Atomic and molecular physics

second written exam

December 11, 2019

1. (30 pts) Separate the covalent and ionic part of the two electron improved valence bond wave function of hydrogen molecule ground state

$$\tilde{\Phi}_{VB}(1,2) = \tilde{\varphi}_a(1) \cdot \tilde{\varphi}_b(2) + \tilde{\varphi}_b(1) \cdot \tilde{\varphi}_a(2)$$

where the one electron orbitals are $\tilde{\varphi}_a = \varphi_a + d \cdot \varphi_b$ and $\tilde{\varphi}_b = \varphi_b + d \cdot \varphi_a$ with variational parameter d. φ_a is centered on nucleus a (likewise with b). (The spin part has been omitted.) What is the percentage of the covalent and ionic components?

2. (35 pts) Derive the construction of sp^2 hybrid orbital wave functions that are symmetry equivalent in trigonal symmetry (C_3). Hint: use the orthonormality requirement (and the symmetry) for the hybrid orbitals.

3. (35 pts) Carry out the symmetry analysis of the vibrational modes of ammonia molecule (NH_3). The character table of C_{3v} point group is:

C_{3v}	E	$2C_3$	$3\sigma_v$	
A_1	1	1	1	z
A_2	1	1	-1	R_z
E	2	-1	0	(x,y) (R_x, R_y)