

## RUBBER BAND HELIUM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.17.

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:

$$(0.1) \quad H = -\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) + \frac{1}{2}m\omega^2 (r_1^2 + r_2^2) - \frac{\lambda}{4}m\omega^2 |\mathbf{r}_1 - \mathbf{r}_2|^2$$

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

$$(0.2) \quad \mathbf{u} \equiv \frac{1}{\sqrt{2}}(\mathbf{r}_1 + \mathbf{r}_2)$$

$$(0.3) \quad \mathbf{v} \equiv \frac{1}{\sqrt{2}}(\mathbf{r}_1 - \mathbf{r}_2)$$

The gradient operators then transform as

$$(0.4) \quad \nabla_u = \frac{1}{\sqrt{2}}(\nabla_1 + \nabla_2)$$

$$(0.5) \quad \nabla_v = \frac{1}{\sqrt{2}}(\nabla_1 - \nabla_2)$$

$$(0.6) \quad \nabla_u^2 = \frac{1}{2}(\nabla_1^2 + \nabla_2^2 + 2\nabla_1 \cdot \nabla_2)$$

$$(0.7) \quad \nabla_v^2 = \frac{1}{2}(\nabla_1^2 + \nabla_2^2 - 2\nabla_1 \cdot \nabla_2)$$

$$(0.8) \quad \nabla_u^2 + \nabla_v^2 = \nabla_1^2 + \nabla_2^2$$

For the potential terms, we have

$$(0.9) \quad u^2 + v^2 = \frac{1}{2} [r_1^2 + r_2^2 + 2\mathbf{r}_1 \cdot \mathbf{r}_2 + r_1^2 + r_2^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2]$$

$$(0.10) \quad = r_1^2 + r_2^2$$

$$(0.11) \quad |\mathbf{r}_1 - \mathbf{r}_2|^2 = r_1^2 + r_2^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2$$

$$(0.12) \quad = 2v^2$$

Thus the hamiltonian separates:

$$(0.13) \quad H = \left[ -\frac{\hbar^2}{2m} \nabla_u^2 + \frac{1}{2} m\omega^2 u^2 \right] + \left[ -\frac{\hbar^2}{2m} \nabla_v^2 + \frac{1}{2} m\omega^2 (1 - \lambda) v^2 \right]$$

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:

$$(0.14) \quad E_0 = \frac{3}{2} \hbar\omega + \frac{3}{2} \hbar\omega \sqrt{1 - \lambda}$$

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.

$$(0.15) \quad \psi = \left( \frac{m\omega}{\pi\hbar} \right)^{3/2} e^{-m\omega(r_1^2 + r_2^2)/2\hbar}$$

This function is an eigenfunction of the first two terms in 0.1 with energy  $3\hbar\omega$  so we have

$$(0.16) \quad \langle H \rangle = 3\hbar\omega + \langle V_\lambda \rangle$$

where

$$(0.17) \quad \langle V_\lambda \rangle = -\frac{\lambda}{4} m\omega^2 \left( \frac{m\omega}{\pi\hbar} \right)^3 \int e^{-m\omega(r_1^2 + r_2^2)/\hbar} |\mathbf{r}_1 - \mathbf{r}_2|^2 d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

$$(0.18) \quad = -\frac{\lambda}{4} m\omega^2 \left( \frac{m\omega}{\pi\hbar} \right)^3 \int e^{-m\omega(r_1^2 + r_2^2)/\hbar} (r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2$$

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

$$(0.19) \quad \langle V_\lambda \rangle = -\frac{3}{4} \lambda \hbar \omega$$

Plugging this back into 0.16 we get

$$(0.20) \quad \langle H \rangle = 3\hbar\omega \left( 1 - \frac{\lambda}{4} \right)$$

This is actually the Taylor expansion with respect to  $\lambda$  of 0.14 up to first order.