for small s. Then

$$
\begin{aligned}
r_{1,2} &= \frac{-\eta \pm \sqrt{\eta^2 - 4mk}}{2m} = \frac{-\eta \pm \eta\sqrt{1 - 4mk/\eta^2}}{2m} \\[2mm]
&\approx \frac{-\eta \pm \eta\left(1 - 2mk/\eta^2 - 2m^2k^2/\eta^4\right)}{2m} \\[2mm]
&= \begin{cases} -k/\eta \left(1 + mk/\eta^2\right) & \approx \quad -\frac{k}{\eta} \\[2mm] -\eta/m \left(1 - mk/\eta^2 - m^2k^2/\eta^4\right) & \approx \quad -\frac{\eta}{m} \end{cases}
\end{aligned}
$$

Both r_1 and r_2 are negative. Since $\eta^2 \gg 4mk$, $|r_2| \gg |r_1|$. Therefore, an overdamped system has a very rapid acceleration phase in which "inertia balancing friction", e.g., $m\ddot{x} = -\eta\dot{x}$, and a relatively slow motion in which "friction balances elasticity", i.e., $\eta\dot{x} = -kx$.

5.2.4 Underdamped system

What happens if $\eta^2 \ll 4mk$? In this case, we have

$$
\begin{aligned}
r_{1,2} &= \frac{-\eta \pm \sqrt{\eta^2 - 4mk}}{2m} = \frac{-\eta \pm i\sqrt{4mk}\sqrt{1 - \eta^2/(4mk)}}{2m} \\[2mm]
&\approx -\frac{\eta}{2m} \pm i\sqrt{\frac{k}{m}}.
\end{aligned}
$$

We have a decaying oscillation with frequency $\omega = \sqrt{k/m}$ and a much slower decaying rate $\eta/(2m) \ll \omega$. On the fast time scale, the inertia balances the elasticity: $m\ddot{x} = -kx$, just like a Harmonic oscillation without damping.

5.3 Mechanistic modeling of biomolecular mechanics

In this section, we shall develop a mathematical model for the phenomenon of "forced biomolecular 'bond' rupture" first observed by Florin, Moy and Gaub in 1994. Their experimental observations were published in Science.[*] However, their "interpretations" were quite erroneous.

The problem, even though it is on a single biological molecule (a protein) and its natural partner (called a ligand) in water, is a very ideal Newtonian mechanical system. One can develop a mechanistic model (or theory) based two laws: Newton's law of motion and van der Waals' formula for the force between two molecules, together with a list of further assumptions.

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[*] Florin, E.L., Moy, V.T. and Gaub, H.E. (1994) Adhesion between individual ligand receptor pair. *Science* 264 415-417.
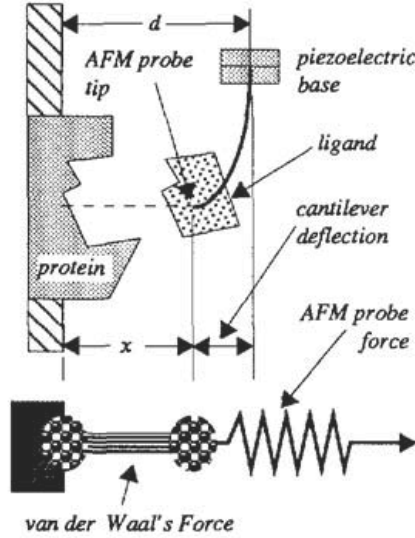
Figure 5.1 *Upper pannel: A schematic overview of protein-ligand complex separation with the AFM. Lower pannel: One-dimensional model. The position of the ligand will be denoted by x.*

We model the external force exerted by a cantilever from an atomic force microscope (AMF) as a linear, harmonic spring:

$$m\frac{d^2x}{dt} = -F_{int}(x) + k(d-x) - \eta\frac{dx}{dt}, \tag{5.16}$$

in which x is the distance between the center-of-mass of the ligand to the center-of-mass of the protein, which is assumed to be fixed.[†] m is the mass of the ligand, η is its frictional coefficient in water, $k(x - x_0)$ represents the force exerted by the AFM cantilever, with d being the position of the base of the cantilever. $F_{int}(x)$ is the interaction force between the ligand and the protein, it has the celebrated van der Waals potential $U_{vdw}(x)$

$$F_{int}(x) = \frac{dU_{vdw}(x)}{dx}, \quad U_{vdw}(x) = -U_0\left[2\left(\frac{x_0}{x}\right)^6 - \left(\frac{x_0}{x}\right)^{12}\right]. \tag{5.17}$$

Because water is a rather viscous medium, we further assume that (1) the mechanical system is *overdamped*, i.e., we can neglect the mass term. Therefore, Eq. (6.13) can

[†] This immediately gives the insight that the internal structure of the protein can change under the pulling. But if our meassurement for x is precisely the distance between the center-of-masses, then it does not matter. However, in real world experiments, this is nearly impossible. So there will be consequences.

be simplified into

$$\eta\frac{dx}{dt} = -F_{int}(x) + k(d - x). \tag{5.18}$$

We now ask the question: When d is slowly increased, i.e., the AFM is pulling the ligand away from the protein, how does the position of the ligand change?

This is in fact a static, force balance problem: $F_{int}(x) = k(d - x)$. That is,

$$\frac{U_0}{x_0}\left[12\left(\frac{x_0}{x}\right)^7 - 12\left(\frac{x_0}{x}\right)^{13}\right] = k(d - x). \tag{5.19}$$

The solution x to the equation, as a function of d, is the answer to our question.

There are many parameters in the equation. But they can be *grouped* together:

$$z = x/x_0, \quad \delta = d/x_0, \quad \text{and} \quad \alpha = kx_0^2/(12U_0),$$

then,

$$\boxed{z^{-7} - z^{-13} = \alpha\left(\delta - z\right)}. \tag{5.20}$$

Note that all three quantities, z, δ, and α are *dimensionless*. non-dimensionalization is a very useful way to simplify mathematical models without involving any approximation. It uses the internal scales as units for physical quantities in a model.

This equation can not be solved in a closed form for $z(\delta)$. However, one can obtain a parametric equation for the function:

$$z = \left(\frac{1 \pm \sqrt{1 - 4\xi}}{2}\right)^{-\frac{1}{6}}, \quad \delta = z + \frac{\xi}{\alpha z}, \quad \xi \in \left[-\infty, \frac{1}{4}\right]. \tag{5.21}$$

Fig. 1 shows several z as functions of δ with different α's. We see with increasing α, i.e., the spring becoming more stiff, the "sluggish" behavior disappears.

One can also understand the behavior in the figure in terms of the "potential energy function":

$$\eta\frac{dx}{dt} = -\frac{dU_{tot}}{dx}, \tag{5.22}$$

where

$$U_{tot}(x) = U_{vdw}(x) + \frac{1}{2}k(x - d)^2 = -U_0\left[2\left(\frac{x_0}{x}\right)^6 - \left(\frac{x_0}{x}\right)^{12}\right] + \frac{1}{2}k(x - d)^2. \tag{5.23}$$

In non-dimensionalized form, it is

$$\frac{U_{tot}(z)}{U_0} = -\left[2\left(\frac{1}{z}\right)^6 - \left(\frac{1}{z}\right)^{12}\right] + 6\alpha(z - \delta)^2. \tag{5.24}$$

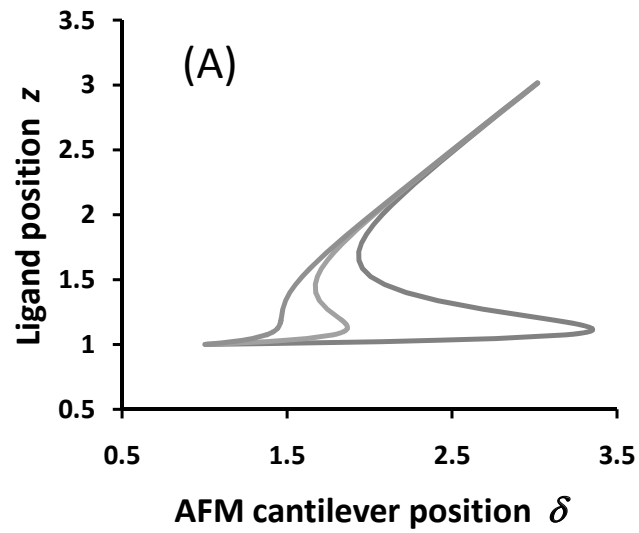Fig. 2 shows the total potential energy function $U_{tot}(z)$ for three different δ.

Figure 5.2 *Mechanical equilibrium position of the ligand, z, as a function of δ, the position of the base of the cantilever, with several different αs, the stiffness of the cantilever. $z = 1$ is the equilibrium position of the ligand in the absent of the AFM force. Red: $\alpha = 0.1$; blue: $\alpha = 0.3$, and green: $\alpha = 0.7$.*
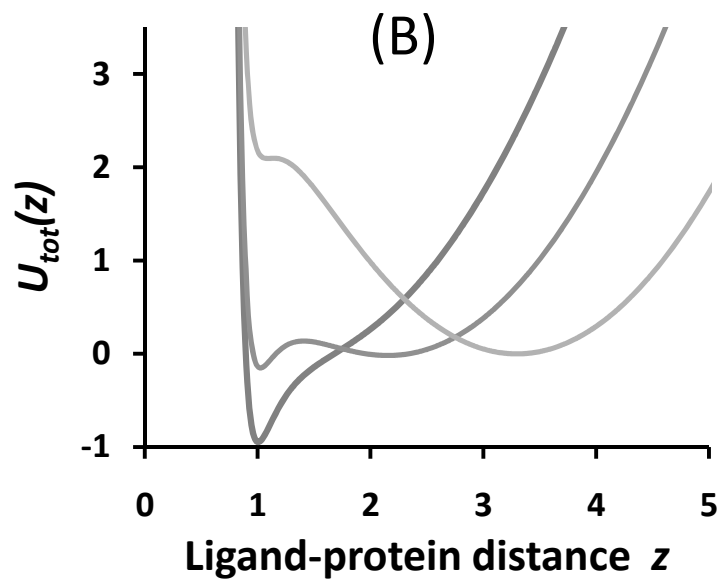
Figure 5.3 *Total mechanical energy, $U_{tot}(z)$, as a function of the ligand-protein (center of masses) distance z for several different values of δs. Red: δ = 1.3, green: δ = 2.2, and orange: δ = 3.3. All with α = 0.1, correspond to the red curve in Fig. 1.*

Snowball Earth

Thermal energy balance states the difference between the influx and radiation energy leads to increasing temperature. For a material with heat capacity R, the heat energy increasing

$$R\frac{dT}{dt} = C(\overline{T} - T) + F_{in}(y) - F_{out}(T), \qquad (11.1)$$

in which R is the heat capacity of the earth, the first term on the right-hand-side represents a heat energy relaxation toward the mean global temperature $\overline{T}$. The numerical value for the relaxation rate $C = 1.6 \times 1.90$ watts per square meter per $°$C.

The $F_{out}(T)$ term is due to radiation. It is a constant term $A + B(T - T_0)$ where A and B are two constants. We shall use $A = 202$ watts per square meter and $B = 1.90$ watts per square meter per $°$C, with $T_0 = 273K$, i.e., $0°$C.

The $F_{in}(y)$ term represents the amount of energy absorbed by the earth per unit area. It is insensitive to the surface temperature T of the earth but depends upon the latitude y due to the *Albedo effect*: A fraction of the solar radiation is reflected back to space without being absorbed, by the earth, due to the ice and snow and the clouds. This term has the form

$$F_{in}(y) = Q\left[1 - S_2\frac{(3y^2 - 1)}{2}\right]\beta(y); \quad \beta(y) = \begin{cases} \beta_1 = 0.68 & |y| < y_s, \\ \beta_0 = 0.53 & |y| = y_s, \\ \beta_2 = 0.38 & |y| > y_s, \end{cases} \quad (11.2)$$

in which $y = \sin\theta$ with θ being the latitude, thus $y \in [0, 1]$. y_s is the latitude of the ice line. The $(3y^2 - 1)$ is the Legendre polynomials of order 2; the origin of this term will become clear in the study of heat equation in spherical coordinates. The constants $Q = 343$ watts per square meter, $S_2 = 0.482$; both are empirically determined.

Putting all together, we have a differential equation

$$R\frac{dT}{dt} = C\left(\overline{T} - T\right) + Q\left[1 - S_2\frac{(3y^2 - 1)}{2}\right]\beta(y) - A - B(T - T_0). \quad (11.3)$$

Eq. 11.3 describes the dynamics of the termpature for each and every t. All parameters are given except two: $\overline{T}$ and y_s hidden in the function $\beta(y)$. It turns out that in this simple ordinary differential equation (ODE) model, the $\overline{T}$, the mean termpature average over different latitudes, is not an independent parameter but actually a function of all the other parameters. In fact, it will be determined through a procedure

called *self-consistet approach*: We shall solve the steady state of ODE (11.3) T^* as a function of y, the latitude, and then

$$\overline{T}^* = \frac{1}{2} \int_{-1}^{1} T^*(y) \mathrm{d}y. \tag{11.4}$$

The steady state temperature T^* according to (11.3)

$$T^*(y) = \frac{C\overline{T}^* + Q\left[1 - \frac{S_2}{2}(3y^2 - 1)\right]\beta(y) - A + BT_0}{B + C}. \tag{11.5}$$

The steady state global mean temperature

$$\overline{T}^* = \frac{1}{2} \int_{-1}^{1} T^*(y) dy = \frac{C\overline{T}^* + Q\overline{\beta} - A + BT_0}{B + C}, \tag{11.6}$$

from which we have

$$\overline{T}^* = \frac{Q\overline{\beta} - A}{B} + T_0. \tag{11.7}$$

In absolute temperature scale of Kelvin, $T_0 = 273K$. We shall use Celsius $°C$, so $T_0 = 0°C$.

The $\overline{\beta}(y_s)$ is obtained

$$\begin{aligned}
\overline{\beta}(y_s) &= \frac{1}{2} \int_{-1}^{1} \left[1 - \frac{S_2}{2}(3y^2 - 1)\right] \beta(y) dy \\
&= \beta_1 \int_{0}^{y_s} \left[1 - \frac{S_2}{2}(3y^2 - 1)\right] dy + \beta_2 \int_{y_s}^{1} \left[1 - \frac{S_2}{2}(3y^2 - 1)\right] dy \\
&= \beta_2 + (\beta_1 - \beta_2) y_s \left(1 + \frac{S_2}{2} - \frac{S_2 y_s^2}{2}\right).
\end{aligned}$$

This is a cubic function of y_s. For our present earth, $\beta_1 = 0.68$, $\beta_2 = 0.38$, $S_2 = 0.482$, and $y_s = 0.95$. Therefore,

$$\overline{\beta}(0.95) = 0.38 + 0.3 \times 0.95 \times \left(1 + 0.241 - 0.241 \times 0.95^2\right) = 0.67.$$

Note this is essentially the same as the ice free β_1.

Substituting Eq. (11.7) into Eq. (11.5), we have

$$T^*(y) = \frac{\frac{C}{B}Q\overline{\beta}(y_s) + Q\left[1 - \frac{S_2}{2}(3y^2 - 1)\right]\beta(y)}{B + C} - \frac{A}{B}. \tag{11.8}$$

This is the Eq. (8.10) in Tung's text, with $\overline{\beta}(y_s) = 1 - \overline{\alpha}$ and $\beta(y) = 1 - \alpha(y)$.

Now according to the model, let us find the ice line which is located at $T = T_c = -10°C$:

$$T_c = \frac{\frac{C}{B}Q\overline{\beta}(y_s) + Q\left[1 - \frac{S_2}{2}(3y_s^2 - 1)\right]\beta(y_s)}{B + C} - \frac{A}{B}. \tag{11.9}$$

Solving y_s as a function of Q, we obtain an important prediction about the location of the ice line as a function of the overall total incoming solar energy to the earth. At the present time, it is about $Q = 343$ watts pers square meter.

Solving $y_s(Q)$ is not easy since the right-hand-side of Eq. (11.9) is cubic of y_s. However, obtaining $Q(y_s)$ is straightforward:

$$Q = \frac{(BT_c + A)(B + C)}{C\overline{\beta}(y_s) + B\left[1 - \frac{S_2}{2}(3y_s^2 - 1)\right]\beta(y_s)}. \tag{11.10}$$
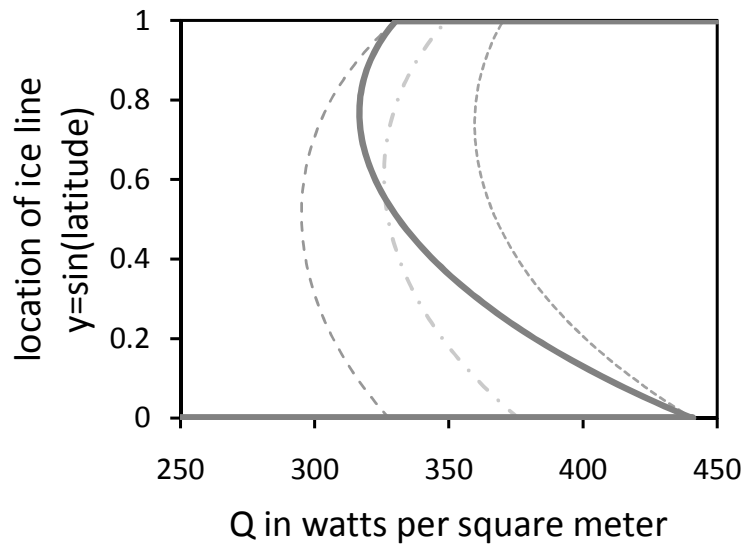
This is shown in Fig. 11.1.

Figure 11.1 *To draw the curve $Q(y_s)$ according to Eq. (11.10), the most delicate issue is to evaluate the function $\beta(y_s)$ which is discontinuous at y_s, as shown in Eq. (11.2). If we choose the $\beta = 0.38$, 0.53, or 0.68, the corresponding $Q(y_s)$ are the blue dotted line, orange line, and green dashed line, respectively. If the discontinuous $\beta(y)$ function is replaced by a continuous function, then the expected $Q(y_s)$ will be like the red line, which is obtained as $Q = (1 - y_s)Q_{0.38} + y_sQ_{0.68}$. The system exhibits the canonical saddle-node bifurcations with catastrophe.*

Now we know y_s as a function, or functions, of Q, using Eq. (11.7), we can determine the global mean temperature T^* as a function, or functions, of Q. This is shown in Fig. 11.2, similar to the Figure 8.4 in Tung's text.
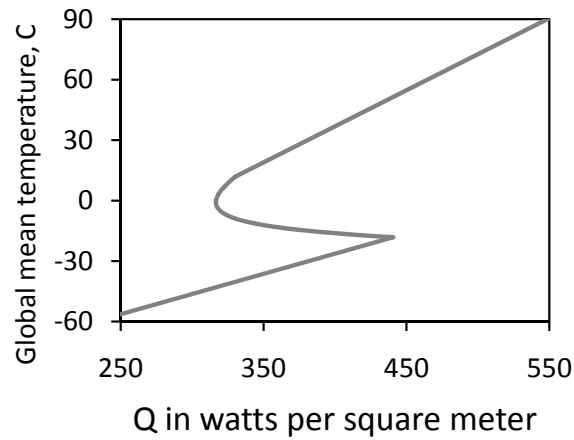
Figure 11.2 *The global mean steady state temperature, $\overline{T}^*$, as a function of Q, according to Eq. (11.7).*

Global warming

We start again an equation similar to that in Eq. (11.1). This time we consider local heat transfer which is represented by the "diffusion term" $\partial^2 T/\partial y^2$:

$$R\frac{\partial T(y,t)}{\partial t} = Qs(y)\beta(y) - (A + BT) + D\frac{\partial^2}{\partial y^2}T(y,t),\qquad (11.11)$$

in which the last term represents the dynamical transport of heat.