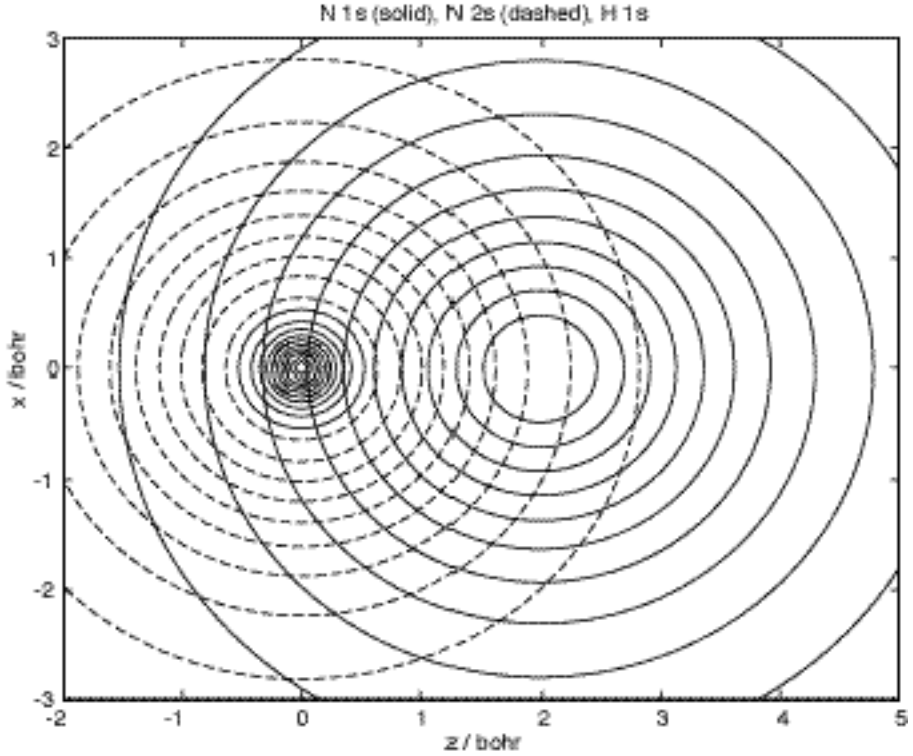
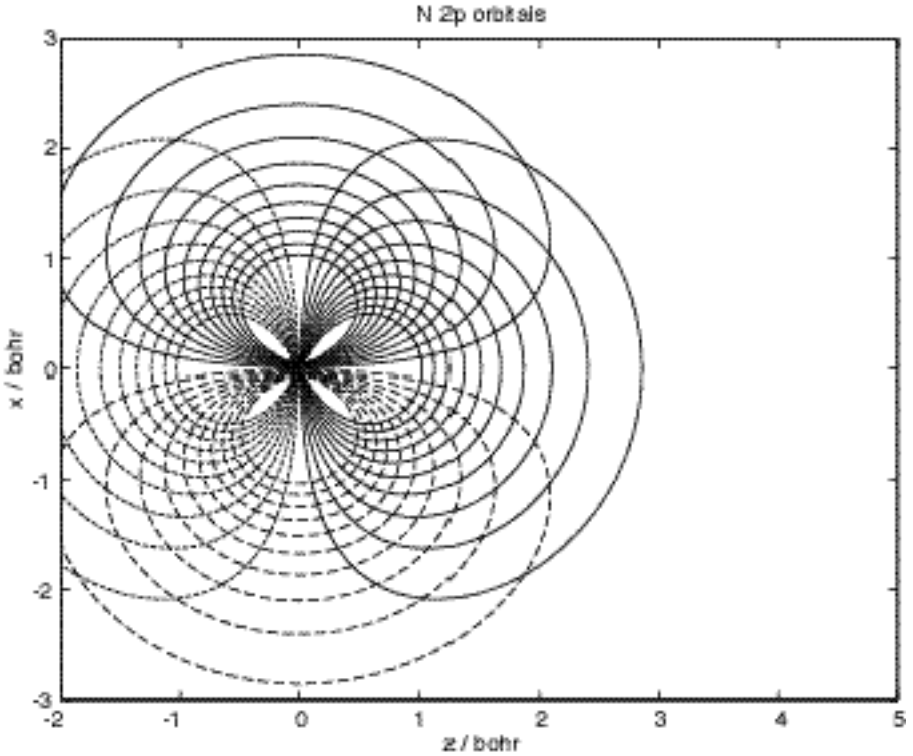
Here are contour plots of N and H sigma orbitals (1*s*, 2*s*, $2p_z$ on N and 1*s* on H). The NH distance is 1.05 Å (1.98 bohr), close to the r_e in the ground $^3\Sigma^-$ state.



And of the π non-bonding orbitals (the $2p_x$ and $2p_y$ on N)

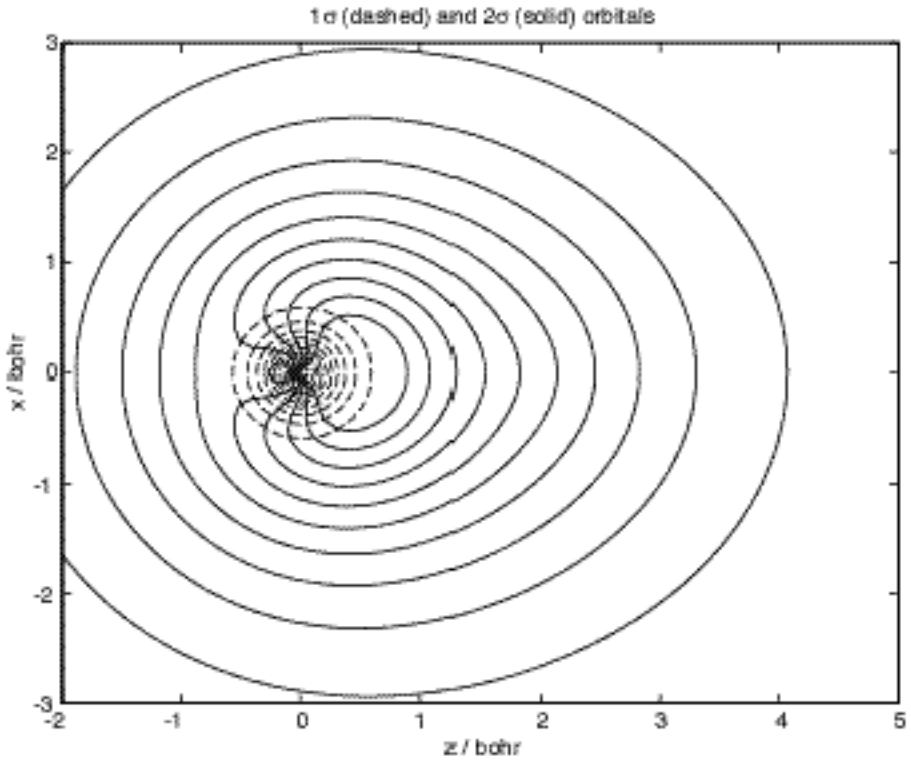


The NH σ molecular orbitals in the $^3\Sigma^-$ state are linear combinations of these atomic orbitals

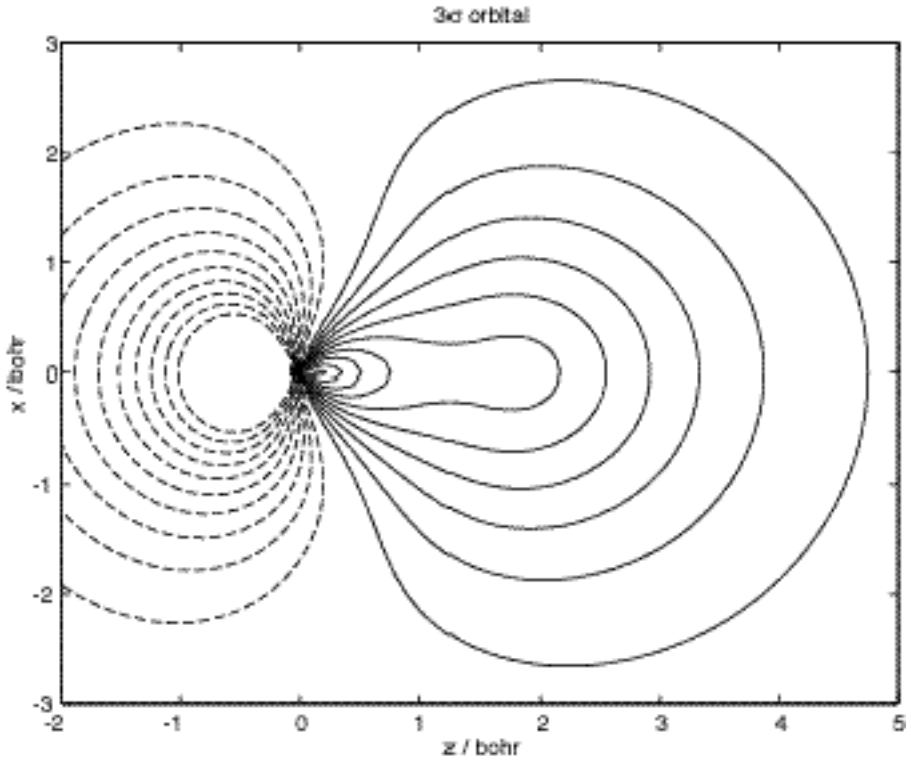
MO	$1s_N$	$2s_N$	$2p_z$	$1s_H$
1σ	0.99133	0.045212	0.007862	–0.01686
2σ	–0.21017	0.83545	0.16467	0.23935
3σ	0.10336	–0.58975	0.66431	0.49299
4σ	0.089038	–0.75158	–0.94876	1.2744

Note, that the H 1*s* orbital makes a contribution to both the 2σ and 3σ bonding orbitals. Nevertheless, overall one can say the the 2σ orbital is primarily the N 2*s* orbital while the 3σ orbital is a linear combination of the 2*s* and 2*p* orbitals on N and the 1*s* orbital on H. The single NH π orbital is identical to the N 2*p* orbital.

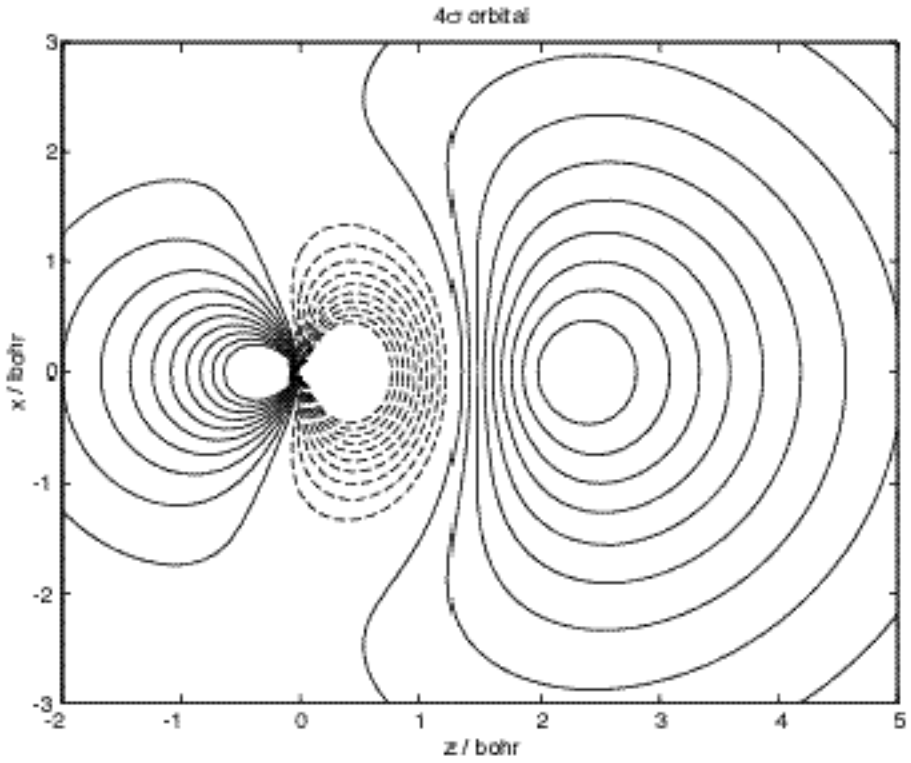
Here is a contour plot of the 1σ and 2σ orbitals



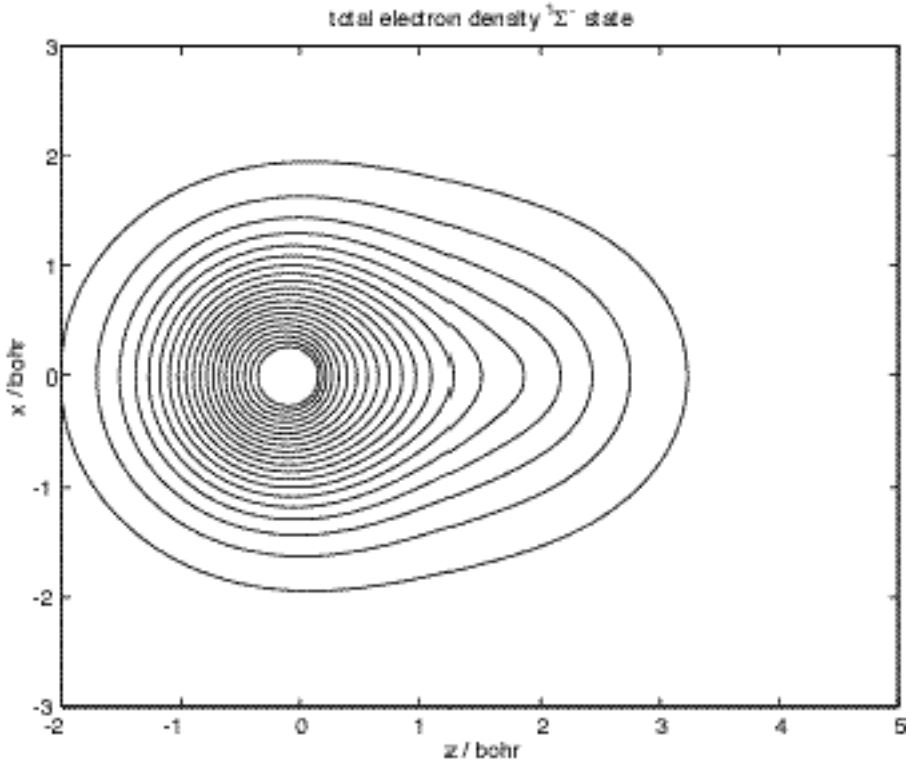
Here is the 3σ orbital



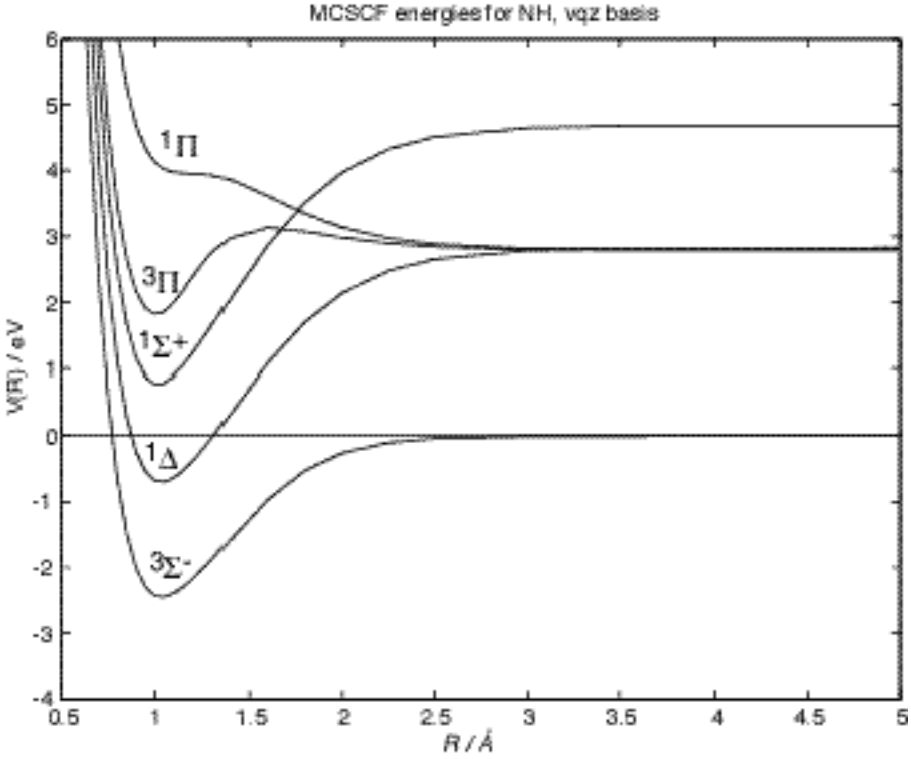
and the anti-bonding (you can see the node between the atoms) 4σ orbital



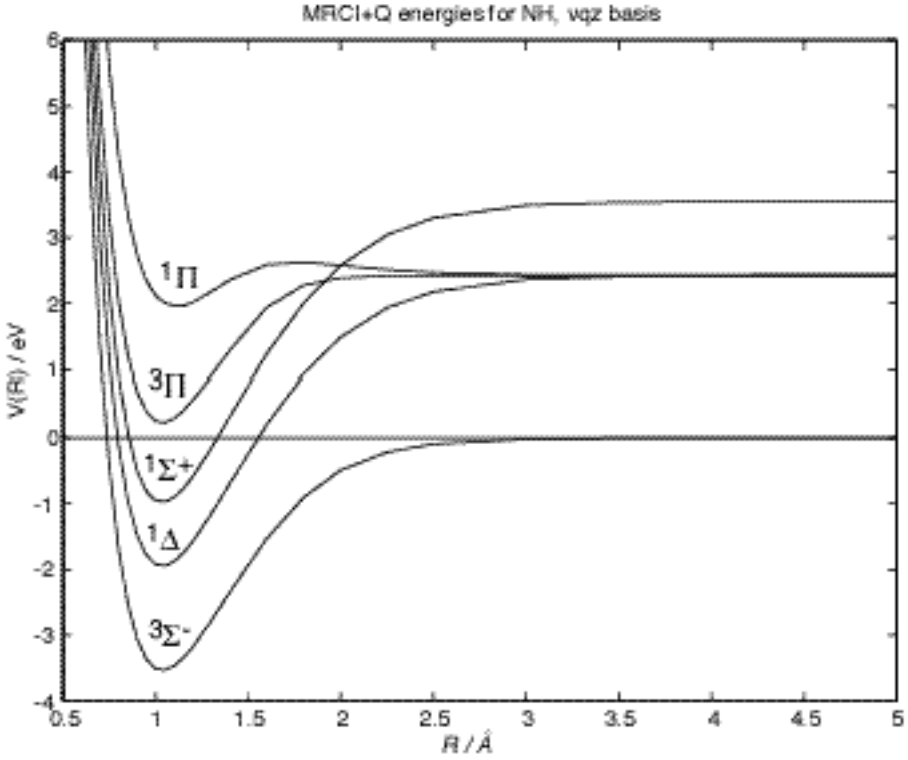
Here is the total electron density (the one-particle density matrix) for NH in the $^3\Sigma^-$ state



Here, now, is a plot of the multi-configuration SCF energies for the lowest states of NH



The $^3\Sigma^-$, $^1\Delta$, and $^1\Sigma^+$ states all correspond to the $1\sigma^2 2\sigma^2 3\sigma^2 1\pi^2$ electronic configuration, while the $^{1,3}\Pi$ states correspond to $1\sigma^2 2\sigma^2 3\sigma^1 1\pi^3$. When configuration interaction is included, to account for dynamic electron correlation, the potential curves are all lowered, as shown in the next figure. Note that the curves go, asymptotically, to the expected atomic limits [N(^{4}S, ^{2}D, ^{2}P)+H].



The calculated spectroscopic properties of the individual states are shown in the next table. This is pretty good agreement!

State	D_o(eV)		T_e (cm^{-1})		r_e (Å)	
	MRCI+Q	exp	MRCI+Q	exp	MRCI+Q	exp
$^3\Sigma^-$	3.33	3.40			1.0318	1.0362
$^1\Delta$			12741	(12566)	1.0353	1.034
$^1\Sigma^+$			20587	21202	1.0342	1.036
$^3\Pi$			30290	29807	1.0359	1.0369
$^1\Pi$			44811	(43744)	1.0079	1.110

Values in parentheses are known with less certainty.