3.3 Hybridization

A closer look at Eq. (3.8) displays one possibility to find a stable state (in time) which is a mixture of several Eigenvectors. Combine several Eigenvectors which belong to the same energy state. In this case we find:

$$\psi\left(t,\vec{r}_i\right)=\sum_j f_{m,j}e^{\frac{iE_m t}{\hbar}}=e^{\frac{iE_m t}{\hbar}}\sum_j f_{m,j} \quad . \tag{3.12}$$

For this mixed state we just see a phase shift as a function of time which is not important for a measurement.

Energy degenerate Eigenfunctions can be mixed!

Very important example: The sp^3 Hybridization

The ground state of the Carbon atom is $1s^2\ 2s^2\ 2p^2$. Combining several or many C-atoms in a solid or a molecule the Hamiltonian of the system changes. As a first consequence we find an excited "ground state" for all C-atoms which is $1s^2\ 2s^{1*}\ 2p^3$. The excited 2s levels and the 2p-levels show the same energy; in consequence each mixture of these four electronic states is stable in time.

For example

$$\begin{aligned}
\psi_1&=\frac{1}{2}\left(\varphi_s+\varphi_{p_x}+\varphi_{p_y}+\varphi_{p_z}\right)\\
\psi_2&=\frac{1}{2}\left(\varphi_s+\varphi_{p_x}-\varphi_{p_y}-\varphi_{p_z}\right)\\
\psi_3&=\frac{1}{2}\left(\varphi_s-\varphi_{p_x}+\varphi_{p_y}-\varphi_{p_z}\right)\\
\psi_4&=\frac{1}{2}\left(\varphi_s-\varphi_{p_x}-\varphi_{p_y}+\varphi_{p_z}\right)
\end{aligned} \tag{3.13}$$

These are the four Tetrahedral-like orbitals of a C- respectively Si-atom.
Which excited state really is found and which mixture of Eigenfunctions is most stable depends on the complete Hamiltonian and is sometimes quite hard to calculate. The energy degenerate states of the excited C atom and the great variety of arrangements of bounded states is the reason for the great variety of organic matter and its stability.
The chemical expressions "Isomery"-and "Mesomery"-stabilized take account for the fact that a system of several symmetric combinations of states almost always will lead to a low energy and thus very stable molecule. The excited "ground state" of the C atom occurs when it is surrounded by other atoms. In this case the sp, sp^2, or sp^3 hybridization of the Carbon atom allow for a large variety of bonds. For some illustrative information you may check the MaWi I script as well.