Molecular Physics solved exercises

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Github: https://github.com/giacThePhantom/MolecularPhysics

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Contents

1 Partial derivatives

1.1 Solving partial derivatives

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

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

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

$$\begin{aligned}f &= xy^3 e^{-\frac{1}{y}} + 5e^{ix^3} y^2 \\ \frac{\partial f}{\partial x} &= y^3 e^{-\frac{1}{y}} + i15x^2 e^{ix^3} y^2 \\ \frac{\partial^2 f}{\partial^2 x} &= i15y^2[(2x)(e^{ix^3}) + (x^2)(i3x^2 e^{ix^3})] \\ &= i15y^2 x e^{ix^3}(2 + i3x^3) \\ \frac{\partial^3 f}{\partial^2 x \partial y} &= i30yxe^{ix^3}(2 + i3x^3) \\ \frac{\partial^4 f}{\partial^2 x \partial^2 y} &= i30xe^{ix^3}(2 + i3x^3) \\ \frac{\partial^5 f}{\partial^2 x \partial^3 y} &= 0\end{aligned}$$

2 Differential operators

2.1 Computing the gradient of a function

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

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

Compute $\mathrm{grad}(f)$ with $f = \sin(x^2yz)$.

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

2.2 Computing the divergence of a function

Compute $\mathrm{div}(\vec{f})$ with $\vec{f} = \begin{pmatrix} xy & y & zx^2 \end{pmatrix}$.

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

2.3 Computing the curl of a function

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

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

2.4 Curl of the grad of a function

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

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

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

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

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

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

3 Spherical coordinates

4 Multidimensional integrals

4.1 Computing multidimensional integrals

Compute $\int\limits_{y=0}^{y=\pi}\int\limits_{x=y}^{x=\pi}\frac{sinx}{x}dxdy$.

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

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

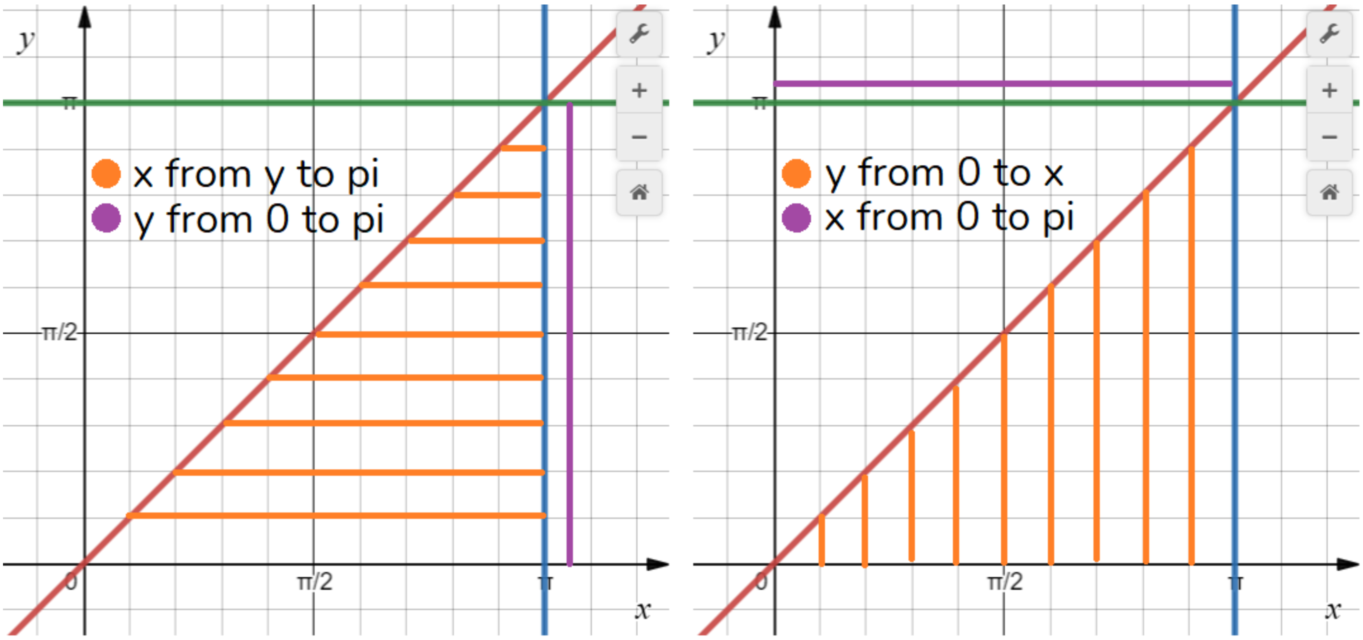

Figure 1: On the left: original order of integration. On the right: inverted order of integration

5 Wave equations

6 Hilbert spaces