WHY DO WE WANT TO DIAGONALIZE?

1) FUNCTIONAL CALCULUS. If \( p(x) = x + x^2 + x^3/4 + x^4/4! \) be a polynomial and \( A \) is a matrix, then \( p(A) = 1 + A + A^2/2! + A^3/3! + A^4/4! \) is a matrix. If \( B = S^{-1}AS \) is diagonal with diagonal entries \( \lambda_i \), then \( p(B) \) is diagonal with diagonal entries \( p(\lambda_i) \). This speeds up the calculation because matrix multiplication costs much. The matrix \( p(A) \) can be written down with three matrix multiplications, because \( p(B) \) is diagonal.

2) SOLVING LINEAR DIFFERENTIAL EQUATIONS. A differential equation \( \dot{v}(t) = Av(t) \) is solved by \( v(t) = e^{At}v(0) \), where \( e^{At} = I + A + A^2/2! + A^3/3! + \ldots \). (Differentiate this sum with respect to \( t \) to get \( Ae^{At}v(t) = Av(t) \).) If we write this in an eigenbasis of \( A \), then \( y(t) = e^{\lambda_i t}y(i) \). Linear differential equations later in this course. It is important motivation.

3) STOCHASTIC DYNAMICS (i.e. MARKOV PROCESSES). Complicated systems can be modeled by putting probabilities on each possible event and computing the probabilities that an event switches to any other event. This defines a transition matrix. Such a matrix always has an eigenvalue 1. The corresponding eigenvector is the stable probability distribution on the states. If we want to understand, how fast things settle to this equilibrium, we need to know the other eigenvalues and eigenvectors.

Molecular Vibrations. While quantum mechanics describes the motion of atoms in molecules, the vibrations can be described classically, when treating the atoms as “balls” connected with springs. Such approximations are necessary when dealing with large atoms, where quantum mechanical computations would be too costly. Examples of simple molecules are white phosphorus \( P_4 \), which has tetrahedral carbon of methane \( CH_4 \), the simplest organic compound or freon, \( C_2F_5Cl \), which is used in refrigerants. Caffeine or aspirin form more complicated molecules.

White Phosphorus Vibrations. (Differential equations appear later, the context is motivation at this stage). Let \( x_1, x_2, x_3, x_4 \) be the positions of the four phosphorus atoms (each of them is a 3-vector). The interatomic forces bonding the atoms is modeled by springs. The first atom feels a force \( x_2 - x_1 \), \( x_3 - x_1 \), \( x_4 - x_1 \), and is accelerated in the same amount. Let’s just choose units so that the force is equal to the acceleration. Then

\[
\begin{bmatrix}
 x_1 \\
 x_2 \\
 x_3 \\
 x_4 \\
\end{bmatrix}
= \begin{bmatrix}
 (x_2 - x_1) + (x_3 - x_1) + (x_4 - x_1) \\
 (x_2 - x_1) + (x_4 - x_1) + (x_2 - x_3) \\
 (x_3 - x_1) + (x_4 - x_1) + (x_2 - x_4) \\
 (x_1 - x_4) + (x_2 - x_4) + (x_3 - x_4) \\
\end{bmatrix}
\]

which has the form \( x = Ax \), where the 4 x 4 matrix

\[
\begin{bmatrix}
 -3 & 1 & 1 & 1 \\
 1 & -3 & 1 & 1 \\
 1 & 1 & -3 & 1 \\
 1 & 1 & 1 & -3 \\
\end{bmatrix}
\]

are the eigenvectors to the eigenvalues \( \lambda_1 = 0, \lambda_2 = -4, \lambda_3 = -4, \lambda_4 = -4 \). With \( S = [v_1, v_2, v_3, v_4] \), the matrix \( B = S^{-1}BS \) is diagonal with entries 0, -4, -4, -4. The coordinates \( y_i = Sx_i \) satisfy \( y_1 = 0, y_2 = -4y_3, y_3 = -4y_4, y_4 = -4y_1 \). We can solve this system which is the center of mass satisfies \( \dot{y}_0 = a + b \) (move molecule with constant speed). The motions \( y_0 = a\cos(2t) + b\sin(2t) \) of the other eigenvectors are oscillations, called normal modes. The general motion of the molecule is a superposition of these modes.