Define test functions

In[151]:=
```
$Assumptions = a > 0
ψ1 = Exp[-a * r]
ψ2 = r * Exp[-a * r]
ψ3 = r/(r^2 + a^2)
ψ4 = 1/(r^2 + a^2)
```

Out[151]= $a > 0$

Out[152]= $e^{-a r}$

Out[153]= $e^{-a r}\, r$

Calculate normalization coefficient

In[154]:=
```
N1 = Integrate[4 * π * r^2 * ψ1^2, {r, 0, ∞}]
N2 = Integrate[4 * π * r^2 * ψ2^2, {r, 0, ∞}]
N3 = Integrate[4 * π * r^2 * ψ3^2, {r, 0, ∞}]
N4 = Integrate[4 * π * r^2 * ψ4^2, {r, 0, ∞}]
```

Out[154]= $\frac{\pi}{a^3}$

Out[155]= $\frac{3\pi}{a^5}$

Integrate: Integral of $4\pi r^2 \psi_3^2$ does not converge on $\{0, \infty\}$.

Integrate: Integral of $4\pi r^2 \psi_3^2$ does not converge on $\{0, \infty\}$.

Out[156]= $\int_0^\infty 4\pi r^2 \psi_3^2 \, dr$

Out[157]= $\frac{\pi^2}{a}$

Clearly the ψ_3 won't work as a test function because we can't normalize it.

Define Laplacian and Hamiltonian operators

In[158]:=
```
lap[ψ_, r_] := 1/(r^2) D[(r^2 * D[ψ, r]), r]
H[ψ_, r_] := (-h^2)/(2 μ) * lap[ψ, r] - (q^2)/(4 * π * ϵ * r) * ψ
```

Calculate Hamiltonains

In[160]:=
```
Hψ₁ = H[ψ₁, r]
Hψ₂ = H[ψ₂, r]
Hψ₄ = H[ψ₄, r]
```

Out[160]= $$-\frac{e^{-a r} q^2}{4 \pi r \epsilon}-\frac{h^2 \left(-2 a e^{-a r} r+a^2 e^{-a r} r^2\right)}{2 r^2 \mu}$$

Out[161]= $$-\frac{e^{-a r} q^2}{4 \pi \epsilon}-\frac{h^2 \left(2 r \left(e^{-a r}-a e^{-a r} r\right)+r^2 \left(-2 a e^{-a r}+a^2 e^{-a r} r\right)\right)}{2 r^2 \mu}$$

Out[162]= $$-\frac{q^2}{4 \pi r \left(a^2+r^2\right) \epsilon}-\frac{h^2 \left(\frac{8 r^4}{\left(a^2+r^2\right)^3}-\frac{6 r^2}{\left(a^2+r^2\right)^2}\right)}{2 r^2 \mu}$$

Integrate against $4\pi r^2$

In[163]:=
```
I₁ = Integrate[4 π * r ^ 2 * ψ₁ * Hψ₁ , {r, 0, ∞}]
```

Out[163]= $$\frac{2 a h^2 \pi \epsilon - q^2 \mu}{4 a^2 \epsilon \mu}$$

In[164]:=
```
I₂ = Integrate[4 π * r ^ 2 * ψ₂ * Hψ₂, {r, 0, ∞}]
```

Out[164]= $$\frac{4 a h^2 \pi \epsilon - 3 q^2 \mu}{8 a^4 \epsilon \mu}$$

In[165]:=
```
I₄ = Integrate[4 π * r ^ 2 * ψ₄ * Hψ₄, {r, 0, ∞}]
```

Out[165]= $$\frac{h^2 \pi^2 \epsilon - 2 a q^2 \mu}{4 a^3 \epsilon \mu}$$

Solve for the expectation value

In[166]:=
```
Expec₁ = I₁ / N₁
Expec₂ = I₂ / N₂
Expec₄ = I₄ / N₄
```

Out[166]= $$\frac{a \left(2 a h^2 \pi \epsilon - q^2 \mu\right)}{4 \pi \epsilon \mu}$$

Out[167]= $$\frac{a \left(4 a h^2 \pi \epsilon - 3 q^2 \mu\right)}{24 \pi \epsilon \mu}$$

Out[168]= $$\frac{h^2 \pi^2 \epsilon - 2 a q^2 \mu}{4 a^2 \pi^2 \epsilon \mu}$$