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Math Methods-I (PHY421)

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Homework-1

1. Given that \mathbf{a} and \mathbf{k} are constant vectors, λ is a constant and $u(\mathbf{r})$ is a well-behaved function.

(a) Evaluate (i) $\nabla e^{i\mathbf{k}\cdot\mathbf{r}}$, (ii) $\nabla \left(\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{|\mathbf{r}|} \right)$ and (iii) $\nabla \cos(\mathbf{k} \cdot \mathbf{r})$.

(b) Evaluate (i) $\nabla \cdot (\mathbf{a} e^{i\mathbf{k}\cdot\mathbf{r}})$ and (ii) $\nabla \times (\mathbf{a} e^{i\mathbf{k}\cdot\mathbf{r}})$.

(c) Evaluate (i) $\nabla^2 \left(\frac{1}{r} \right)$ and (ii) $\nabla^2 \left(\frac{e^{-\lambda r}}{r} \right)$.

(d) Show that

$$-\hbar^2 \nabla_{\mathbf{r}}^2 [u(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}] = e^{i\mathbf{k}\cdot\mathbf{r}} [-i\hbar \nabla + \hbar \mathbf{k}]^2 u(\mathbf{r}).$$

2. Given a vector field $\mathbf{A} = yz\hat{i} + xz\hat{j} + xy\hat{k}$.

(a) Check that $\nabla \cdot \mathbf{A} = 0$ and $\nabla \times \mathbf{A} = 0$.

(b) Find a scalar field $f(x, y, z)$ such that $\nabla f(x, y, z) = \mathbf{A}$.

(c) Find a vector field \mathbf{B} such that $\nabla \times \mathbf{B} = \mathbf{A}$.

3. Given $\mathbf{A} = \mathbf{a} e^{i\mathbf{k}\cdot\mathbf{r}}$.

(a) Show that

$$I = \oint_S \mathbf{A} \cdot d\mathbf{S} = 4\pi R^3 (i\mathbf{k} \cdot \mathbf{a}) \left[\frac{\sin(kR) - kR \cos(kR)}{(kR)^3} \right].$$

Here S is the surface of a sphere of radius R centered at the origin and V is the volume of the sphere.

(b) Plot I [in units of $4\pi R^3 (i\mathbf{k} \cdot \mathbf{a})$] vs kR .

(c) Obtain approximate expressions of I for the two limiting cases: (i) $kR \rightarrow 0$ and (ii) $kR \rightarrow \infty$ and compare with the plot.

4. The angular momentum operator is $\mathbf{L} = \mathbf{r} \times \mathbf{p} = -i\hbar[\mathbf{r} \times \nabla]$. Here \mathbf{r} is the position vector and $\mathbf{p} = -i\hbar\nabla$ is the momentum operator.

(a) Verify the relations:

$$(i) \mathbf{r} \cdot \mathbf{p} = \mathbf{p} \cdot \mathbf{r} + 3i\hbar, \quad (ii) \mathbf{L} = \mathbf{r} \times \mathbf{p} = -(\mathbf{p} \times \mathbf{r}), \quad (iii) \mathbf{r} \cdot \mathbf{L} = 0, \quad (iv) \mathbf{p} \cdot \mathbf{L} = 0.$$

Note: The last three results are also true for classical angular momentum vector.

(b) Obtain the Cartesian components L_j (with $j = x, y, z$) of the angular momentum operator \mathbf{L} .

(c) Using the differential forms of the angular momentum operators, verify the commutation relations

$$\begin{aligned} (i) \quad [L_k, x_l] &= i\epsilon_{klm}x_m, & (ii) \quad [L_k, p_l] &= i\epsilon_{klm}p_m, & (iii) \quad [L_k, L_l] &= i\epsilon_{klm}L_m \\ (iv) \quad [L_k, \mathbf{r}^2] &= 0, & (ii) \quad [L_k, \mathbf{p}^2] &= 0, & (iii) \quad [L_k, \mathbf{r} \cdot \mathbf{p}] &= 0. \end{aligned}$$

5. The kinetic momentum ($\mathbf{\Pi}$) of a particle with charge $q > 0$ and mass m in presence of the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ is $\mathbf{\Pi} = (-i\hbar\nabla - q\mathbf{A})$. Here $\mathbf{p} = -i\hbar\nabla$ is the canonical momentum operator and \mathbf{A} is a vector potential corresponding to the magnetic field \mathbf{B} .

- (a) Show that $\mathbf{\Pi} \times \mathbf{\Pi} = i\hbar q\mathbf{B}$ and the commutator $[\Pi_x, \Pi_y] = i\hbar qB$, without choosing any specific form of the vector potential.
- (b) Find a symmetric and an asymmetric form of \mathbf{A} for the uniform magnetic field $\mathbf{B} = B \hat{\mathbf{z}}$. Sketch these vector potentials. Check that \mathbf{A} is divergenceless in both the cases.
- (bi) Consider both form of the vector potential and calculate the line integral $\int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{A} \cdot d\mathbf{r}$ along the straight line joining between \mathbf{r}_1 and \mathbf{r}_2 points and show that its value is the magnetic flux passing through the triangle spanned by the vectors $\mathbf{r}_1 = x_1\hat{i} + y_1\hat{j}$, $\mathbf{r}_2 = x_2\hat{i} + y_2\hat{j}$ and $\mathbf{r}_2 - \mathbf{r}_1$. Check that Stokes' theorem is satisfied.

(bii) Show that

$$H = \frac{\mathbf{\Pi}^2}{2m} = \frac{\mathbf{\Pi} \cdot \mathbf{\Pi}}{2m} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{qB}{2m}L_z + \frac{q^2B^2}{8m}(x^2 + y^2)$$

with $L_z = [\mathbf{r} \times (-i\hbar\nabla)]_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$ is the angular momentum operator.

6. A vector field is given by $\mathbf{A} = (-y\hat{i} + x\hat{j})/2$. Verify the Stokes' theorem for two different cases:
- (a) An open surface of the northern/southern hemisphere with its base of radius R centered at the origin lying on the xy plane.
- (b) A circular disk of the same radius R centered at the origin lying on the xy plane.

You will see that the results do not depend on the two open surfaces you are considering, depends only on the circle of radius R , which is boundary of the both the open surfaces.

7. (a) Show that the gradient operator in spherical coordinates is

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}.$$

Obtain the expression $\nabla^2 f = \nabla \cdot (\nabla f)$ in spherical coordinates. Note: The partial derivatives $\frac{\partial}{\partial \theta}$ and $\frac{\partial}{\partial \phi}$ in the left-hand ∇ operator act on the unit vectors $\hat{r}, \hat{\theta}, \hat{\phi}$ of right-hand ∇ operator.

- (b) Show that the angular momentum operator $\mathbf{L} = -i\hbar[\mathbf{r} \times \nabla]$ in spherical coordinates is

$$\mathbf{L} = -i\hbar\left[-\hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial \phi} + \hat{\phi}\frac{\partial}{\partial \theta}\right].$$

Obtain the form of \mathbf{L} at the equator from the above expression.

- (c) Given that

$$\begin{aligned}\hat{\mathbf{i}} &= \hat{\mathbf{r}}\sin\theta\cos\phi + \hat{\boldsymbol{\theta}}\cos\theta\cos\phi - \hat{\boldsymbol{\phi}}\sin\phi, & \hat{\mathbf{r}} &= \hat{\mathbf{i}}\sin\theta\cos\phi + \hat{\mathbf{j}}\sin\theta\sin\phi + \hat{\mathbf{k}}\cos\theta \\ \hat{\mathbf{j}} &= \hat{\mathbf{r}}\sin\theta\sin\phi + \hat{\boldsymbol{\theta}}\cos\theta\sin\phi + \hat{\boldsymbol{\phi}}\cos\phi, & \hat{\boldsymbol{\theta}} &= \hat{\mathbf{i}}\cos\theta\cos\phi + \hat{\mathbf{j}}\cos\theta\sin\phi - \hat{\mathbf{k}}\sin\theta \\ \hat{\mathbf{k}} &= \hat{\mathbf{r}}\cos\theta - \hat{\boldsymbol{\theta}}\sin\theta, & \hat{\boldsymbol{\phi}} &= -\hat{\mathbf{i}}\sin\phi + \hat{\mathbf{j}}\cos\phi.\end{aligned}$$

Show that

$$\begin{aligned} L_x &= -i\hbar \left[-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right] \\ L_y &= -i\hbar \left[\cos\phi \frac{\partial}{\partial\theta} - \sin\phi \cot\theta \frac{\partial}{\partial\phi} \right] \\ L_z &= -i\hbar \frac{\partial}{\partial\phi}. \end{aligned}$$

(d) Show that

$$\mathbf{L} \times \mathbf{L} = i\hbar \mathbf{L}.$$

(e) Show that

$$\mathbf{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] = -\hbar^2 \left[r^2 \nabla_{\mathbf{r}}^2 - \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right].$$

Obtain the form of \mathbf{L}^2 at the equator from the above expression.

(f) Show that $[L_k, \mathbf{L}^2] = 0$ with $k = x, y, z$. This is the reason the operator \mathbf{L}^2 plays an important role for systems having spherically symmetric potential. You will see in quantum mechanics that the operator \mathbf{L}^2 is one of the operators in the Complete Set of Commuting Observables (CSCO).

(g) Defining the raising and lowering angular momentum operators as $L_{\pm} = L_x \pm iL_y$. Show that L_{\pm} operators in the spherical coordinates are

$$L_{\pm} = \hbar e^{\pm i\phi} \left[\pm \frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi} \right].$$

8. Sketch the following functions:

$$(i) \lim_{\epsilon \rightarrow 0} \tanh(x/\epsilon), \quad (ii) \lim_{\epsilon \rightarrow 0} \frac{\sin(x/\epsilon)}{\pi x}, \quad (iii) \lim_{\epsilon \rightarrow 0} \frac{\epsilon/\pi}{x^2 + \epsilon^2} = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi\epsilon} \frac{1}{1 + \frac{x^2}{\epsilon^2}} \quad (iv) \lim_{\epsilon \rightarrow 0} \frac{1}{2\epsilon} \frac{1}{\cosh^2(\frac{x}{\epsilon})}.$$

9. The Fermi-Dirac distribution function is given by

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1},$$

where $\beta = 1/(k_B T)$ and μ is a real constant.

(a) Sketch the Fermi-Dirac distribution function $f(E)$ and its derivative $f'(E) = \frac{\partial f(E)}{\partial E}$ as $T \rightarrow 0$. In the limit of $T \rightarrow 0$, express $f(E)$ and its derivative $f'(E)$ in terms of the generalized distribution functions (unit step function and Dirac delta function).

(b) Sketch the following function $g(E) = 1 - f(E)$ and its derivative $g'(E) = \frac{\partial g(E)}{\partial E}$ as $T \rightarrow 0$:

$$g(E) = \frac{e^{\beta(E-\mu)}}{e^{\beta(E-\mu)} + 1},$$

where μ is a real constant.

In the limit of $T \rightarrow 0$, express $g(E)$ and its derivative $g'(E)$ in terms of the generalized distribution functions (unit step function and Dirac delta function).

(c) Express $f(E)$ and $f'(E) = \frac{\partial f(E)}{\partial E}$ in terms of hyperbolic functions.

$$f(E) = \frac{1}{2} \left[1 - \tanh \left(\frac{\beta \xi}{2} \right) \right], \quad f'(E) = -\frac{\beta}{4} \operatorname{sech}^2 \left(\frac{\beta \xi}{2} \right).$$

where $\xi = (E - \mu)$ and $\beta = 1/(k_B T)$.

(d) Expand $f(E)$ around $E = \mu$ (keeping first two non-vanishing terms only) for $\mu \ll k_B T$.

$$f(E) \simeq \frac{1}{2} - \frac{1}{k_B T} (E - \mu) + \dots$$

Sketch the above expanded function around $E = \mu$ and estimate the width of the variation of $f(E)$.

10. The Bose occupation number is given by

$$f_B(E) = \frac{1}{e^{\beta(E-\mu)} - 1},$$

where μ is a real constant, $E \geq 0$ and $\beta = 1/(k_B T)$.

Sketch the Bose occupation number $f_B(E)$ for $\mu = 0$, and $\mu < 0$ as $T \rightarrow 0$.

Is it possible to have $\mu > 0$ for any physical system having $E \geq 0$?

11. Evaluate the following integrals:

(a)

$$D_3(E) = \int_V \frac{d^3 k}{(2\pi)^3} \delta \left(E - \frac{\hbar^2 k^2}{2m} \right).$$

Here $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ is three-dimensional wavevector. The final result will give you the density of states of a free electron with mass m .

(b)

$$D_2(E) = \int_S \frac{d^2 k}{(2\pi)^2} \delta \left(E - \frac{\hbar^2 k^2}{2m} - \alpha k \right).$$

Here α is a constant having suitable dimension and $k = \sqrt{k_x^2 + k_y^2}$ is two-dimensional wavevector. What happens to $D_2(E)$ for $\alpha = 0$ case?

(c)

$$D_g(E) = \int_S \frac{d^2 k}{(2\pi)^2} \delta(E - \beta k).$$

Here β is a constant having suitable dimension and $k = \sqrt{k_x^2 + k_y^2}$ is two-dimensional wavevector.

Answers:

$$\begin{aligned} (a) \quad D_3 &= \frac{1}{6\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}, \quad (b) \quad D_2 = \frac{m}{2\pi\hbar^2} \left[1 - \sqrt{\frac{E_\alpha}{E + E_\alpha}} \right] \text{ with } E_\alpha = \frac{m\alpha^2}{2\hbar^2}, \\ (c) \quad D_g &= \frac{E}{2\pi\beta^2}. \end{aligned} \tag{1}$$

12. (a) Find the points x_n , the range of values of the summation index n and the coefficients c_n in the following expansion

$$\delta(\sin x - \cos x) = \sum_n c_n \delta(x - x_n).$$

Answers: $x_n = (n + 1/4)\pi, n = 0, \pm 1, \pm 2, \dots, c_n = 1/\sqrt{2}$.

- (b) Evaluate the following integral:

$$I = \int_{-\infty}^{\infty} dx e^{-a|x|} \delta(\sin x), \quad a > 0.$$

Answer: $I = \coth(a\pi/2)$.

13. Show that

$$\nabla \cdot \left(\frac{\hat{r}}{r^2} \right) = 4\pi \delta^3(\mathbf{r}).$$

Evaluate the following volume integral using (i) direct integration and (ii) using the above result:

$$J = \int_V e^{-r} \left[\nabla \cdot \left(\frac{\hat{r}}{r^2} \right) \right] d\tau,$$

where V is a sphere of radius R , centered at origin. Try to understand role of the auxiliary function e^{-r} in the integrand.

[Hints: In direct integration, use $\nabla \cdot (f\mathbf{A}) = f\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla f$ and Gauss divergence theorem. Here $f \equiv f(\mathbf{r})$ is a scalar function.]

14. Show that

$$\nabla \times \left(\frac{\hat{\phi}}{\rho} \right) = 2\pi \delta^2(\boldsymbol{\rho}),$$

with $\boldsymbol{\rho} = x\hat{i} + y\hat{j}$.

Note that $\mathbf{B} = \frac{\mu_0 I}{2\pi} \left(\frac{\hat{\phi}}{\rho} \right)$ is the magnetic field of an infinitely long current (I) carrying wire located at $\boldsymbol{\rho} = 0$. This problem is equivalent of calculating curl of the magnetic field and the final result should be consistent with the Maxwell equation: $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$, where $\mathbf{J} = I\delta^2(\boldsymbol{\rho})\hat{z}$ is the current density flowing in the wire.

Evaluate the following surface integral using (i) direct integration and (ii) using the above result:

$$J = \int_S e^{-\rho} \left[\nabla \times \left(\frac{\hat{\phi}}{\rho} \right) \right] \cdot d\mathbf{a},$$

where S is a circular disk of radius R , centered at origin. Try to understand role of the auxiliary function $e^{-\rho}$ in the integrand.

[Hints: In direct integration, use $\nabla \times (f\mathbf{A}) = \nabla f \times \mathbf{A} + f\nabla \times \mathbf{A}$ and Stokes theorem.]

15. Consider the following well-defined function $f(\mathbf{r}) = \nabla^2 \delta^3(\mathbf{r})$, where the three-dimensional δ -function is represented by the Gaussian distribution as

$$\delta^3(\mathbf{r}) = \lim_{\epsilon \rightarrow 0} \frac{1}{(2\pi\epsilon^2)^{3/2}} e^{-\frac{r^2}{2\epsilon^2}}.$$

- (a) Obtain simplified expression of $f(\mathbf{r})$ by acting the Laplacian ∇^2 on $\delta^3(\mathbf{r})$.
- (b) Obtain the value of r at which $f(\mathbf{r}) = 0$. Sketch $f(r)$.
- (c) Evaluate the following integral all over the space:

$$\int_V f(\mathbf{r}) d^3r.$$

16. Show that

(a)

$$\nabla_{\mathbf{r}}^4 e^{-kr} = \nabla_{\mathbf{r}}^2 \nabla_{\mathbf{r}}^2 e^{-kr} = \left(-\frac{4k^3}{r} + k^4 \right) + 8\pi k \delta^3(\mathbf{r}).$$

(b)

$$[\nabla_{\mathbf{r}}^2 + k^2] \left(\frac{e^{\pm ikr}}{r} \right) = -4\pi \delta^3(\mathbf{r}).$$

(c)

$$\left[\frac{d^2}{dx^2} + k^2 \right] e^{\pm ik|x-x'|} = \pm 2ik \delta(x-x').$$

[Hints: Express $|x-x'|$ in terms of the unit step function:

$$|x-x'| = (x-x')\theta(x-x') - (x-x')\theta(x'-x).$$

(d) Sketch the following functions:

$$(i) f(x), \quad (ii) \frac{df(x)}{dx}, \quad (iii) \frac{d^2f(x)}{dx^2}$$

for two different functions: $f(x) = |x|$ and $f(x) = e^{-|x|}$. Comment on nature of the functions and their derivatives at $x = 0$.