Physics 651: Assignment 4

(to be submitted by Thursday, October 6, 2023)

1. A triatomic molecule consists of three identical atoms of mass m, each sitting at the corner of an equilateral triangle and bonded to its two neighbours by a Hooke's law interaction. Motion of the ith atom away from its equilibrium position is characterized by x_i and y_i, which are measures of the displacement in the two orthogonal directions in the plane of the triangle. We choose to ignore any displacements out of the plane. The instantaneous positions are

$$r_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}, \quad r_2 = \begin{pmatrix} L \\ 0 \end{pmatrix} + \begin{pmatrix} x_2 \\ y_2 \end{pmatrix}, \quad r_3 = \begin{pmatrix} L/2 \\ \sqrt{3}L/2 \end{pmatrix} + \begin{pmatrix} x_3 \\ y_3 \end{pmatrix}.$$

Furthermore, we suppose that atom 1 sits in a laser trap that works to keep it pinned at the coordinate origin. Hence, the total energy

$$E_{\text{kin}} + \underbrace{E_{\text{bond}} + E_{\text{laser}}}_{E_{\text{pot}}} = \frac{m}{2}\sum_{i=1}^{3} v_i^2 + \frac{K}{2}\big[(\ell_{1,2} - L)^2 + (\ell_{2,3} - L)^2 + (\ell_{1,3} - L)^2\big] + \frac{K'}{2}|r_1|^2$$

is a sum of the kinetic energy, the elastic potential energy cost of chemical bond deformation, and the optical potential energy cost of ascending the quadratic well of the laser trap. We have made use of these definitions for the instantaneous velocity and the pairwise bond length:

$$v_i = |\dot{r}_i| = \left(\dot{r}_i^T \dot{r}_i\right)^{1/2} = (\dot{r}_i \cdot \dot{r}_i)^{1/2},$$
$$\ell_{i,j} = |r_j - r_i| = \left[(r_j - r_i)^T (r_j - r_i)\right]^{1/2}.$$

The Mathematica Notebook triatomic-molecule.nb shows how the equations of motion in the linear response regime ($x_i, y_i \ll L$) can be obtained from

$$m\ddot{x}_i = -\lim_{L\to\infty} \frac{dE_{\text{pot}}}{dx_i} \quad \text{and} \quad m\ddot{y}_i = -\lim_{L\to\infty} \frac{dE_{\text{pot}}}{dy_i}.$$

In matrix form, with the composite coordinates ordered as $(x_1, x_2, x_3, y_1, y_2, y_3)$, the equations of motion are

$$m\frac{d^2}{dt^2}\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ y_2 \\ y_3 \end{pmatrix} = -K \begin{pmatrix} 5/4 + 2\kappa & -1 & -1/4 & \cdots \\ -1 & 5/4 & -1/4 & \\ -1/4 & -1/4 & 1/2 & \\ \vdots & & & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ y_2 \\ y_3 \end{pmatrix} = -KA \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ y_2 \\ y_3 \end{pmatrix},$$

where $\kappa = K'/K$ is the relative coupling strength of the laser trap and A is the (dimensionless) dynamical matrix.

   (a) Explain how the equations of motion can be recast as an eigenvalue/vector problem in the normal modes:

$$-m\omega^2 \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_6 \end{pmatrix} = -KA \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_6 \end{pmatrix} \quad \Leftrightarrow \quad \omega^2 \xi = \frac{K}{m} A\xi.$$

   Hint: Consider $x_i(t) = \xi_i \cos\omega t$, $y_i(t) = \xi_{i+3}\cos\omega t$ as an ansatz for periodic motion.

   (b) Use Mathematica to evaluate the characteristic polynomial (with `Det` and `IdentityMatrix` or, even more simply, with the built-in `CharacteristicPolynomial` function) of the dynamical matrix A as a function of $\lambda = \omega^2$ and κ. Viewed as a series expansion around $\kappa = 0$, you should be able to express the result (via `Series`) as

$$\begin{aligned}\mathcal{P}(\lambda;\kappa) = \big|\lambda I - A(\kappa)\big| = {}& (3-2\lambda)^2(\lambda-3)\lambda^3 \\ & + 2\lambda^2(27 - 60\lambda + 40\lambda^2 - 8\lambda^3)\kappa \\ & + 8\lambda(-3 + 9\lambda - 8\lambda^2 + 2\lambda^3)\kappa^2 + O(\kappa^3),\end{aligned}$$

which captures how the roots shift as the laser is turned on.

(c) Provide a plot of the function $\mathcal{P}(\lambda;\kappa = 0)$ that highlights the roots and their multiplicity.

(d) Continuing in the no-laser-trap case ($\kappa = 0$), sketch the mode shape of the corresponding eigenvector for each of the nonzero eigenvalues you identified in part (c).

(e) Continuing in the no-laser-trap case ($\kappa = 0$), explain what the zero eigenvalues in part (d) represent and why there are exactly three.

(f) Now add the laser trap. Consider the case $K' = 100K$, in which the energetics are dominated by the beam strength of the so-called optical tweezers. Again compute the eigenvalues and eigenvectors. Explain why there are two high-frequency modes and only one zero mode.

2. The quantum Hamiltonian

$$\hat{H} = \sigma^x \otimes \sigma^z + \sigma^z \otimes \sigma^x$$

is a tensor product of Pauli matrices and describes the behaviour of two spin-half objects. Its effect is to flip each of the spins with an overall sign that depends on the sign of the other. The action of the Hamiltonian on each of the four possible spin configurations is

$$\begin{aligned}\hat{H}(|\uparrow\rangle \otimes |\uparrow\rangle) &= \hat{H}|\uparrow\uparrow\rangle = |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle,\\ \hat{H}(|\uparrow\rangle \otimes |\downarrow\rangle) &= \hat{H}|\uparrow\downarrow\rangle = -|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle,\\ \hat{H}(|\downarrow\rangle \otimes |\uparrow\rangle) &= \hat{H}|\downarrow\uparrow\rangle = |\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle,\\ \hat{H}(|\downarrow\rangle \otimes |\downarrow\rangle) &= \hat{H}|\downarrow\downarrow\rangle = -|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle.\end{aligned}$$

The corresponding matrix elements are given by the four-index object

$$H_{i,k;j,l} = \langle i,k|\hat{H}|j,l\rangle = \sigma^x_{i,j}\sigma^z_{k,l} + \sigma^z_{i,j}\sigma^x_{k,l}.$$

(a) Adopt the basis ordering convention $\{\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow\} = \{1,1;1,2;2,1;2,2\}$ for the index pairs i,k and j,l. Show that

$$H = \begin{pmatrix} H_{1,1;1,1} & H_{1,1;1,2} & H_{1,1;2,1} & H_{1,1;2,2} \\ H_{1,2;1,1} & H_{1,2;1,2} & H_{1,2;2,1} & H_{1,2;2,2} \\ H_{2,1;1,1} & H_{2,1;1,2} & H_{2,1;2,1} & H_{2,1;2,2} \\ H_{2,2;1,1} & H_{2,2;1,2} & H_{2,2;2,1} & H_{2,2;2,2} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \end{pmatrix}.$$

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Subscript[\[Sigma], x] = PauliMatrix[1]
Subscript[\[Sigma], z] = PauliMatrix[3]
H[i_, k_, j_, l_] := Subscript[\[Sigma], x][[i, j]] Subscript[\[Sigma], z][[k, l]]
   + Subscript[\[Sigma], z][[i, j]] Subscript[\[Sigma], x][[k, l]]
HH = Partition[
   Flatten[Table[H[i, j, k, l], {i, 1, 2}, {j, 1, 2}, {k, 1, 2}, {l, 1, 2}]], 4];
HH // MatrixForm
```

(b) Compute that characteristic polynomial $\mathcal{P}(\epsilon) = |H - \epsilon I|$ and find its roots.

(c) Find the four eigenvalue/eigenvector pairs $(\Psi^{(m)}, \epsilon_m)$ that satisfy the time-independent Schrödinger equation:

$$\sum_{j,l=1}^{2} H_{i,k;j,l}\Psi^{(m)}_{j,l} = \epsilon_m \Psi^{(m)}_{j,l}.$$

(d) Ensure that the $\Psi^{(m)}$ vectors are properly normalized. Show explicitly that

$$\Psi^{(m)^T}\Psi^{(n)} = \sum_{i,k=1}^{2} \Psi^{(m)}_{i,k}\Psi^{(n)}_{i,k} = \delta_{m,n},$$

$$\sum_{m=1}^{4} \Psi^{(m)^T}\epsilon_m \Psi^{(m)} = \sum_{m=1}^{4}\sum_{i,k=1}^{2} \Psi^{(m)}_{i,k}\epsilon_m \Psi^{(m)}_{i,k} = H.$$

An equivalent way to think about this is that if you concatenate vectors $\Psi^{(1)}, \ldots, \Psi^{(4)}$ to form the columns of a matrix V, then $V^{-1} = V^\dagger$ and

$$VV^\dagger = V^\dagger V = I \text{ and } VHV^\dagger = \begin{pmatrix} -2 & & & \\ & 2 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}.$$

(e) Show that the ground state

$$|\Psi^{(1)}\rangle = \frac{1}{2}\left(-|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)$$

is not an eigenstate of the magnetization

$$M = \frac{1}{2}\left(\sigma^z \otimes I + I \otimes \sigma^z\right).$$

(f) Construct the ground-state density operator $\rho = |\Psi^{(1)}\rangle\langle\Psi^{(1)}|$. Verify that the matrix representation $\rho_{i,k;j,l} = \Psi^{(1)}_{i,k}\Psi^{(1)}_{j,l}$ is hermitian and has real, non-negative eigenvalues.

(g) Prove the following two equalities:

$$\operatorname{tr}\rho M \overset{1}{=} \langle\Psi^{(1)}|M|\Psi^{(1)}\rangle \overset{2}{=} 0.$$

The first says that the expectation value of the magnetization in the ground state is a trace of the product of the density and magnetization operators. The second says that the magnetization vanishes.