Properties of the Laplacian

Show that the Laplacian is a linear, Hermitian, operator.

To show that ∇^2 is linear, we need only recall that it is the second derivative operator. We know that differentiation is a linear operator. I.e., differentiation of a constant times a function is equal to a constant, times the value obtained by differentiating the function. Similarly, differentiation of a sum of functions is equal to summing the derivatives of the functions. Mathematically,

$$\frac{d^k}{dx^k}\text{constant} \cdot f(x) = \text{constant} \cdot \frac{d^k f}{dx^k}$$

and

$$\frac{d^k\left(f(x)+g(x)\right)}{dx^k} = \frac{d^k f(x)}{dx^k} + \frac{d^k g(x)}{dx^k}$$

So ∇^2 (corresponding to $k=2$) is linear.

One can show that ∇^2 is Hermitian using integration by parts, similar to how we did in the course notes. You can also recognize that the Hermitian property follows directly from Green's second identity . (In both cases you use the fact that the wavefunction and its derivatives vanish at the end of the interval of integration.)

However, we also know that ∇^2 is closely related to the momentum operator.

$$\hat{p}^2 = -i\hbar\nabla \cdot -i\hbar\nabla = -\hbar^2\nabla^2$$

In atomic units, then, $\nabla^2 = -\hat{p}^2$. The following math uses the fact that the momentum operator is Hermitian.

We need to show that

$$\int \Phi(x)^* \nabla^2 \Psi(x) dx = \int \left(\nabla^2 \Phi(x)\right)^* \Psi(x) dx$$

To this end, we start with the relationship between the Laplacian and the momentum operator, then (repeatedly) invoke the fact the momentum operator is Hermitian. So:

$$\begin{aligned}
\int \Phi(x)^* \nabla^2 \Psi(x) dx &= \int \Phi(x)^* \left(-\hat{p}^2\right) \Psi(x) dx \\
&= -\int \Phi(x)^* \left(\hat{p}\hat{p}\right) \Psi(x) dx \\
&= -\int \left(\hat{p}\Phi(x)\right)^* \hat{p}\Psi(x) dx \\
&= -\int \left(\hat{p}\hat{p}\Phi(x)\right)^* \Psi(x) dx \\
&= \int \left(-\hat{p}^2\Phi(x)\right)^* \Psi(x) dx \\
&= \int \left(\nabla^2\Phi(x)\right)^* \Psi(x) dx
\end{aligned}$$

Show that the Laplacian is negative definite.

One can show that ∇^2 is negative-definite using Green's first identity or integration by parts. However, as with the first part of this problem, one can also directly invoke the connection to the momentum operator, $\nabla^2 = -\hat{p}^2$. Since the square of an operator is positive definite, it's clear that the negative of the square of an operator is negative definite. However, more explicitly:

$$\begin{aligned}
\int \Psi(x)^* \nabla^2 \Psi(x) dx &= \int \Psi(x)^* \left(-\hat{p}^2\right) \Psi(x) dx \\
&= -\int \Psi(x)^* \hat{p}\hat{p}\Psi(x) dx \\
&= -\int \left(\hat{p}\Psi(x)\right)^* \hat{p}\Psi(x) dx \\
&= -\int \left|\hat{p}\Psi(x)\right|^2 dx \\
&< 0
\end{aligned}$$