrm{e}^{-2r^2}\, dr$. Then use $\int u\, dv = uv - \int v\, du$

$$u = r \qquad dv = r\mathrm{e}^{-2r^2}\, dr$$
$$du = dr \qquad v = -\frac{1}{4}\mathrm{e}^{-2r^2}\,,$$

so

$$\int \psi(r)^* \psi(r) d\mathbf{r} = 4\pi A^2 \int_{r=0}^{\infty} r^2 \mathrm{e}^{-2r^2} dr$$
$$= 4\pi A^2 \left(\left[-\frac{r}{4}\mathrm{e}^{-2r^2} \right]_0^{\infty} - \int_{r=0}^{\infty} -\frac{1}{4}\mathrm{e}^{-2r^2} dr \right)$$
$$= \pi A^2 \int_{r=0}^{\infty} \mathrm{e}^{-2r^2} dr\,.$$

CONT...

Let $u = \sqrt{2}r$, so $du/dr = \sqrt{2}$ and $dr = \frac{1}{\sqrt{2}}du$. Then

$$\begin{aligned}
\int \psi(r)^* \psi(r) d\mathbf{r} &= \pi A^2 \int_{r=0}^{\infty} \mathrm{e}^{-2r^2} dr \\
&= \frac{\pi A^2}{\sqrt{2}} \int_{u=0}^{\infty} \mathrm{e}^{-u^2} du \\
&= \frac{\pi A^2}{\sqrt{2}} \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{e}^{-u^2} du \\
&= \left(\frac{\pi}{2}\right)^{3/2} A^2 \,,
\end{aligned}$$

so finally,

$$\left(\frac{\pi}{2}\right)^{3/2} A^2 = 1 \quad \Rightarrow \quad A = \left(\frac{2}{\pi}\right)^{3/4} .$$

Useful Gaussian Integrals

Gaussian Functions

$$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x^2\, e^{-ax^2}\,dx = \frac{1}{4a}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x^4\, e^{-ax^2}\,dx = \frac{3}{8a^2}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x^{2n}\, e^{-ax^2}\,dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty x\, e^{-ax^2}\,dx = \frac{1}{2a}$$

$$\int_0^\infty x^3\, e^{-ax^2}\,dx = \frac{1}{2a^2}$$

$$\int_0^\infty x^5\, e^{-ax^2}\,dx = \frac{1}{a^3}$$

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

Exponential Functions

$$\int_0^\infty x^n\, e^{-ax}\,dx = \frac{n!}{a^{n+1}}$$

https://www.colby.edu/chemistry/PChem/notes/Integral.pdf

Problem 4

We have constructed our normalized wavefunction from problem 3.

$$\psi(r) = \left(\frac{2}{\pi}\right)^{3/4} \mathrm{e}^{-r^2}$$

Compute

- $\langle r \rangle$
- $\left\langle r^2 \right\rangle$
- $\langle p_r \rangle$ given $p_r = \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial r}$
- $\left\langle p_r^2 \right\rangle$
- $\langle P_r \rangle$ given $P_r = \frac{\hbar}{\mathrm{i}} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right)$
- $\left\langle P_r^2 \right\rangle$

Note: There are two ways you could define "radial momentum". $p_r = \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial r}$ is considered the "radial component of the momentum operator", however, this operator is not a valid *Hermitian* operator and thus it is seldom used. An alternative definition is $p_r = \frac{\hbar}{\mathrm{i}} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right)$, which is known as the "radial momentum operator".

https://physics.stackexchange.com/questions/9349/how-to-construct-the-radial-component-of-the-momentum-operator

Problem 4: Solution

```
ψ[r_] := A * Exp[-r^2];
A = (2/π)^(3/4);
Integrate[ψ[r]^* × ψ[r] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
```

1

```
pr = ħ/i (D[#1, r]) &;
Pr = ħ/i (D[#1, r] + #1/r) &;
```

$\langle p_r \rangle$ & $\langle p_r{}^2 \rangle$

```
Integrate[ψ[r]^* × pr[ψ[r]] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
Integrate[ψ[r]^* × pr[pr[ψ[r]]] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
```

$2\, i \sqrt{\frac{2}{\pi}}\, \hbar$

$-\hbar^2$

$\langle r \rangle$ & $\langle r^2 \rangle$

```
Integrate[ψ[r]^* r ψ[r] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
Integrate[ψ[r]^* r^2 ψ[r] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
```

$\sqrt{\frac{2}{\pi}}$

$\frac{3}{4}$

$\langle P_r \rangle$ & $\langle P_r{}^2 \rangle$

```
Integrate[ψ[r]^* × Pr[ψ[r]] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
Integrate[ψ[r]^* × Pr[Pr[ψ[r]]] * r^2 Sin[θ], {r, 0, ∞}, {θ, 0, π}, {ϕ, 0, 2π}]
```

0

$3\hbar^2$

Questions?

Want My Slides?

https://github.com/KyleBryenton/slides-posters

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