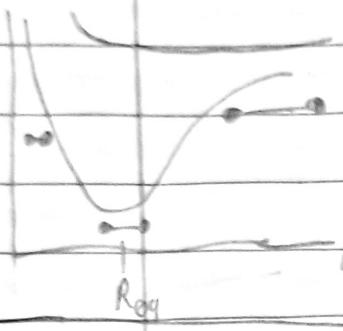
Lecture 13 review:

Schrö.

- Quantum interference: for 1 e⁻, add/subtract atomic wavefunctions ; still satisfies equation.
- Hartree: for multiple e⁻, multiply wavefunctions: $\Psi(x_1, x_2 \ldots) = \psi_1(x_1)\psi_2(x_2)\ldots$
- Fock (accounts for spin): to satisfy $P\psi$, $\Psi(x_1, x_2 \ldots) = \psi_1(x_1)\psi_2(x_2)\ldots - \psi_1(x_2)\psi_2(x_1)\ldots$
- Determinant: $\Psi = \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) \\ \psi_2(x_1) & \psi_2(x_2) \end{vmatrix}$

- For H_2, V(R), where R is internuclear distance

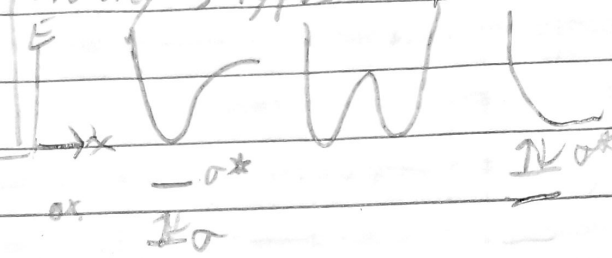


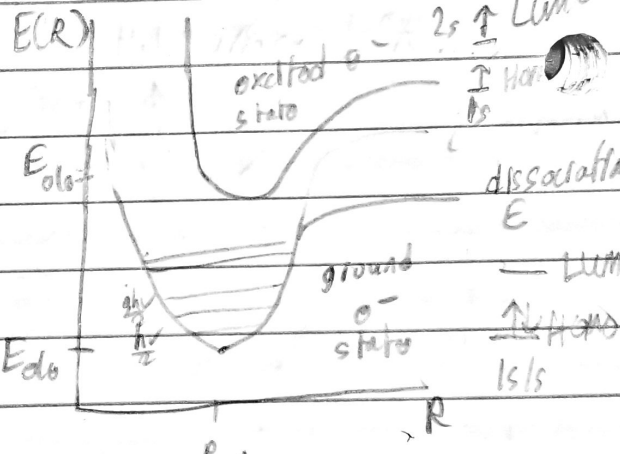
ex. IQmol

Lecture 14: Potential Surfaces & Spectroscopy

"Science Question": Can spectroscopy detect alien life?

- When doing QM calculations, there are only 3 types of potential curves.





- Excited electronic states can sometimes be stable (↓) or always dissociative (↑).
- Bottom of electronic states approximately parabola: harmonic oscillator solutions can be used. These describe nucleus motion, the vibrational energy levels. Squeezing + stretching. Access by IR.

- Molecules can also rotate. For each vibrational E level, there are multiple rotational E levels.