THE ADIABATIC APPROXIMATION

Many of the quantum mechanical calculations which have been made with hyperspherical coordinates have made use of an approximation which was first introduced by J. Macek (1968). This approximation (which is sometimes called the adiabatic approximation) is closely analogous to the Born-Oppenheimer approximation. (An excellent discussion of the Born-Oppenheimer approximation has been given by C.J. Ballhausen and Aage E. Hansen, Annual Rev. Phys. Chem. 23, 15-38, (1972)).

In Macek's method, one solves the Schrödinger equation involving the hyperangles for various fixed values of the hyperradius. The resulting energies as a function of the hyperradius are then used as an effective potential for the radial part of the Schrödinger equation. This procedure is closely analogous to the Born-Oppenheimer approximation, in which one solves the electronic Schrödinger equation for various fixed nuclear positions, thus obtaining an effective potential for the nuclear motion.

As an illustration of the adiabatic approximation, let us consider a system of N particles interacting through Coulomb forces. The Schrödinger equation for such a system can be written in the form shown in equation (5-41):

\[ (-\frac{1}{2} \Delta - \frac{Z(\Omega)}{r})\psi = E\psi \]  

(11-1)

Here \( \Delta \) is the generalized Laplacian operator.
\[ \Delta = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2} \]  \hspace{1cm} (11-2) \\

in a d-dimensional space, where \( d = 3N \).

In the adiabatic approximation, one tries to construct a solution of the form:

\[ \psi = r^{\frac{d}{2}(1-d)} \sum_{\tau} R_\tau (r) \phi_\tau (r, \Omega) \]  \hspace{1cm} (11-3) \\

Then, since

\[ \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} [r^{\frac{d}{2}(1-d)} R_\tau (r)] \]

\[ = r^{\frac{d}{2}(1-d)} \left[ - \frac{(d-1)(d-3)}{4r^2} + \frac{\partial^2}{\partial r^2} \right] R_\tau (r) \]  \hspace{1cm} (11-4) \\

substitution of (11-3) into (11-1) yields

\[ \sum_{\tau} \left[ \frac{\partial^2}{\partial r^2} - \Lambda^2 + \frac{(d-1)(d-3)}{4r^2} + \frac{2Z(\Omega)}{r} + 2E \right] R_\tau (r) \phi_\tau (r, \Omega) = 0 \]  \hspace{1cm} (11-5) \\

Let us now suppose that we have found a set of functions \( \phi_\tau (r, \Omega) \) which are solutions to the angular part of the Schrödinger equation at various fixed values of the hyperradius. In other words, the set of functions satisfies the equations