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The solution to the secular problem, or more conveniently the diagonalization of the Hamiltonian matrix, defines the full configuration interaction or Full CI solution.

Problem set 2: Szabo and Ostlund: Chapter II (up to page

Solution set 2: Chapter 1: Szabo and Ostlund I will be brief in my solution set. I expect your home works to be more complete than my solution set! S&O 1.1: a. $i j j i k i k j j i k j j i k i j j j O e e O e O e e O e e O O O \hat{I} = \hat{a} \dots = \hat{a} \dots = \hat{a} \dots = \hat{a} \dots \hat{a} \dots \hat{a} \dots \hat{a} \dots r r r r r r r r b.$

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Over 150 exercises, designed to help the reader acquire a working knowledge of the material, are embedded in the text. The book is largely self-contained and requires no prerequisite other than a solid undergraduate physical chemistry course; however, some exposure to quantum chemistry will enhance the student's appreciation of the material.

Modern Quantum Chemistry: Introduction to Advanced

3. The attempt at a solution I've solved the unnormalized function into: $\Phi_{1sCGF} = 0.3696 * \exp(-0.4166*r^2)$ I'm a little bit confused which overlap integral has to be used in the Appendix A. There is a 2-center overlap integral mentioned, but I don't get the hang of it. Actually I don't even understand how Gaussian functions are contracted.

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