

Molecular Physics solved exercises

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Contents

1	Partial derivatives	1
1.1	Solving partial derivatives	1
2	Differential operators	2
2.1	Computing the gradient of a function	2
2.2	Computing the divergence of a function	2
2.3	Computing the curl of a function	3
2.4	Curl of the grad of a function	3
2.5	Divergence of the curl of a function	3
2.6	Divergence of the gradient of a function	3
3	Spherical coordinates	4
4	Multidimensional integrals	4
4.1	Computing multidimensional integrals	4
5	Wave equations	4
6	Hilbert spaces	4

1 Partial derivatives

1.1 Solving partial derivatives

Compute all first order partial derivatives of $f(x, y, z) = ze^{-x^2-y^2}$.

$$\begin{aligned}\frac{\partial f}{\partial x} &= -2xze^{-x^2-y^2} \\ \frac{\partial f}{\partial y} &= -2yze^{-x^2-y^2} \\ \frac{\partial f}{\partial z} &= e^{-x^2-y^2}\end{aligned}$$

Compute both first order partial derivatives of $f = e^{ix}(x^3 + y^3 + 1)$.

$$\begin{aligned}\frac{\partial f}{\partial x} &= ie^{ix}(x^3 + y^3 + 1) + e^{ix}(3x^2) \\ &= e^{ix}(ix^3 + iy^3 + i + 3x^2) \\ \frac{\partial f}{\partial y} &= 3y^2 e^{ix}\end{aligned}$$

Compute $\frac{\partial^5 f}{\partial^2 x \partial^3 y}$ with $f = xy^3 e^{-\frac{1}{y}} + 5e^{ix^3} y^2$.

$$\begin{aligned}f &= xy^3 e^{-\frac{1}{y}} + 5e^{ix^3} y^2 \\ \frac{\partial f}{\partial x} &= y^3 e^{-\frac{1}{y}} + i15x^2 e^{ix^3} y^2 \\ \frac{\partial^2 f}{\partial^2 x} &= i15y^2 [(2x)(e^{ix^3}) + (x^2)(i3x^2 e^{ix^3})] \\ &= i15y^2 x e^{ix^3} (2 + i3x^3) \\ \frac{\partial^3 f}{\partial^2 x \partial y} &= i30y x e^{ix^3} (2 + i3x^3) \\ \frac{\partial^4 f}{\partial^2 x \partial^2 y} &= i30x e^{ix^3} (2 + i3x^3) \\ \frac{\partial^5 f}{\partial^2 x \partial^3 y} &= 0\end{aligned}$$

2 Differential operators

2.1 Computing the gradient of a function

Compute $\text{grad}(f)$ with $f = x^2 + y^2 + z^2$.

$$\begin{aligned}\text{grad}(f) &= \vec{\nabla} f = \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \\ &= (2x \quad 2y \quad 2z)\end{aligned}$$

Compute $\text{grad}(f)$ with $f = \sin(x^2 y z)$.

$$\begin{aligned}\text{grad}(f) &= \vec{\nabla} f = \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \\ &= (xyz \cos(x^2 y z) \quad x^2 z \cos(x^2 y z) \quad x^2 y \cos(x^2 y z))\end{aligned}$$

2.2 Computing the divergence of a function

Compute $\text{div}(\vec{f})$ with $\vec{f} = (xy \quad y \quad zx^2)$.

$$\begin{aligned}\text{div}(\vec{f}) &= \vec{\nabla} \cdot \vec{f} = \begin{pmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} f_x & f_y & f_z \end{pmatrix} \\ &= \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z} \\ &= \frac{\partial(xy)}{\partial x} + \frac{\partial(y)}{\partial y} + \frac{\partial(zx^2)}{\partial z} \\ &= y + 1 + x^2\end{aligned}$$

2.3 Computing the curl of a function

Compute $\text{rot}(\vec{f})$ with $\vec{f} = (y \ -x \ 0)$.

$$\begin{aligned}\text{rot}(\vec{f}) &= \vec{\nabla} \times \vec{f} = \begin{pmatrix} \frac{\partial f_z}{\partial y} - \frac{\partial f_y}{\partial z} & \frac{\partial f_x}{\partial z} - \frac{\partial f_z}{\partial x} & \frac{\partial f_y}{\partial x} - \frac{\partial f_x}{\partial y} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial(0)}{\partial y} - \frac{\partial(-x)}{\partial z} & \frac{\partial(y)}{\partial z} - \frac{\partial(0)}{\partial x} & \frac{\partial(-x)}{\partial x} - \frac{\partial(y)}{\partial y} \end{pmatrix} \\ &= (0 - 0 \quad 0 - 0 \quad -1 - -1) \\ &= (0 \quad 0 \quad -2)\end{aligned}$$

2.4 Curl of the grad of a function

Compute $\text{rot}(\text{grad}(\vec{f}))$.

$$\begin{aligned}\text{rot}(\text{grad}(\vec{f})) &= \vec{\nabla} \times (\vec{\nabla} \vec{f}) = \vec{\nabla} \times \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \\ &= \det \begin{vmatrix} \vec{e}_x & \vec{e}_y & \vec{e}_z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{vmatrix} \\ &= \begin{pmatrix} \frac{\partial^2 f}{\partial y \partial z} - \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z \partial x} - \frac{\partial^2 f}{\partial x \partial z} & \frac{\partial^2 f}{\partial x \partial y} - \frac{\partial^2 f}{\partial y \partial x} \end{pmatrix} \\ &\text{since you can change the order of derivation} \\ &= (0 \quad 0 \quad 0)\end{aligned}$$

Notice that $\text{rot}(\text{grad}(\vec{f}))$ is equal to the zero vector regardless of f .

2.5 Divergence of the curl of a function

Compute $\text{div}(\text{rot}(\vec{f}))$.

$$\begin{aligned}\text{div}(\text{rot}(\vec{f})) &= \vec{\nabla} \cdot (\vec{\nabla} \times \vec{f}) = \vec{\nabla} \cdot \begin{pmatrix} \frac{\partial f_z}{\partial y} - \frac{\partial f_y}{\partial z} & \frac{\partial f_x}{\partial z} - \frac{\partial f_z}{\partial x} & \frac{\partial f_y}{\partial x} - \frac{\partial f_x}{\partial y} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial f_z}{\partial y} - \frac{\partial f_y}{\partial z} & \frac{\partial f_x}{\partial z} - \frac{\partial f_z}{\partial x} & \frac{\partial f_y}{\partial x} - \frac{\partial f_x}{\partial y} \end{pmatrix} \\ &= \frac{\partial^2 f_z}{\partial y \partial x} - \frac{\partial^2 f_y}{\partial z \partial x} + \frac{\partial^2 f_x}{\partial z \partial y} - \frac{\partial^2 f_z}{\partial x \partial y} + \frac{\partial^2 f_y}{\partial x \partial z} - \frac{\partial^2 f_x}{\partial y \partial z} \\ &\text{then, changing the order of the terms we notice that} \\ &= \frac{\partial^2 f_z}{\partial y \partial x} - \frac{\partial^2 f_z}{\partial x \partial y} + \frac{\partial^2 f_x}{\partial z \partial y} - \frac{\partial^2 f_x}{\partial y \partial z} + \frac{\partial^2 f_y}{\partial x \partial z} - \frac{\partial^2 f_y}{\partial z \partial x} \\ &\text{since you can change the order of derivation} \\ &= 0\end{aligned}$$

Notice that $\text{div}(\text{rot}(\vec{f}))$ is equal to zero vector regardless of f .

2.6 Divergence of the gradient of a function

Demonstrate that $\Delta f = \text{div}(\text{grad}(f))$

$$\begin{aligned}\text{div}(\text{grad}(\vec{f})) &= \vec{\nabla} \cdot (\vec{\nabla} \vec{f}) = \vec{\nabla} \cdot \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \end{pmatrix} \\ &= \frac{\partial^2 f}{\partial^2 x} + \frac{\partial^2 f}{\partial^2 y} + \frac{\partial^2 f}{\partial^2 z} \\ &= f \left(\frac{\partial^2}{\partial^2 x} + \frac{\partial^2}{\partial^2 y} + \frac{\partial^2}{\partial^2 z} \right) \\ &= \Delta f\end{aligned}$$

3 Spherical coordinates

4 Multidimensional integrals

4.1 Computing multidimensional integrals

Compute $\int_{y=0}^{y=\pi} \int_{x=y}^{x=\pi} \frac{\sin x}{x} dx dy$.

$$\begin{aligned}
 \int_{y=0}^{y=\pi} \int_{x=y}^{x=\pi} \frac{\sin x}{x} dx dy &= \int_{x=0}^{x=\pi} \int_{y=0}^{y=x} \frac{\sin x}{x} dy dx && \text{change order of integration} \\
 &= \int_{x=0}^{x=\pi} \left[y \frac{\sin x}{x} \right]_{y=0}^{y=x} dx && \text{integrate over } y \\
 &= \int_{x=0}^{x=\pi} \left(x \frac{\sin x}{x} - 0 \frac{\sin x}{x} \right) dx && \text{evaluate over interval of } y \\
 &= \int_{x=0}^{x=\pi} \sin x dx && \text{simplify} \\
 &= [-\cos x]_{x=0}^{x=\pi} && \text{integrate over } x \\
 &= (-\cos \pi - \cos 0) && \text{evaluate over interval of } x \\
 &= -(-1) - (-1) = 2
 \end{aligned}$$

Notice how the integration region changes when swapping order of integration. To understand how the integration region changes, look at 1.

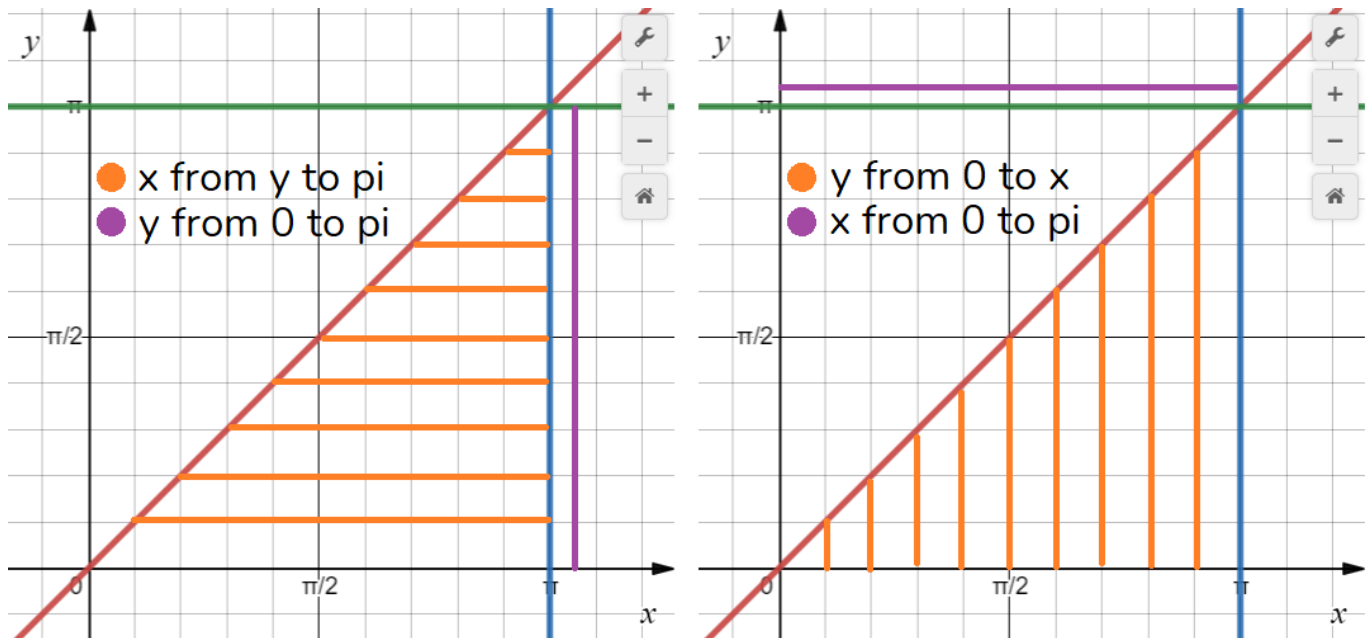


Figure 1: On the left: original order of integration. On the right: inverted order of integration

5 Wave equations

6 Hilbert spaces