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Triatomic Vibrational Energies

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The generator coordinate approximation theory is formally applied to H_3^+. A "secular equation" with an eigenvector of three dimensions and "matrix" elements of six dimensions results. Numerical solutions of this equation are the vibrational energy levels of H_3^+.

1. INTRODUCTION

The generator coordinate approximation (GCA) is an approximation proposed to solve collective system problems, such as many-body nuclei and molecules. It stands as an approximation much as the Born–Oppenheimer approximation (Gasiorowicz, 1974) and the adiabatic approximation (Kolos, 1970). It was first proposed by Hill and Wheeler (1953). Griffin and Wheeler (1957) simplified and further developed it. Substantial further work has been done on it (Lathouwers and Van Leuven (1982). More specifically, the GCA was applied to calculate numerically the vibration-rotation energy levels of H_2^+ (Deumens *et al.*, 1986). Other aspects of the application of the GCA to H_2^+ have been treated (Lathouwers *et al.*, 1987; Broeckhove *et al.*, 1990, 1995). It is natural therefore to extend and apply the GCA to triatomic systems.

In this paper, we develop the formal aspects of the application of the GCA to triatomic systems. It will be seen that a "secular equation" with an eingenvector of three dimensions and a "matrix" of six dimensions results for the vibrational energy levels.

This paper is organized as follow. Section 2 summarizes the GCA theory. Section 3 outlines the application of the GCA to diatomic systems. Finally, Section 4 details the application of the GCA to triatomic systems.

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2. GENERATOR COORDINATE APPROXIMATION

The GCA (Lathouwers and Van Leuven, 1982) proposes for the wave function $\psi(x)$

$$\psi(x) = \int_a^b F(\alpha)\chi(x|\alpha)\, d\alpha \tag{1}$$

where $F(\alpha)$ is a "continuous superposition index" called the weight function, $\chi(x|\alpha)$ is a basis called the intrinsic state, and α is a parameter called the generator coordinate. We then form the variational energy,

$$E[F(\alpha)] = \frac{\langle\psi(x)|H|\psi(x)\rangle}{\langle\psi(x)|\psi(x)\rangle} \tag{2}$$

where H is the Hamiltonian of the system being considered. $E[F(\alpha)]$ becomes

$$E[F(\alpha)] = \frac{\int\int F^*(\alpha)H(\alpha,\beta)F(\beta)\, d\alpha\, d\beta}{\int\int F^*(\alpha)\Delta(\alpha,\beta)F(\beta)\, d\alpha\, d\beta} \tag{3}$$

where

$$H(\alpha,\beta) = \langle\chi(\alpha)|H|\chi(\beta)\rangle \tag{4}$$

$$\Delta(\alpha,\beta) = \langle\chi(\alpha)|\chi(\beta)\rangle \tag{5}$$

$H(\alpha,\beta)$ is called the Hamiltonian kernel and $\Delta(\alpha,\beta)$ the overlap kernel.

Minimizing the variational energy expression (2) with respect to $F(\alpha)$, one obtains the Wheeler equation,

$$\int_a^b [H(\alpha,\beta) - E\Delta(\alpha,\beta)]F(\beta)\, d\beta = 0 \tag{6}$$

Solution of the Wheeler equation then gives the upper bound energy levels of the system.

3. DIATOMIC SYSTEMS

The Hamiltonian of the diatomic system is (Deumens *et al.*, 1986)

$$H = -\frac{1}{2\mu}\Delta_{\vec{R}} - \frac{1}{2m}\sum_i \Delta_{\vec{r}_i} - \frac{1}{2M}\left(\sum_i \vec{\nabla}_{\vec{R}i}\right)^2 + \frac{Z_1Z_2}{R} - \sum_i \frac{Z_1}{|\vec{r}_i - \vec{R}_1|} - \sum_i \frac{Z_2}{|\vec{r}_i - \vec{R}_2|} + \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \tag{7}$$

where Z_1 and M_1 are the charge and mass of one nucleus, Z_2 and M_2 are the

charge and mass of the second nucleus, m is the mass of the electron, $\bar{R}_1$ and $\bar{R}_2$ are the position vectors of the two nuclei, r_i are the position vectors of the electrons, μ is the reduced mass,

$$\mu = \frac{M_1 M_2}{M} \tag{8}$$

$$M = M_1 + M_2 \tag{9}$$

$$\bar{R} = \bar{R}_2 - \bar{R}_1 \tag{10}$$

and the origin of the reference frame is the center of mass of the nuclei. We can separate the Hamiltonian into an electronic Hamiltonian and a nuclear kinetic energy part,

$$H(r, \bar{R}) = -\frac{1}{2\mu} \Delta_{\bar{R}} + H_e(r, \bar{R}) \tag{11}$$

The solution for the electronic Hamiltonian $H_e(r, \bar{R})$ is

$$H_e(r|\bar{\alpha})\phi(r|\bar{\alpha}) = U(\alpha)\phi(r|\bar{\alpha}) \tag{12}$$

where $\bar{\alpha}$ is chosen to be the equilibrium $\bar{R}$ parameter. $U(\alpha)$ is the effective potential energy curve.

For the intrinsic state $\chi(r, \bar{R}|\bar{\alpha})$ we can form the product

$$\chi(r, \bar{R}|\bar{\alpha}) = \phi(r, \bar{\alpha})\Phi\left(\frac{|\bar{R} - \bar{\alpha}|}{W}\right)^5 \tag{13}$$

where $\Phi(|\bar{R} - \bar{\alpha}|/W)$ is a nuclear wave function and W is the width of the nuclear wave function. Demanding the limit

$$\lim_{W \to 0} \Phi\left(\frac{|\bar{R} - \bar{\alpha}}{W}\right) = \delta(\bar{R} - \bar{\alpha}) \tag{14}$$

we have the adiabatic approximation wave function,

$$\begin{aligned} \psi(r, \bar{R}) &= \int F(\bar{\alpha})\phi(r|\bar{\alpha})\delta(\bar{R} - \bar{\alpha})\, d\bar{\alpha} \\ &= F(\bar{R})\phi(r|\bar{R}) \end{aligned} \tag{15}$$

$\chi(r, \bar{R}|\bar{\alpha})$ thus formed, we have for the GCA wave function

$$\psi(r, \bar{R}|W) = \int F(\bar{\alpha}|W)\phi(\bar{r}|\bar{\alpha})\Phi(\bar{R}|\bar{\alpha}, W)d\bar{\alpha} \tag{16}$$

and for the Wheeler equation,

$$\int [H(\bar{\alpha},\bar{\beta}|W) - E(W)\Delta(\bar{\alpha}, \bar{\beta}|W)]F(\bar{\beta}|W)\, d\bar{\beta} = 0 \tag{17}$$

where

$$H(\bar{\alpha}, \bar{\beta}|W) = \langle\chi(\bar{\alpha}, W)|H|\chi(\bar{\beta}, W)\rangle \tag{18}$$

$$\Delta(\bar{\alpha}, \bar{\beta}|W) = \langle\chi(\bar{\alpha}, W)|\chi(\bar{\beta}, W)\rangle \tag{19}$$

Expanding now the weight function in terms of Wigner functions (Deumens *et al.*, 1986; Thompson, 1994)

$$F(\bar{\alpha}|W) = \sum_{JM} e^{iM\phi_\alpha} d^J_{MK}(\theta_\alpha) e^{iK\gamma_\alpha} f^J_{MK}(\alpha|W) \tag{20}$$

we have for the GCA wave function

$$\psi_{JM}(r, \bar{R}|W) = \int f^J_{MK}(\alpha|W) e^{iM\phi_\alpha}\, d^J_{MK}(\theta_\alpha) e^{iK\gamma_\alpha} \times \phi_K(r|\bar{\alpha})\Phi(\bar{R}|\bar{\alpha}, W)\, d\bar{\alpha} \tag{21}$$

The most general wave function will be

$$\psi(r, \bar{R}|W) = \sum_{JM} \psi_{JM}(r, \bar{R}|W) \tag{22}$$

Furthermore, using unitary rotation operators (Lathouwers and Van Leuven, 1982), we can write the GCA wave function in terms of angular momentum projection operators.

$$\psi_{JM}(r, \bar{R}|W) = \int f^J_{MK}(\alpha|W) e^{iM\phi_\alpha}\, d^J_{MK}(\theta_\alpha) e^{iK\gamma_\alpha} \times \mathcal{R}_e(\phi_\alpha, \theta_\alpha, \gamma_\alpha)\phi_K(r|\alpha\hat{e_z})\mathcal{R}_n(\phi_\alpha, \theta_\alpha, \gamma_\alpha) \times \Phi(\bar{R}|\alpha\hat{e_z}, W)\alpha^2\, d\alpha\, d\phi_\alpha \sin\theta_\alpha\, d\theta_\alpha\, d\gamma_\alpha \tag{23}$$

$$= \int_0^\infty f^J_{MK}(\alpha|W) P^J_{MK}\, \chi_K(r, \bar{R}|\alpha\hat{e_z}, W)\alpha^2\, d\alpha \tag{24}$$

Here

$$P^J_{MK} = \frac{2J+1}{8\pi^2} \int d\Omega\, D^{J*}_{MK}(\Omega) R(\Omega) \tag{25}$$

is the angular momentum projection operator; in addition,

$$D^J_{MK}(\Omega) \equiv e^{-iM\phi_\alpha} d^J_{MK}(\theta_\alpha) e^{-iK\gamma_\alpha} \tag{26}$$

are the Wigner functions,

$$\begin{aligned} R(\Omega) &= R_e(\Omega)\, R_n(\Omega) \\ R_e(\Omega) &\equiv e^{-i\phi_\alpha J_z}\, e^{-i\theta_\alpha J_y} e^{-i\gamma_\alpha J_z} \\ R_n(\Omega) &\equiv e^{-i\phi_\alpha J_z} e^{-i\theta_\alpha J_y}\, e^{-i\gamma_\alpha J_z} \end{aligned} \tag{27}$$

are the unitary rotation operators, where $R_e(\Omega)$ is the unitary rotation operator for the electron wave function and $R_n(\Omega)$ is the unitary rotation operator for the nuclear wave function, and

$$\Omega \equiv (\phi_\alpha, \theta_\alpha, \gamma_\alpha) \tag{28}$$

$$d\Omega \equiv \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\gamma \tag{29}$$

are the Euler angles.

Applying the variational principle again to the variational energy (2) using (23), we have the Wheeler equation,

$$\int_0^{\infty} [H^J_{KK}(\alpha, \beta|W) - E^J_K(W)\Delta^J_{KK}(\alpha, \beta|W)]\, f^J_K(\beta|W)\beta^2\, d\beta = 0 \tag{30}$$

where

$$H^J_{KK}(\alpha, \beta|W) = \langle \chi_K(\alpha\hat{e_z}, W)|HP^J_{KK}|\chi_K(\beta\hat{e_z}, W)\rangle \tag{31}$$

$$\Delta^J_{KK}(\alpha, \beta|W) = \langle \chi_K(\alpha\hat{e_z}, W)|P^J_{KK}|\chi_K(\beta\hat{e_z}, W)\rangle \tag{32}$$

are the angular momentum projected kernels.

Expanding now the $f^J(\alpha|W)$ in an oscillator basis $\{f_n\}$,

$$f^J(\alpha|W) = \sum_n d^J_n(W) f_n(\alpha) \tag{33}$$

we find that the Wheeler equation (30) reduces to the algebraic equation (Deumens *et al.*, 1986; Deumens and Lathouwers, 1983)

$$\sum_n [H^J_{mn}(W) - E\Delta^J_{mn}(W)]\, d^J_n(W) = 0 \tag{34}$$

where

$$H^J_{mn} = \int f_m(\alpha) H^J(\alpha, \beta|W) f_n(\beta)\, d\alpha\, d\beta \tag{35}$$

and

$$\Delta^J_{mn}(W) = \int f_m(\alpha)\Delta^J(\alpha, \beta|W) f_n(\beta)\, d\alpha\, d\beta \tag{36}$$

The solutions of equation (34) give the vibrational energy levels for a given total angular momentum J.

4. TRIATOMIC SYSTEMS

We treat the simplest triatomic system, H_3^+. Generalization to unequal-mass nuclei is easily done. For this system we demand first that (Lathouwers and Van Leuven, 1982)

$$\bar{\alpha}_{10} + \bar{\alpha}_{20} + \bar{\alpha}_{30} = 0 \tag{37}$$

where the subscript denotes the chosen reference frame. This will insure that the translational energy of the center of mass of H_3^+ will not be taken into account.

We next demand that (Lathouwers and Van Leuven, 1982; Wigner, 1959)

$$\begin{aligned} \bar{\alpha}_{10} &= \alpha_{10}\hat{e}_z \\ \bar{\alpha}_{20} &= \alpha_{20x}\hat{e}_z + \alpha_{20z}\hat{e}_z \end{aligned} \tag{38}$$

This will insure that we do not take into account different systems that differ only by a rotation of the H_3^+ system as a whole.

Then,

$$\begin{aligned} \alpha_{20x} + \alpha_{30x} &= 0 \\ \alpha_{30y} &= 0 \\ \alpha_{10} + \alpha_{20z} + \alpha_{30z} &= 0 \end{aligned} \tag{39}$$

We relabel,

$$\begin{aligned} \alpha_{10} &= \mu_1 \\ \alpha_{20x} &= \mu_2 \\ \alpha_{20z} &= \mu_3 \end{aligned} \tag{40}$$

Now, the GCA wave function becomes,

$$\begin{aligned} \psi(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|W) = \int & F(\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3|W)\phi(\bar{r}_1, \bar{r}_2|\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3) \\ & \times \Phi(\bar{R}_1, \bar{R}_2, \bar{R}_3|\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, W)\, d\bar{\alpha}_1\, d\bar{\alpha}_2\, d\bar{\alpha}_3 \end{aligned} \tag{41}$$

where $\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3$ denote the reference frame $\bar{\alpha}_{10}, \bar{\alpha}_{20}, \bar{\alpha}_{30}$ rotated through the Euler angles $\Omega \equiv (\phi, \theta, \gamma)$. Since there are only three internal generator coordinates μ_1, μ_2, μ_3, we expand (Lathouwers and Van Leuven, 1982)

$$F^{JM} = \sum_{\bar{J}\bar{M}} f^J_{MK}(\mu_1, \mu_2, \mu_3|W) D^{J*}_{MK}(\Omega) \tag{42}$$

The GCA wave function becomes

$$\begin{aligned}
&\psi(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|W) \\
&\quad = \sum_{\bar{J}\bar{M}} \int f^J_{MK}(\mu_1, \mu_2, \mu_3|W) e^{iM\phi} d^J_{MK}(\theta) e^{iK\gamma} \\
&\quad \times \phi(\bar{r}_1, \bar{r}_2|\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3) \Phi(\bar{R}_1, \bar{R}_2, \bar{R}_3|\bar{\alpha}_1, \bar{\alpha}_2, \bar{\alpha}_3, W)\, d\mu_1\, d\mu_2\, d\mu_3\, d\Omega \\
&= \sum_{\bar{J}\bar{M}} \int f^J_{MK}(\mu_1, \mu_2, \mu_3|W) e^{iM\phi} d^J_{MK}(\theta) e^{iK\gamma} \\
&\quad \times \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\mu_1, \mu_2, \mu_3, \Omega, W)\, d\mu_1\, d\mu_2\, d\mu_3\, d\Omega \\
&= \sum_{\bar{J}\bar{M}} \int f^J_{MK}(\mu_1, \mu_2, \mu_3|W) P^J_{MK} \\
&\quad \times \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\mu_1, \mu_2, \mu_3, 0, W)\, d\mu_1\, d\mu_2\, d\mu_3
\end{aligned} \tag{43}$$

The Wheeler equation is then

$$\begin{aligned}
\int_0^\infty \int_0^\infty \int_0^\infty & [H^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\
& - E^J_{MK}(W) \Delta^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\
& \times f^J_{MK}(\nu_1, \nu_2, \nu_3|W)\, d\nu_1\, d\nu_2\, d\nu_3
\end{aligned} \tag{44}$$

where

$$\begin{aligned}
&H^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\
&\quad = \langle \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\mu_1, \mu_2, \mu_3, 0, W)|HP^J_{MK}| \\
&\times \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\nu_1, \nu_2, \nu_3, 0, W)\rangle
\end{aligned} \tag{45}$$

and

$$\begin{aligned}
&\Delta^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\
&\quad = \langle \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\mu_1, \mu_2, \mu_3, 0, W)|P^J_{MK}| \\
&\times \chi^J_{MK}(\bar{r}_1, \bar{r}_2, \bar{R}_1, \bar{R}_2, \bar{R}_3|\nu_1, \nu_2, \nu_3, 0, W)\rangle
\end{aligned} \tag{46}$$

We now expand $f^J_{MK}(\nu_1, \nu_2, \nu_3|W)$ in oscillator bases,

$$\begin{aligned} f^J_{MK}(\nu_1, \nu_2, \nu_3|W) &= \sum_i A^J_i(\nu_2, \nu_3, W) f_i(\nu_i) \\ &= \sum_i \left(\sum_j B^J_{ij}(\nu_3, W) f_j(\nu_2) \right) f_i(\nu_1) \\ &= \sum_i \sum_j B^J_{ij}(\nu_3, W) f_j(\nu_2) f_i(\nu_1) \\ &= \sum_i \sum_j \left(\sum_k C^J_{ijk}(W) f_k(\nu_3) \right) f_j(\nu_2) f_i(\nu_1) \\ &= \sum_i \sum_j \sum_k C^J_{ijk}(W) f_k(\nu_3) f_j(\nu_2) f_i(\nu_1) \end{aligned} \tag{47}$$

The Wheeler equation becomes

$$\begin{aligned} &\int_0^\infty \int_0^\infty \int_0^\infty [H^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\ &\quad - E^J_{MK}(W) \Delta^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W)] \\ &\quad \times \left[\sum_i \sum_j \sum_k C^J_{ijk}(W) f_k(\nu_3) f_j(\nu_2) f_i(\nu_1) \right] d\nu_1\, d\nu_2\, d\nu_3 \end{aligned} \tag{48}$$

Integrating with $f_l(\mu_3) f_m(\mu_2) f_n(\mu_1)$, we have

$$\begin{aligned} &\int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty f_l(\mu_3) f_m(\mu_2) f_n(\mu_1) \\ &\quad \times [H^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W) \\ &\quad - E^J_{MK}(W) \Delta^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3|W)] \\ &\quad \times \left[\sum_i \sum_j \sum_k C^J_{ijk}(W) f_k(\nu_3) f_j(\nu_2) f_i(\nu_1) \right] \\ &\quad \times d\nu_1\, d\nu_2\, d\nu_3\, d\mu_1\, d\mu_2\, d\mu_3 = 0 \end{aligned} \tag{49}$$

or

$$\sum_i \sum_j \sum_k [H^J_{lmnkji}(W) - E^J_{MK}(W) \Delta^J_{lmnkji}(W)] C^J_{ijk}(W) = 0 \tag{50}$$

where

$$H^J_{lmnkji}(W) = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty f_l(\mu_3) f_m(\mu_2) f_n(\mu_1) \times H^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3 | W) f_k(\nu_3) f_j(\nu_2) f_i(\nu_1) \times d\nu_1\, d\nu_2\, d\nu_3\, d\mu_1\, d\mu_2\, d\mu_3 \quad (51)$$

and

$$\Delta^J_{lmnkji}(W) = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty f_l(\mu_3) f_m(\mu_2) f_n(\mu_1) \times \Delta^J_{MK}(\mu_1, \mu_2, \mu_3, \nu_1, \nu_2, \nu_3 | W) f_k(\nu_3) f_j(\nu_2) f_i(\nu_1) \times d\nu_1\, d\nu_2\, d\nu_3\, d\mu_1\, d\mu_2\, d\mu_3 \quad (52)$$

We thus have a "secular equation" with a three-dimensional eigenvector $C^J_{ijk}(W)$ and six-dimensional "matrix" elements. The solutions of this "secular equation" will give vibrational energy levels for a given J and W.

5. CONCLUSION

Following the application of the generator coordinate approximation to diatomic systems to calculate the vibrational energies, we have applied the generator coordinate approximation to H_3^+ to calculate also the vibrational energies. We have presented the formal aspects of this application. It is seen that a "secular equation" with a three-dimensional eigenvector and six-dimensional "matrix" elements results.

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