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Established March 2007. References: Szabo, A. and Ostlund, N. S. Modern Quantum Chemistry

Problem 3 solution - Solution set 2 Chapter 1 Szabo and ...

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The full derivation is in Szabo & Ostlund in sec. 3.8.7. This problem is long and may be submitted the week after. Parts 1, 2 and 3 are due next week. Part 4 may be submitted the week after. I'd rather you solved this properly rather than in a hurry. Reading assignment for this week and the next: Chapter 5 in Molecular Electronic Structure Theory.

Modern Quantum Chemistry: Introduction to Advanced ...

Szabo & Ostlund Chapter 2, pages 39-97 Lecture notes: Limitations of the MO model The homework is officially due Wednesday, April 6, but you have an extension till Monday April 18. This due date is strict as I have to grade the homeworks. We will put electronic structure theory into perspective and define the general problem that has to be solved.

Modern Quantum Chemistry

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Exercise. This is the solution to exercise 1.13 in the book. Solution. If we consider matrix $U = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$ such that $U^\dagger A U = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$. then we get $\theta = \frac{1}{2} \arctan \frac{2b}{a-c}$, or $2\theta = \arctan \frac{2b}{a-c}$, hence $\theta = \frac{1}{2} \arctan \frac{2b}{a-c}$. Therefore

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