

VANDERBILT UNIVERSITY

MATH 3120 – INTRO DO PDES

Practice problems on the Schrödinger equation

Question 1. In this question you will derive the Laplacian in spherical coordinates (see class notes). Recall that spherical coordinates are given by

$$x = r \sin \phi \cos \theta,$$

$$y = r \sin \phi \sin \theta,$$

$$z = r \cos \phi,$$

and

$$r^2 = x^2 + y^2 + z^2,$$

$$\sin \phi = \frac{x^2 + y^2}{r},$$

$$\tan \theta = \frac{y}{x}.$$

(a) Show that

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin \phi \cos \theta,$$

and find similar expressions for $\frac{\partial r}{\partial y}$ and $\frac{\partial r}{\partial z}$.

(b) Show that

$$\frac{\partial \phi}{\partial x} = \frac{x \cos^2 \phi}{z^2 \tan \phi} = \frac{\cos \phi \cos \theta}{r},$$

and

$$\frac{\partial \theta}{\partial x} = -\frac{\sin \theta}{r \sin \phi},$$

and find similar expressions for the derivatives with respect to y and z .

(c) Use the chain rule to show that

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} \\ &= \sin \phi \cos \theta \frac{\partial}{\partial r} + \frac{\cos \phi \cos \theta}{r} \frac{\partial}{\partial \phi} - \frac{\sin \theta}{r \sin \phi} \frac{\partial}{\partial \theta}, \end{aligned}$$

and find similar expressions for $\frac{\partial}{\partial y}$ and $\frac{\partial}{\partial z}$.

(d) Use the above to find $\frac{\partial^2}{\partial x^2}$, $\frac{\partial^2}{\partial y^2}$, and $\frac{\partial^2}{\partial z^2}$ in spherical coordinates, i.e., write $\frac{\partial^2}{\partial x^2}$, $\frac{\partial^2}{\partial y^2}$, and $\frac{\partial^2}{\partial z^2}$ in terms of (r, θ, ϕ) and $\frac{\partial}{\partial r}$, $\frac{\partial}{\partial \phi}$, and $\frac{\partial}{\partial \theta}$.

(e) Use the results of part (d) to write the Laplacian in spherical coordinates.

The equations mentioned in the questions below are from the notes on the Schrödinger equation posted on the course webpage.

Question 2. Explain why condition (1.3) is enough to ensure (1.2).

Question 3. Derive equations (2.8) and (2.9).

Question 4. Explain condition (2.13), and derive (2.14) and (2.15).

Question 5. Derive equation (2.18), (2.21), and (2.23).

Question 6. Show that (2.26) diverges, unless (2.27) holds.

Question 7. Explain how (2.28) is obtained.

Question 8. Derive (2.35), giving precise conditions that guarantee that the integrals at ∞ vanish as stated in the text. Compare such conditions with (1.3), and comment whether they are reasonable.

Question 9. Derive (2.40), (2.44), and (2.46).

Question 10. Explain why γ has to be a positive integer.

Question 11. In the table of section 3, where are the numerical factors, such as $\sqrt{\pi}$, coming from?