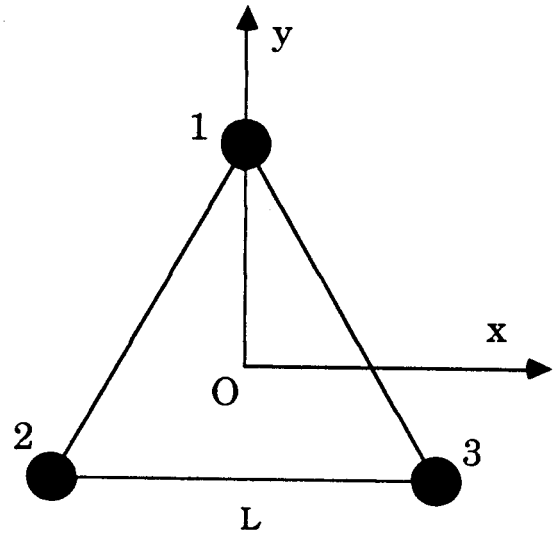
QM Spring 96 B

A molecule consists of three equal atoms which form an equilateral triangle of side L as shown. The eigenstates of an electron in this molecule can be considered as linear combinations of orthonormal basis states, ϕ_i, centered on each atom $i = 1,2,3$. In this basis the Hamiltonian has diagonal matrix elements $\langle \phi_i | H | \phi_i \rangle = \varepsilon$, and off-diagonal matrix elements between neighboring basis states i and j, $\langle \phi_i | H | \phi_j \rangle = -t$, where the energy $t > 0$.



(a) Define the operator R which operates on the basis functions as follows: $R\phi_i = \phi_{i+1}$, $i = 1,2$; $R\phi_3 = \phi_1$. Note that R has the effect of rotating the basis functions around the triangle and that $R^3 = 1$. Show that R commutes with the Hamiltonian.

(b) The eigenstates ψ_n of R with eigenvalues λ_n can be expressed as $\psi_n = \sum_{i=1}^{3} a_{ni}\, \phi_i$. Find the expansion coefficients a_{ni} and the eigenvalues λ_n. [Hint: note that $\lambda_n^3 = 1$.]

(c) Give the energy eigenvalues in terms of ε and t and give their degeneracies.

(d) Now suppose an electric field of strength F is switched on in the +x-direction. The only effect is to change the diagonal matrix elements of the Hamiltonian at each site by an amount eFx_i, where x_i is the x position of the center of atom i, and -e is the charge of the electron. Find the new energy eigenvalues to linear order in F.