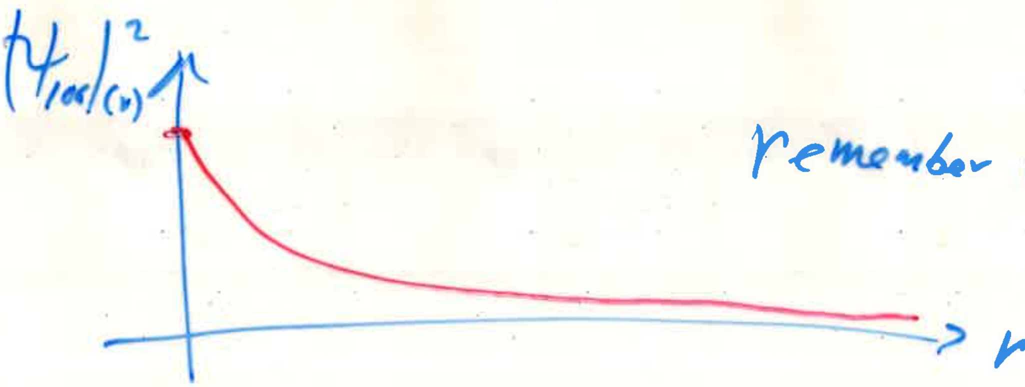
H ground state

$$n(\vec{r}) \propto |\psi_{\underset{n\ \ell\ m}{100}}(\vec{r})|^2 = \psi^*_{100}(\vec{r})\,\psi_{100}(\vec{r})$$

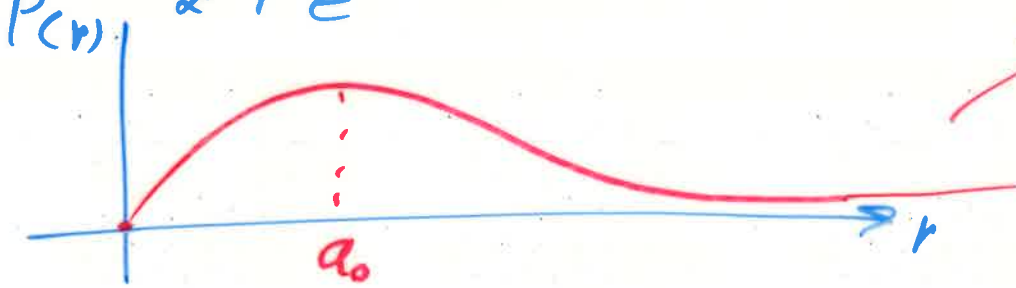
$$|\psi_{100}(\vec{r})|^2 = \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}}$$

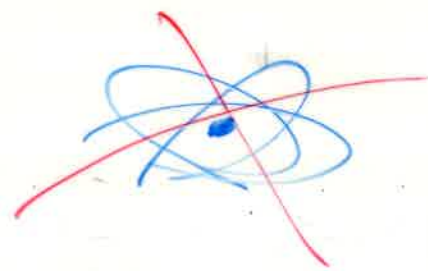
a_0 = Bohr radius



remember $dV = r^2 \sin\theta \, dr \, d\theta \, d\varphi$

$P(r) \propto r^2 e^{-2r/a_0}$





$$S_{\vec{G}} = \iiint n(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV = \frac{16}{(4+|\vec{G}|^2 a_0^2)^2}$$

$$= \int_{\varphi=0}^{2\pi} d\varphi \int_{\theta=0}^{\pi} \sin\theta \int_{r=0}^{\infty} r^2 \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}} e^{-i|\vec{G}| r \cos\theta} \, d\theta \, dr$$

Choose $\vec{G}$ along $\hat{z}$

Chapter 3

5 types of binding

- van der Waals
- ionic
- covalent
- metal
- hydrogen

usually some mixture

e.g. xtal 90% ionic
10% covalent.

Cohesive energy of xtal

energy required to pull the xtal apart into neutral atoms ∞ly far apart, $\underbrace{\text{not moving}}_{\text{no K.E.}}$, in the same electronic configuration they had in the xtal.

Call potential energy at ∞ $U=0$

$\Rightarrow$ then cohesive energy < 0.

Lattice energy for ionic xtals

- pull ions apart, not neutral atoms.

van der Waals - London binding

- neutral atoms do not feel a Coulomb force.
- atoms without a permanent electric dipole moment

should not feel a Keesom force.