RUBBER BAND HELIUM

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We've looked at the helium atom using the variational principle. Although the helium atom using the correct Coulomb potential cannot be solved exactly, a variant known as 'rubber band helium' can be. Here we use simple harmonic oscillator potentials. The hamiltonian is then:

$$H=-\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)+\frac{1}{2}m\omega^2\left(r_1^2+r_2^2\right)-\frac{\lambda}{4}m\omega^2\left|\mathbf{r}_1-\mathbf{r}_2\right|^2 \tag{1}$$

By introducing a change of variables, we can decouple the hamiltonian. Let

$$\mathbf{u}\equiv\frac{1}{\sqrt{2}}\left(\mathbf{r}_1+\mathbf{r}_2\right) \tag{2}$$

$$\mathbf{v}\equiv\frac{1}{\sqrt{2}}\left(\mathbf{r}_1-\mathbf{r}_2\right) \tag{3}$$

The gradient operators then transform as

$$\nabla_u=\frac{1}{\sqrt{2}}\left(\nabla_1+\nabla_2\right) \tag{4}$$

$$\nabla_v=\frac{1}{\sqrt{2}}\left(\nabla_1-\nabla_2\right) \tag{5}$$

$$\nabla_u^2=\frac{1}{2}\left(\nabla_1^2+\nabla_2^2+2\nabla_1\cdot\nabla_2\right) \tag{6}$$

$$\nabla_v^2=\frac{1}{2}\left(\nabla_1^2+\nabla_2^2-2\nabla_1\cdot\nabla_2\right) \tag{7}$$

$$\nabla_u^2+\nabla_v^2=\nabla_1^2+\nabla_2^2 \tag{8}$$

For the potential terms, we have

$$u^2+v^2 = \frac{1}{2}\left[r_1^2+r_2^2+2\mathbf{r}_1\cdot\mathbf{r}_2+r_1^2+r_2^2-2\mathbf{r}_1\cdot\mathbf{r}_2\right] \tag{9}$$

$$= r_1^2+r_2^2 \tag{10}$$

$$|\mathbf{r}_1-\mathbf{r}_2|^2 = r_1^2+r_2^2-2\mathbf{r}_1\cdot\mathbf{r}_2 \tag{11}$$

$$= 2v^2 \tag{12}$$

Thus the hamiltonian separates:

$$H = \left[-\frac{\hbar^2}{2m}\nabla_u^2+\frac{1}{2}m\omega^2u^2\right]+\left[-\frac{\hbar^2}{2m}\nabla_v^2+\frac{1}{2}m\omega^2(1-\lambda)v^2\right] \tag{13}$$

which is the sum of two 3-d harmonic oscillators. The exact ground state energy of this system are then just the sum of the two separate oscillator energies:

$$E_0 = \frac{3}{2}\hbar\omega+\frac{3}{2}\hbar\omega\sqrt{1-\lambda} \tag{14}$$

To test the variational principle for this potential, we can start with the (known) ground state wave function for the 3-d harmonic oscillator as the test function.

$$\psi = \left(\frac{m\omega}{\pi\hbar}\right)^{3/2}e^{-m\omega\left(r_1^2+r_2^2\right)/2\hbar} \tag{15}$$

This function is an eigenfunction of the first two terms in 1 with energy $3\hbar\omega$ so we have

$$\langle H\rangle = 3\hbar\omega+\langle V_\lambda\rangle \tag{16}$$

where

$$\langle V_\lambda\rangle = -\frac{\lambda}{4}m\omega^2\left(\frac{m\omega}{\pi\hbar}\right)^3\int e^{-m\omega\left(r_1^2+r_2^2\right)/\hbar}|\mathbf{r}_1-\mathbf{r}_2|^2\,d^3\mathbf{r}_1d^3\mathbf{r}_2 \tag{17}$$

$$= -\frac{\lambda}{4}m\omega^2\left(\frac{m\omega}{\pi\hbar}\right)^3\int e^{-m\omega\left(r_1^2+r_2^2\right)/\hbar}\left(r_1^2+r_2^2-2r_1r_2\cos\theta_2\right)d^3\mathbf{r}_1d^3\mathbf{r}_2 \tag{18}$$

The term with $\cos\theta_2$ integrates to zero when we do the θ_2 integral, so we're left with two Gaussian integrals and we get

$$\langle V_\lambda\rangle = -\frac{3}{4}\lambda\hbar\omega \tag{19}$$

Plugging this back into 16 we get

$$\langle H \rangle = 3\hbar\omega \left(1 - \frac{\lambda}{4}\right) \tag{20}$$

This is actually the Taylor expansion with respect to λ of 14 up to first order.