Final Spring 2022
Physics 6562/4488: Statistical Mechanics
http://www.physics.cornell.edu/sethna/teaching/562/
Due midnight, Tuesday May 17, submitted via the course Canvas site
Last correction at May 9, 2022, 9:33 am

Open Book Exam. Work on your own for this exam. You may consult your notes, homeworks and answer keys, books and published work, or Web pages as you find useful. The problems have been designed to be doable given only material already presented in the course. If you find something in the literature or on the Web that is particularly helpful (*e.g.*, solves the problem), feel free to use it. However, just as in a publication, cite your source.

Some of the parts are as basic as they seem. Our goal here was to present deep and powerful ideas in the simplest possible context.

Exercises (1-3 for everyone, 4-5 for 6562 only)
Everyone (4488 and 6562)
Questions 1-3

1. **Convexity and phase separation.** ③

A piston, initially completely filled with water vapor, compresses the gas until it is completely liquid (connecting the marked positions in Fig. 1). The piston is held at temperature $T = 550$K at all times.

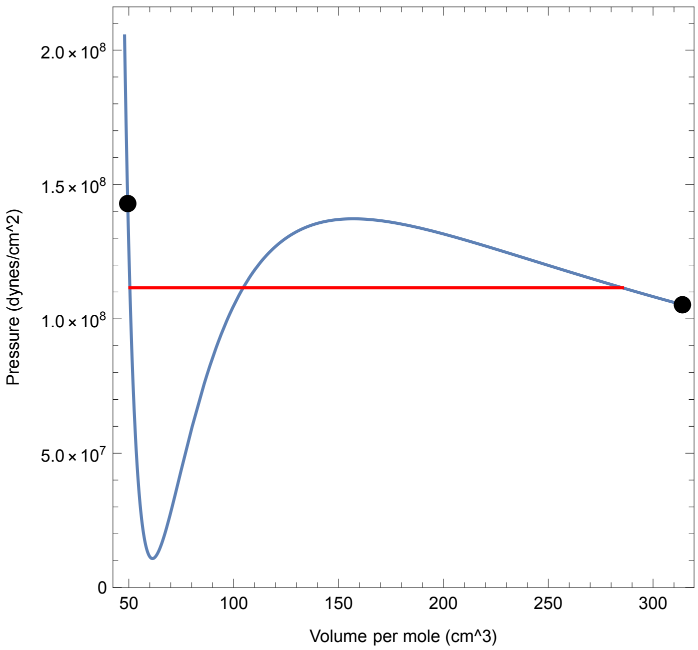

Fig. 1 Pressure vs. volume for the van der Waals model applied to one mole of H_2O at $T = 550$K. The red line shows the vapor pressure P_v at this temperature.

(a) *Draw the path on Fig. 1 taken if the piston moves slowly enough that the system remains in thermal equilibrium at all times.*

(b) *Sketch a path on Fig. 1 taken if the piston moves fast enough so that the pressure rises past the vapor pressure (say, to* 1.2×10^8 *dynes/cm*^{2}*) before a liquid water drop nucleates, but slowly enough so that the subsequent condensation of vapor into the water stays in equilibrium.*

Figure 2 shows the chemical potential for the van der Waals model as a function of density at this same temperature. Remember that the Gibbs free energy is μN, so this is also the Gibbs free energy per molecule. Note that the van der Waals solution assumes that the system is filled with molecules at a uniform density ρ, not a mixture of liquid and gas.

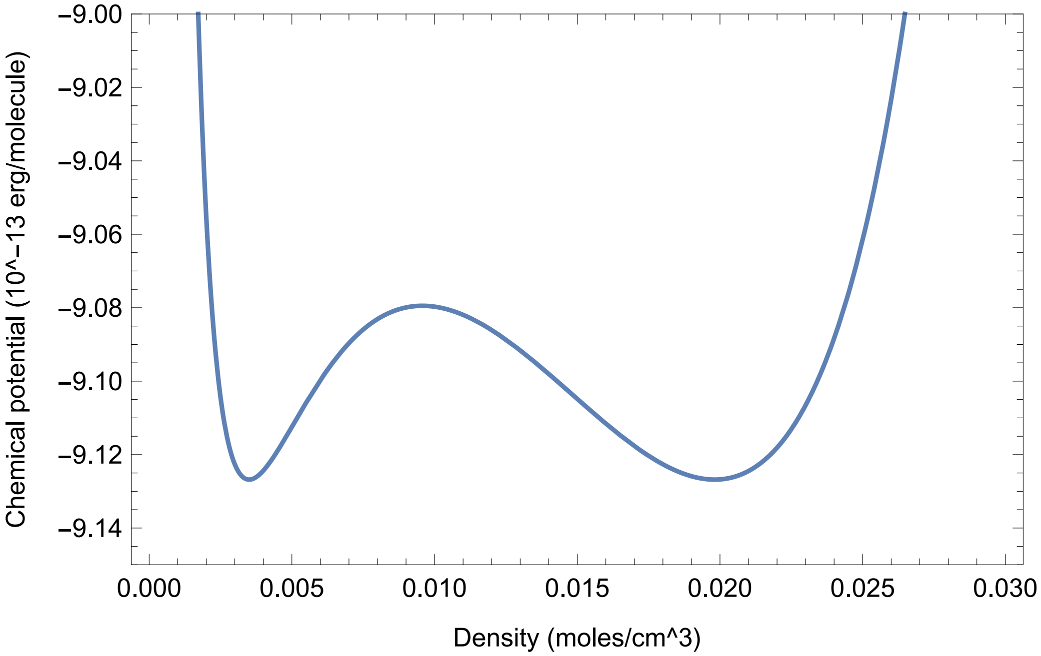

Fig. 2 Chemical potential μ **vs. density** ρ for the van der Waals model for H_2O at $T = 550$K.

(c) *Sketch on a copy of Fig. 2 the free energy one would obtain by allowing for the separation of the water into coexisting liquid and gas.* (Ignore the small contribution of surface tension.)

If a system can be broken up into two weakly interacting subsystems, then the minimum free energy for the system in the limit of infinite size must be convex (see note 4 on page 322).

(d) *In your solution to part (c), what are the two weakly interacting subsystems? Why did we need to take the limit of infinite size to ignore surface tension? Is your answer convex?*

2. **Spinodals vs. Nucleation.** ③

Here we explore the predicted edges of metastability for the liquid and gas, which are called *spinodals* in the older literature. Spinodals provide some insight into the behavior of materials near abrupt transitions, but should not be taken literally – fluctuations ignored by models like these cause the crossover from nucleation to 'spinodal decomposition' to become blurred.

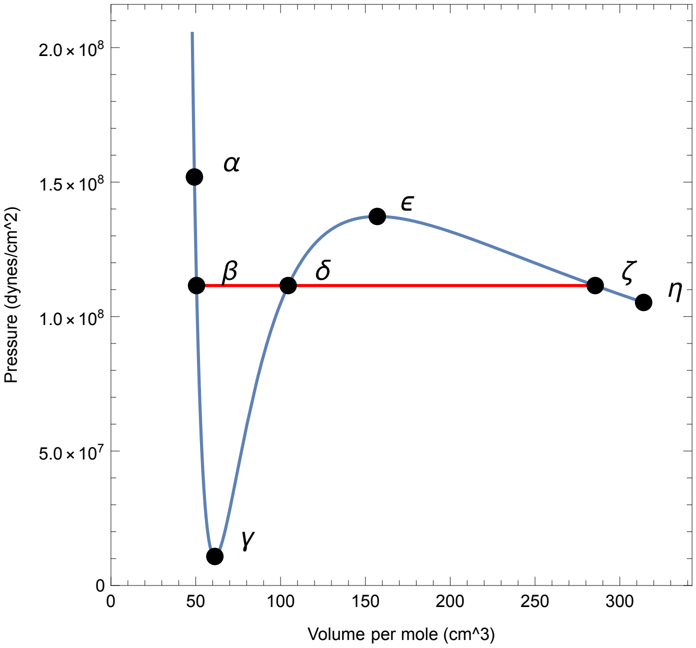

Fig. 3 Volume vs. pressure for the van der Waals model applied to one mole of H_2O at $T = 550\,\mathrm{K}$. The red line shows P_v at this temperature.

Let us explore how the Gibbs free energy per particle $G/N = \mu$ (Fig. 4) varies as we move between different points on the $P{-}V$ diagram Fig. 3.

(a) *At point α in Fig. 3 at the highest pressure, how many other solutions are there with that pressure? Which of the labeled points in the free energy plots of Fig. 4 corresponds to the state α?*

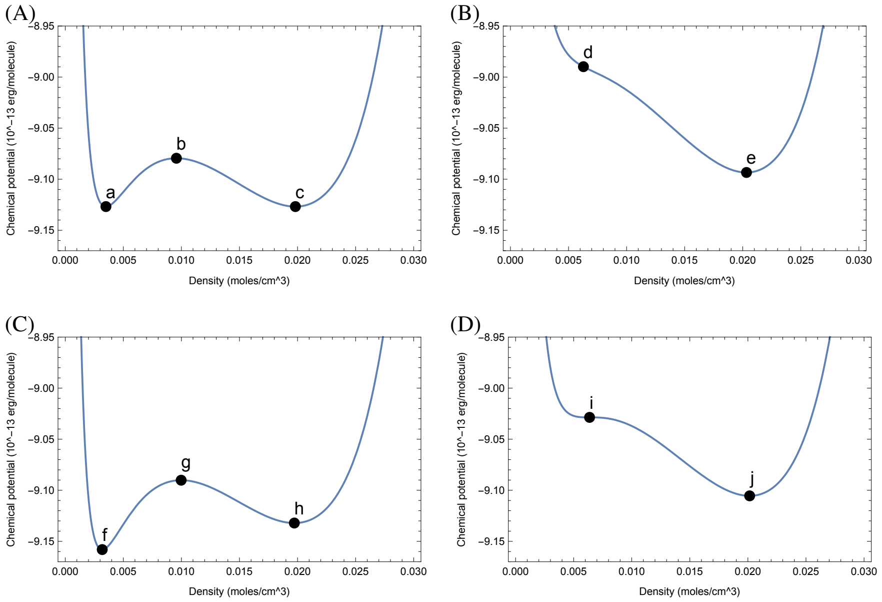

Fig. 4 Chemical potential vs. density at a few of the labeled points α–ζ in Fig. 3. The labeled points *a-j* here are solutions to the van der Waals model.

(b) *Is the system at point δ in Fig. 3 stable, unstable, or metastable? Which point a–j in Fig. 4 corresponds to δ? Explain what about the free energy tells you whether a state is stable, unstable, or metastable.*

We gradually compress a hot water vapor at 550 K. We first study this in the $P - V$ plane and in terms of the chemical potential.

(c) *At which labeled point in Fig. 3 does the metastable gas state go unstable?* This is called a spinodal point. *Which point a–j in Fig. 4 corresponds to this spinodal point for the gas phase?* In Exercise 11.3, we saw that the surface tension energy for nucleating a bubble is related to the barrier in free energy between the two phases. *At the spinodal point, does the free energy barrier between the two phases disappear?*

If one quickly changes the temperature or volume or other parameter across an abrupt phase transition line, the phase transition qualitatively happens in one of two ways. It can be nucleated by slow-forming bubbles or droplets. Or, if one moves into the unstable region, it can undergo *spinodal decomposition*, spontaneously separating into two phases without a nucleation barrier, with small random density fluctuations growing on many length scales. The boundary between these two is blurry except in mean-field theories like that of van der Waals.

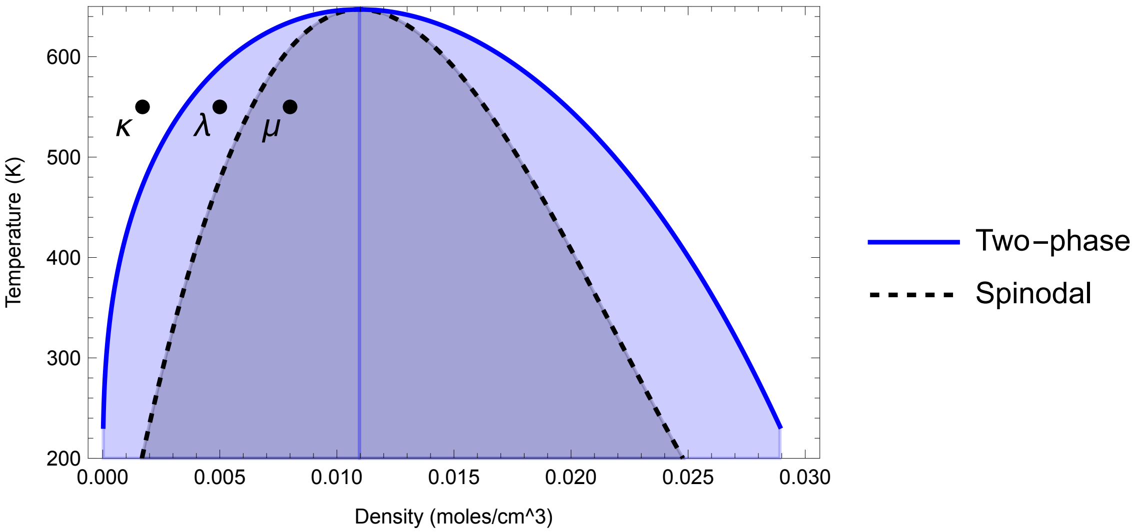

Fig. 5 Spinodal and two-phase regions for van der Waals water, as we vary density ρ and temperature T.

The three points κ, λ, and μ in Fig. 5 correspond to our compression experiment in part (c). We prepare the state at λ and μ by quickly decreasing from state κ at $t = 0$ while cooling to keep T fixed, starting each in a uniformly compressed state with only microscopic fluctuations. Assume the system is in very low gravity (so the liquid water, when it forms, does not quickly fall to the bottom). For each, consider the density $\rho_\lambda(h, t)$ and $\rho_\mu(h, t)$ along a one-dimensional line h rising from the bottom to the top.

(d) *Roughly sketch* $\rho_\lambda(h, t)$ *as a function of* h *for three times:* $t = 0$ *just after compression, a time* t_{droplets} *when the line passes through a nucleated droplet or two (which have yet to grow to equilibrium or fall to the bottom), and a much later time* t_{equilib} *when it is fully phase separated.* (Hint: What fraction of the volume will be liquid?) *Label your density axis with the equilibrium densities of the liquid and gas at 550 K, and with the initial density* ρ_λ.

After evolving for a while at the same final conditions, a system which was launched quickly with spinodal decomposition or slowly by nucleation will evolve into a rather similar late-time state which coarsens with time.

(e) *Roughly sketch* $\rho_\mu(h, t)$ *as a function of* h *at a time* t_{spinodal} *when tiny random thermal density fluctuations have been noticably magnified by the instability, but have yet to approach the equilibrium densities of the two phases. Label your density axis with the equilibrium densities of the liquid and gas at 550 K, and with the initial density* ρ_μ.

3. Cell signaling and mutual information.[1] ③

To survive, living systems must accurately measure and and respond to their environment. For example, *E. coli* bacteria famously execute a process called chemotaxis. By sensing gradients in nutrients, they decide whether to to run (propel themselves forward) or tumble (change direction) using their propellor-like *flagella* (see Exercises 2.19 and 2.22). The environmental signal is transmitted from the receptors on the cell surface to the motors that control the flagella via a cascade of chemical reactions. These cascades involve kinases – protein enzymes that are activated (phosphorylated) by reactions that are catalyzed by upstream enzymes (the cell membrane receptors or another kinase). The activated kinase has a finite lifetime, with dephosphorylation reactions catalyzed by so-called phosphatase enzymes. Fluctuations in active kinase populations carry the signal through the cascade. Multi-level cascades can amplify signals, enabling sensitive detection of the environment, but also introduce noise due to the stochastic nature of enzymatic reactions. In this problem we will investigate how cells can mitigate this noise, optimizing the information transmitted by the signaling circuit.

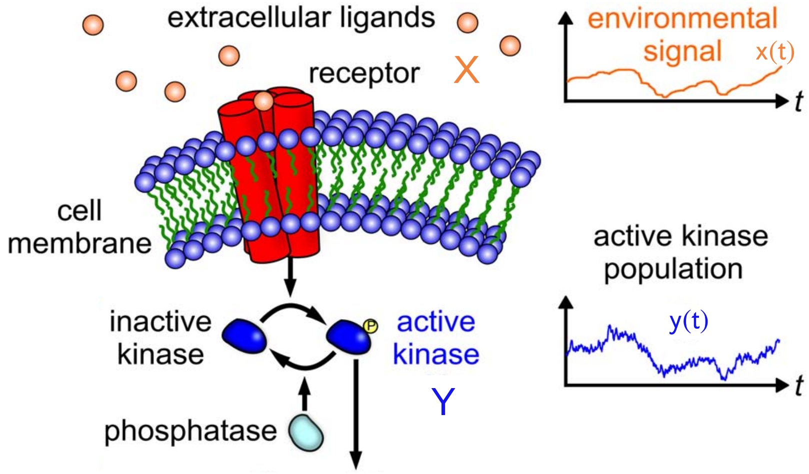

Fig. 6 The simplest cellular signaling circuit involves: (i) the environmental signal from extracellular ligands X, (ii) an kinase population Y within the cell, activated by the membrane receptors. This minimal model is a coarse-grained representation of actual chemical circuits that regulate chemotaxis in *E. coli*, olfactory (smell) sensing in mammals, and yeast response to osmotic pressure [5, 2].

Let $X(t)$ be the local concentration of food as the bacteria swims forward. This concentration randomly fluctuates, driven by noise ξ_x due to both to the bacteria's movement and coupling to the environment, but changes relatively slowly, with a long correlation time γ_x^{-1}. The dynamics of X are given by a Langevin equation, $\dot{X} = A_x - \gamma_x X + \xi_x(t)$, where A_x keeps the mean food level $\overline{X} = A_x/\gamma_x$ positive. The cell's measurement of this signal is noisy: small numbers of food molecules randomly bump into the receptors,

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[1] This exercise was developed in collaboration with David Hathcock.

which in turn causes activation of R kinase within the cell. The dynamics of active kinase population Y are given by, $\dot{Y} = A_y + R(X - \overline{X}) - \gamma_y Y + \xi_y(t)$, where ξ_y is the measurement noise, A_y is the background activation rate, and γ_y is the deactivation rate, determined by phosphatase concentrations. As with X, γ_y^{-1} sets the time-scale for fluctuations in Y. How can the cell tune γ_y to filter out the measurement noise at the receptors and gain the most information about the food in its environment?

For our calculations, we will assume the terms $\xi_a(t)$ with $a = x, y$ are white noise with correlation[2] $\langle \xi_a(t)\xi_b(t')\rangle = 2F_a\delta_{ab}\delta(t - t')$. Information is carried by the fluctuations in X and Y about the mean values, $\overline{X} = A_x/\gamma_x$ and $\overline{Y} = A_y/\gamma_y$; the bacteria wants to swim toward locations where there is more food than average. Subtracting off the means, $x = X - \overline{X}$ and $y = Y - \overline{Y}$, we are left with,

$$\dot{x} = -\gamma_x x + \xi_x(t) \quad \dot{y} = -\gamma_y y + Rx + \xi_y(t) \tag{1}$$

The calculations in this exercise are somewhat involved, so we shall provide many intermediate results to allow you to bypass parts if you get stuck. *If you use a computer algebra system (Mathematica™, SymPy, ...) please provide your code. If you use paper and pencil, please show your steps and prune your dead ends.*

(a) *Fourier transform eqn (1) and solve for* $\widetilde{x}(\omega)$ *and* $\widetilde{y}(\omega)$. *Express your answers in terms of the Fourier transformed noise* $\widetilde{\xi}_x(\omega)$, $\widetilde{\xi}_y(\omega)$ *as well as* γ_x, γ_y, *and* R.

If $C_{ab}(\tau) = \langle a(t+\tau)b(t)\rangle$ is the correlation between a and b, then $\widetilde{C}_{ab}(\omega) = \widetilde{a}(\omega)\widetilde{b}^*(\omega)$ (see Appendix A). For example, the noise correlation relation becomes $\widetilde{\xi}_a(\omega)\widetilde{\xi}_b^*(\omega) = 2F_a\delta_{ab}$ and the equal time correlation is $C_{ab}(0) = 1/(2\pi)\int d\omega\, \widetilde{a}(\omega)\widetilde{b}^*(\omega)$. For the next parts, the following integrals are useful:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{-i\omega t}d\omega}{\omega^2 + c^2} = \frac{e^{-c|t|}}{2c} \qquad \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{d\omega}{(\omega^2 + c^2)(i\omega + d)} = \frac{1}{2c(c+d)}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{d\omega}{(\omega^2 + c^2)(\omega^2 + d^2)} = \frac{1}{2cd(c+d)}$$

(b) *Show that* $x(t)$ *has exponential time correlations,* $C_{xx}(\tau) = F_x/\gamma_x \exp(-\gamma_x|\tau|)$. As we mentioned above the signal has a correlation time scale set by γ_x^{-1}.

(c) *Show that the equal time correlations are* $C_{xx}(0) = F_x/\gamma_x$, $C_{xy}(0) = F_x R/(\gamma_x^2 + \gamma_x\gamma_y)$ *and* $C_{yy}(0) = F_x R^2/(\gamma_x^2\gamma_y + \gamma_x\gamma_y^2) + F_y/\gamma_y$. To simplify the notation below, we will define $\sigma_x^2 = C_{xx}(0)$, $\sigma_y^2 = C_{yy}(0)$, and $\text{cov}_{xy} = C_{xy}(0)$.

So far, we have understood the fluctuations and correlations in two chemical populations: food molecules in the environment and signaling proteins within the cell. How can we use these to quantify the information gained by the bacteria? Fortunately,

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[2] If the number of molecules attaching to the receptor is the cause of the noise (this is called *shot noise*), then $F_x = A_x$ and $F_y = A_y$.

Shannon explored this question in his seminal work on information theory. He developed the machinery of information entropy when working for the telephone company.[3] The phones in those days had lots of static. How could one calculate when the static noise made it impossible to hear the words? Shannon introduced the idea of a *mutual information* between the original signal and the noisy final signal.

Suppose the probability distribution of an original message x is $\rho_X(x)$, and the probability distribution of x being turned into a noisy final message y is $\rho_T(y|x)$ (the probability of y given x). This transmitted probabilty distribution can be written in terms of the joint probability distribution $\rho_{X,Y}(x,y)$ – the likelihood of a random transmission having original message x and final noisy message y. Note that $\rho_X(x) = \int dy\, \rho_{X,Y}(x,y)$ and similarly for $\rho_Y(y)$.

(d) *Express in words the true statement* $\rho_T(y|x)\rho(x) = \rho_{X,Y}(x,y)$ *in a way that would convince a non-scientist.*

The mutual information[4] is defined to be

$$\mathcal{I}(X,Y) = k_S \int dx \int dy\, \rho_{X,Y}(x,y) \log\left(\frac{\rho_{X,Y}(x,y)}{\rho_X(x)\rho_Y(y)}\right), \tag{2}$$

The mutual information is symmetric in X and Y. How can it be used to study how much the noisy final signal y tells us about the original signal x?

(e) *Show that* $\mathcal{I}(X,Y) = S(X) - S(X|Y)$*, the entropy of the probability distribution of general noisy input signals* $\rho_X(x)$ *minus the entropy of the noisy signals resulting in a particular received signal* y*,* $\rho_T(x|y)$*, averaged over* y (Hint: the identity from part (d) also holds if we swap x and y. Plug this in and separate the log into a difference of two terms). *Explain in words why the first measures your ignorance of the message* X *before getting a telephone call* Y*, and the latter is your average ignorance after a call.*

To compute the mutual information for the cell signaling system, we require the joint distribution $\rho_{X,Y}(x,y)$. In general, for systems driven by white-noise (with delta-function correlations), this is done by converting the Langevin equations into a Fokker-Planck equation (see Exercise 8.22), which can then be solved to obtain the equilibrium distribution. When the equations are linear (as is the case for our model, eqn (1)), one finds that the joint distribution is a bivariate Gaussian[5],

$$\rho_{X,Y}(x,y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-r^2}} \exp\left(-\frac{1}{2\,(1-r^2)}\left(\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} - \frac{2rxy}{\sigma_x\sigma_y}\right)\right). \tag{3}$$

Here, the standard deviations $\sigma_x = \langle x^2\rangle^{1/2}$ and $\sigma_y = \langle y^2\rangle^{1/2}$ and correlation $r = \langle xy\rangle/(\sigma_x\sigma_y) = \mathrm{cov}_{xy}/(\sigma_x\sigma_y)$ are precisely those you computed in part (c).

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[3] This was in the olden days, when there was only one phone company in the US, Bell Telephone.

[4] The mutual information is also the distance in probability space between the joint distribution $\rho_{X,Y}(x,y)$ and the uncorrelated case $\rho_X(x)\rho_Y(y)$, using a distance measure called the Kullback–Liebler divergence (see Exercise 1.16).

[5] This is a generalization of a familiar result from statistical mechanics: the Boltzmann distribution for an over-damped harmonic oscillator (which feels forces linear in the displacement) is Gaussian.

(f) *Argue that the marginal distributions* $\rho_X(x)$ *and* $\rho_Y(y)$ *are also Gaussian, with widths* σ_x *and* σ_y *respectively. Show that the mutual information for the bivariate Gaussian is* $-(k_S/2)\log(1-r^2)$*. Interpret this result for* $r \to 0$ *and* $r \to 1$*. Is the mutual information dependent on the magnitude of the fluctuations?* (Hint: what happens if we scale $x \to \alpha x$).

Biologically, the rate γ_y is easiest to tune (e.g. through evolution and natural selection). This rate is controlled by concentrations of phosphatase in the cell, whereas the activation rate R requires energy dissipation.

(g) *Argue that maximizing mutual information is equivalent to maximizing* r^2*. Show that* $r^2 = Z\Lambda/((1+Z)(1+Z+\Lambda))$*, where* $Z = \gamma_y/\gamma_x$ *and* $\Lambda = F_x R^2/(F_y \gamma_x^2)$*. Maximize* r^2 *with respect to* γ_y*. Show that when the information transmission is optimized,* $\gamma_y = \gamma_x\sqrt{1+\Lambda}$ *and* $\mathcal{I} = \frac{1}{2}[k_S \log(1+\sqrt{1+\Lambda}) - 1]$*.*

With all else fixed, there is an ideal response time: γ_y^{-1} must be faster than γ_x^{-1} by the factor $1/\sqrt{1+\Lambda}$. If γ_y is too small, Y will integrate over the changes in X, filtering out too much of the the signal. On the other hand, if γ_y is too large, Y will fail to filter out enough of the noise introduced at the cell receptors. The mutual information quantifies how much information the cell has about the current state of its environment, obtained by measuring the history of the signal and filtering out receptor noise. The dimensionless parameter Λ serves as a measure of the signal fidelity. When $F_x \gg F_y$, then $\Lambda \gg 1$: it is easy to reproduce the signal if the magnitude of fluctuations in X are large compared to the noise introduced by the receptors. On the other hand if $F_x \approx F_y$, $\Lambda = R^2/\gamma_x^2$, which measures the sensitivity of Y to changes in the X population over the timescale γ_x^{-1}. Real biological signaling circuits, like those in yeast and *E. coli*, tend to lie in the range $\Lambda = 100 - 1000$.

(h) *For the range of* Λ *listed above, how much information, in bits, can the cell learn about its environment from monitoring* $Y(t)$*?*

Graduate (6562 only)
Questions 4-5

4. **Emittance and particle beams.**[6] ③

Particle accelerators take bunches of protons and antiprotons up to near the speed of light, and smash them head-on to see what happens. Electron microscopes take bunches of electrons and focus them to image materials at the atomic scale. X-ray sources accelerate electrons to near the speed of light, and use undulators to wiggle them to create X-rays (synchrotron X-ray sources) or free electron lasers (coherent beams of X-rays). In all of these applications, in addition to the energy per ion and the number of ions, the key property of a good bunch is its *emittance*. In this exercise, we shall explain why emittance is important, relate it to the entropy of the bunch, analyze its quantum limit, and explore the use of electron bunches to cool bunches of protons.

The 3D emittance of a bunch is loosely given by the product of the volume it occupies in position space and in momentum space:

$$\varepsilon = (\Delta q_x \Delta p_x)(\Delta q_y \Delta p_y)(\Delta q_z \Delta p_z). \tag{4}$$

For our purposes, Δq and Δp will represent the standard deviations of the positions and momenta in the center of mass frame of the bunch. Here z is the 'longitudinal' direction in which the beam is moving, and x and y are 'transverse'. For synchrotrons, y is the direction perpendicular to the circular orbit and x the direction in the plane of the circle perpendicular to the motion. One also speaks of the 2D emittance of the transverse directions $(\Delta q_x \Delta p_x)(\Delta q_y \Delta p_y)$ perpendicular to the velocity of the bunch, or the 1D emittance along one of the axes.

Emittance is a limiting parameter in the performance of any accelerator. In electron microscope/diffraction accelerators, the emittance limits the resolution; in colliders, it limits the luminosity; in free electron lasers, it limits the gain length and the minimum wavelength of the laser. Reducing beam emittance is therefore desirable, and it is a central research goal of the Center for Bright Beams (CBB), a collaboration in which Cornell plays a leading role.

At the Large Hadron Collider (LHC), the bunches have $N = 1.2 \times 10^{11}$ protons, a bunch radius of $\sigma_q = 3.5\,\mu$m, and a transverse emittance of $3.75\,\mu\text{rad} = 1.88\,10^{-24}\,\text{kg}\,\text{m}^2/\text{s}$, implying a RMS bunch momentum of $\sigma_p = 5.4 \times 10^{-19}\,\text{kg}\,\text{m/s}$.

The ions in a bunch are often nearly noninteracting and uncorrelated, with all ions having nearly the same probability distribution in phase space. In this case, $\rho_N(\mathbb{P}, \mathbb{Q}) = \prod_{n=1}^{N} \rho(\mathbf{p}_n, \mathbf{q}_n)$. In this exercise, we shall focus on Gaussian bunches. We roughly approximate the LHC bunch as a spherically symmetric Gaussian

$$\rho_{\text{LHC}}(\mathbf{p}, \mathbf{q}) = \frac{e^{-\mathbf{q}^2/2\sigma_q^2} e^{-\mathbf{p}^2/2\sigma_p^2}}{(2\pi\sigma_q^2)^{3/2}(2\pi\sigma_p^2)^{3/2}}. \tag{5}$$

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[6] This exercise was developed in collaboration with Michael Kaemingk. We have used real numbers as input for this exam, but our assumptions for the calculations are not reliable. For example, real bunches are not as tidy as our Gaussian model bunches, and their momentum spread is not thermal.

(a) *Write the formula for the 3D emittance of the bunch in eqn 4.* Note that the kinetic energy has the form of a thermal distribution. *Write a formula for the temperature of the bunch. Write the entropy*

$$\begin{aligned} S &= -k_B\langle \log \rho\rangle = -k_B \int \rho \log \rho \\ &= -k_B \int \mathrm{d}\mathbb{P}\, \mathrm{d}\mathbb{Q}\, \rho(\mathbb{P},\mathbb{Q}) \log \rho(\mathbb{P},\mathbb{Q}) - 3Nk_B \log h. \end{aligned} \tag{6}$$

(Warning: There is an error in the corresponding eqn 5.20 in the text.) *Evaluate the temperature and the entropy of the bunch using the LHC parameters above. Write a formula for the emittance in terms of* $\exp(S/Nk_B)$*.* We may view your last result as a more rigorous definition of the emittance.

Thus, the emittance, like the entropy, can only grow as the bunch passes through accelerating fields and focusing magnets.[7] Making a low emittance bunch, and keeping the emittance low during its acceleration and focusing, is key to all accelerator applications.

Why do we care about the momentum spread Δp in eqn 4, if we want a dense beam or a sharp focus? The conservation of emittance forces a tradeoff between a narrow beam and one that stays narrow as it moves.

The angular dispersion of a beam is due to the momentum spread σ_p: the momentum in the transverse direction will make the beam grow in width. The angular spread in a beam is given by the ratio of the transverse momentum spread Δp over the mean momentum of the ions in the forward direction. The latter, mv for nonrelativistic motion (with m the particle mass) becomes $mv/\sqrt{1-v^2/c^2} = \beta\gamma mc$ for a relativistic beam, with $\beta = v/c$ and $\gamma = 1/\sqrt{1-v^2/c^2}$. Thus the angular spread $\Delta\theta = \Delta p/\beta\gamma mc$ radians with respect to the direction of motion.

(b) *An electron microscope has a beam with velocity* $v = 0.62c$*, a width* $\sigma_q^i = 200\,\mu\mathrm{m}$ *and a vertical emittance* $\varepsilon = 2.7 \times 10^{-30}\,\mathrm{kg\,m^2/s}$*. What is its vertical momentum spread* σ_p*? What is its angular spread* $\Delta\theta_i$ *in radians?* A lens system focuses the beam into a smaller width $40\,\mu\mathrm{m}$, without increasing the entropy or changing its velocity. *What is the new angular spread* $\Delta\theta_f$*, in terms of* $\Delta\theta_i$*? How far can it propagate before the new spread gives the beam a width larger than the original width* σ_q^i*?* (Rough estimates are fine.)

One might be surprised that the ions in a bunch can be treated as non-interacting, given the strong Coulomb interactions between particles. Indeed, these 'space-charge' effects are important when the bunch is first formed. But as it reaches near the speed of light, these interactions become much less important. Using an ultrafast electron diffraction apparatus at Cornell as an example, the current state-of-the-art photoemission bunch starts out as a bunch of radius $20\,\mu\mathrm{m}$ in the transverse directions, and a duration of 200 femtoseconds. Suppose this beam is now placed in an X-ray Free Electron Laser and accelerated to a speed very close to that of light (but leaving its duration fixed). The

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[7] The beam can lower its emittance by emitting X-rays, which is important in synchrotrons and undulators.

packet in the laboratory frame is $60\,\mu$m long (roughly spherical). But the packet in the laboratory frame is Lorentz contracted by a factor of $\gamma \approx 34000$, so in the center of mass frame it is a long tube of length $\gamma \times 60\,\mu\mathrm{m} = 1.3\,\mathrm{m}$. The force on the electrons in the beam are mostly due to the charges within a distance along the tube roughly given by the distance of the electron from the center of the tube ($20\,\mu$m), which in turn is roughly $1/\gamma$ of the total. Furthermore, the motion due to these forces in the lab frame takes γ times longer to happen in the lab frame due to time dilation. The two effects combined imply that the Coulomb interactions are suppressed by $1/\gamma^2$, making them basically negligible.

Strong transverse bunch shape anisotropy is also seen in electron beams in synchrotrons. At the Cornell Electron Storage Ring (CESR), $\varepsilon_x \approx 500\,\mathrm{eV\,m/c} = 2.7 \times 10^{-25}\,\mathrm{kg\,m^2/s}$ along the horizontal (x) direction, and $\varepsilon_y \approx 0.1\,\mathrm{eV\,m/c} = 5.3 \times 10^{-29}\,\mathrm{kg\,m^2/s}$ along the vertical direction:[8] a factor of 1000 anisotropy! Indeed, one of the ambitious goals in the accelerator community is to get the transverse emittance down to the *quantum limit*.

(c) *What would the vertical emittance* $\Delta q_y \Delta p_y$ *be at the quantum limit, set by the uncertainty principle? By what factor must CESR shrink their emittance to approach this goal?*

Liouville's theorem implies that reducing the entropy or the emittance cannot be done simply with the standard tools of accelerators (magnetic lenses, focusing solenoids, bunchers, etc.). Instead, the beam must be coupled to another system into which the entropy can be dumped. There are different methods for doing this, such as synchrotron cooling, electron cooling, and stochastic cooling (for which Simon van der Meer received the Nobel Prize in 1984). Here we will consider a simplified model of electron cooling.

Electron cooling is a mechanism by which an electron beam is used to reduce the momentum spread, and therefore the entropy, of a beam of heavier ions. It is being used in the Relativistic Heavy Ion Collider (RHIC), colliding gold ions to create a quark-gluon plasma. The electron and gold ion beams are overlapped with nearly the same velocity.

(d) *Suppose a gold ion bunch with initial temperature* T_{Au} *is put into thermal equilibrium with an electron bunch of the same radius* σ_q*, the same number of particles* N *and a temperature* $T_e \ll T_{\mathrm{Au}}$*. What will the final temperature* T_f *of the gold ion beam be?* (You may ignore the interactions between the various ions.) *Calculate the ratio of the emittances* $\varepsilon_{\mathrm{Au}}/\varepsilon_e$ *and the beam angular dispersion* $\Delta\theta_{\mathrm{Au}}/\Delta\theta_e$ *of the resulting gold ion and electron bunches.*

As the gold ion beam travels through the electron gas, it will experience two effects. One is a drag force proportional to the velocity with respect to the center of mass. The other is fluctuations due to individual scattering events with the electrons. In Exercise 6.18, you found a fluctuation-response relationship between the noise and the drag coefficient

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[8] The horizontal width is large because of the randomness introduced by the emission of X-ray photons as the beam circles around.

in simulations of Langevin dynamics for one-dimensional motion. The relationship you found in that exercise was $k_B T = \langle \Delta p^2 \rangle / 2\eta\Delta t$. We express this relation in terms of η, the inverse of the mobility, so the force on a moving gold ion is $F = -\eta v$. (The mobility is called γ in Exercise 6.18.) For us, Δp is the root-mean-square momentum change due to each collision, T is the temperature of the electron beam, and Δt is the time between collisions.

So, to find the drag force for a moving gold ion, we shall calculate the noise on a stationary ion and use this relationship.

The geometry of collisions between electrons and ions via the Coulomb interaction is complicated. One simplifying concept is that of a scattering cross section – the effective circular disk that would suffer the same forces. For the densities of electrons and gold ions in our two bunches, you may assume that a gold ion near the center of the electron bunch has a cross section $\Sigma = 0.1\,\mathrm{nm}^2 = 10^{-19}\,\mathrm{m}^2$. The momentum exchange in a collision with that disk will solely depend on the momentum p_x of the electron, where x is the axis perpendicular to that disk.

How big a momentum change will a gold ion have during a collision with an electron? (How much momentum is exchanged when a ping-pong ball hits a car?)

(e) *Taking the limit $m_{\mathrm{Au}}/m_e \to \infty$, what is the net change Δp for the gold disk, given a head-on elastic collision with an electron with x momentum p_x?*

We can get the frequency of collisions from the cross section Σ, the density per unit volume n and the momentum distribution of the electrons.

(f) *What will the average time Δt be between collisions with the stationary ion disk of area Σ? What will the average squared momentum transfer Δp^2 be for these collisions? What is the temperature $k_B T$ of the bath?* (Rough estimates are fine.)

At the Relativistic Heavy Ion Collider (RHIC) work is underway to cool gold ions with an electron beam. In one scheme, a gold ion beam circles a ring with circumference $C = 3.9$km, and each turn passes through a segment of length $0.0078C$ with a co-moving electron gas of density $10^8\,\mathrm{cm}^{-3} = 10^{14}/\mathrm{m}^3$ and momentum spread $1.2\,10^{-23}\,\mathrm{kg\,m/s}$. The electrons are refreshed continuously using a Cornell-invented energy recovery Linac. The bunches are moving fast – their value of $\gamma = 1/\sqrt{1 - v^2/c^2} = 105$. Time dilation makes the interaction time needed larger by a factor of γ.

(g) *Using this result along with the temperature definition given above and the relation from Exercise 6.18, find a formula for the inverse mobility eta. Using $F = -\eta v = \dot{p}$, find a formula for the exponential decay time τ for the gold ion velocity in the center of mass frame. Evaluate it for RHIC's electron cooling scenario.*

i. *What is the exponential decay time for the gold ion beam in the lab frame of RHIC?*

5. **Nonabelian defects.**[9] Mathematics ③

In this problem, we will try to understand the defects that occur in a liquid crystal composed of a planar tri-headed molecule (Figure 7). The ordered states of this system have all molecules in the same orientation, but with liquid translational order (randomly placed centers). This exercise will explore subtle questions regarding classification of nonabelian defects. It will explore *braiding* with mathematics related to the problems of anyon statistics and topological quantum computing. And it will provide a complete analysis of the transformation of one defect as it is pulled around another, explored in the case of fingerprints in Exercise 9.17.

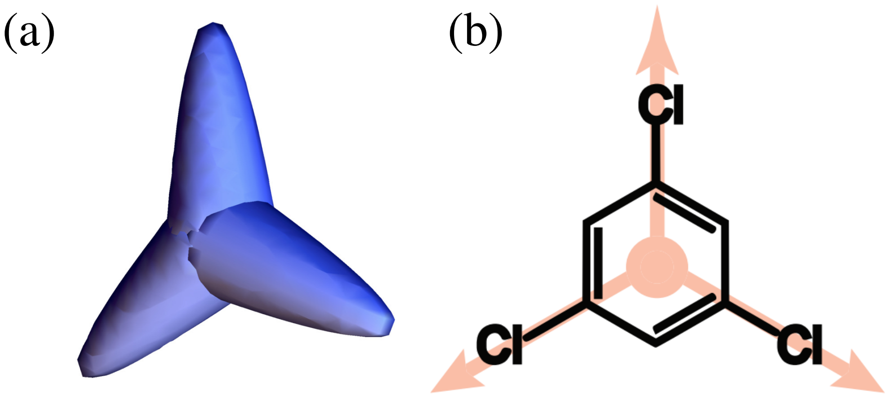

Fig. 7 Dihedral molecules. (a) The tri-headed molecule studied in this problem. (b) The molecular structure of $1, 3, 5$-Trichlorobenzene, with a representation of a tri-headed molecule superimposed [1]. If these molecules were to form a liquid crystal, the liquid crystal would have the types of defects described in this exercise.

If the molecule $1, 3, 5$-Trichlorobenzene (Fig. 7b), which has the same symmetry as our cartoon molecule, had a liquid crystalline phase[10] where they oriented parallel to one another, one would find the defects we study here [1]. These systems are generally called *dihedral* liquid crystals for reasons that we will explore shortly.[11]

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[9] This exercise was developed in collaboration with Stephen Thornton.

[10] There is currently no experimental evidence for this specific type of liquid crystal.

[11] Note: Most papers on dihedral liquid crystals confine the molecules to the plane. We are allowing them to rotate in 3 dimensions.

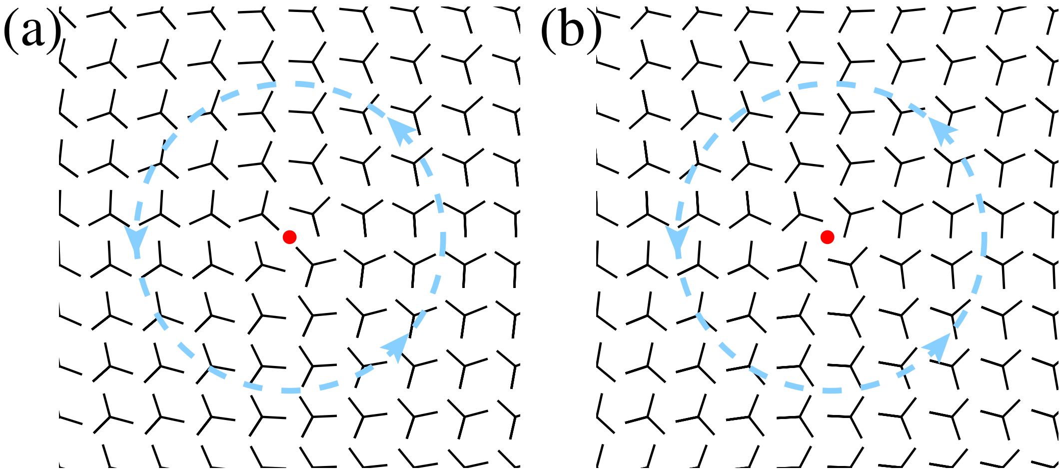

Fig. 8 Defects with molecules confined to the plane. Note that the molecules are at random positions; the orientations are shown on a square lattice for convenience.

Figure 8 shows two defects (red points) around which the molecules swirl. Recall that the winding number is defined as the fraction of a full rotation $\Delta\phi/2\pi$ an object does as we travel around a defect counterclockwise in real space. $\Delta\phi$ has a sign associated with it. Is the defect labeled by the winding number? In part (a) we find that the answer is yes if the molecular “legs” are confined to the plane, but otherwise no:

(a) *What are the winding numbers of the defects shown in Figure 8? If we allow the molecules to rotate in three dimensions, are these two defects topologically equivalent?* (Hint: Try applying a rotation about various axes to all the molecules.)

We saw in part (a) that the molecular orientation, after following the path around a defect, must return to an orientation related by the symmetry group of the molecule. Our molecule has a dihedral symmetry group D_3 (hence the name dihedral liquid crystal). We imagine that the homotopy group (the nonequivalent possible circular paths in the order parameter space) will be related somehow to D_3.

D_3 is a six element group, generated[12] by two elements: a $2\pi/3$ counter-clockwise rotation a about an axis normal to the plane of the molecule (taken to face out of the page for the planar configurations), and a flip x, rotating by π about a particular leg of the molecule (the ‘bra’ in eqn 7). The multiplication rules can be discovered by the three relations in the ‘ket’:

$$D_3 = \left\langle x, a \;\middle|\; x^2 = 1, a^3 = 1, xax^{-1} = a^{-1} \right\rangle . \tag{7}$$

We can also write out the full multiplication table (Table 1).

The group element gh is found in the row labeled by g and the column labeled by h. This is important because D_3 is nonabelian.

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[12] A group is *generated* by a subset of elements (called *generators*) if every member of the group can be represented by repeatedly multiplying generators and their inverses.

$\mathbf{D_3}$	$\mathbf{1}$	$\mathbf{a}$	$\mathbf{a^2}$	$\mathbf{x}$	$\mathbf{xa}$	$\mathbf{xa^2}$
$\mathbf{1}$	1	a	a^2	x	xa	xa^2
$\mathbf{a}$	a	a^2	1	xa^2	x	xa
$\mathbf{a^2}$	a^2	1	a	xa	xa^2	x
$\mathbf{x}$	x	xa	xa^2	1	a	a^2
$\mathbf{xa}$	xa	xa^2	x	a^2	1	a
$\mathbf{xa^2}$	xa^2	x	xa	a	a^2	1

Table 1: Multiplication table for the dihedral group D_3. Note that the group is nonabelian: gh is not equal to hg. The element gh would be found in the row labeled by g and the column labeled by h.

(b) *What are the symmetry group elements given by the paths in Fig. 8 (a) and (b)? Explain in words why* $xax^{-1} = a^{-1}$. *Use the multiplication rules to calculate* $xa^2 \otimes xa$ *and* $xa \otimes xa^2$. *Compare your answers to those in the table.*

We know from part (a) that two different dihedral symmetry group elements can be topologically equivalent – so the defect strength is not just given by the element of D_3. We shall explore this further below. But first, let us see if the same dihedral symmetry group element can correspond to two non-equivalent topological defects.

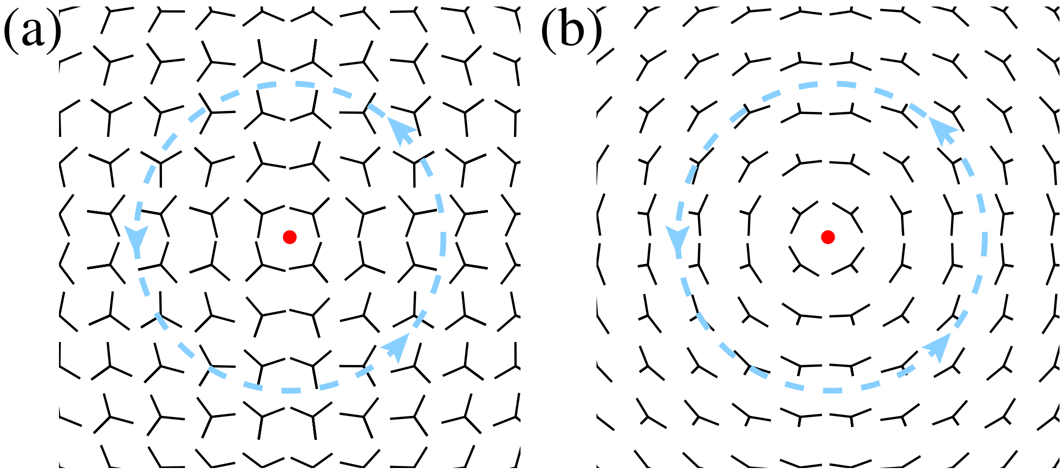

Fig. 9 Two equivalent defects, one with the molecules confined to the plane, and the other with one leg rotated to point 'upward'.

(c) *What is the winding number of the defect shown in Fig. 9(a)? If* D_3 *were the homotopy group, and we were to assign this defect an element of* D_3*, which element would it be? What does this suggest about the defect?* Can we heal this defect by rotating into the third dimension? *Does the rotation into the third dimension shown in Fig. 9(b) heal the defect in the order parameter field?*

We need a homotopy group that somehow has a category for a defect that returns the molecule to its original orientation trivially (the identity element in D_3), and somehow also allows a defect to return the molecule differently (nontrivially) to the same labelling of the legs (the element a^3). There is a wonderful treatment of the topological theory of defects by Mermin [3], which we draw upon here.

How can a 2π rotation in three dimensions be different from the identity? For those experienced in quantum physics, rotating a spin ½ electron by 2π changes the sign of the wavefunction. This is because the spin wavefunction is represented not by a vector, but by a 2×2 unitary matrix in SU(2), and there are two SU(2) matrices for every rotation in SO(3). Similarly, in our problem for every rotation g in D_3 there are two rotations $\pm g$ in Dic_3: the 12-element *dicyclic* group, which is the first homotopy group for our dihedral liquid crystal.[13] The multiplication rules for Dic_3 are

$$\mathrm{Dic}_3 = \left\langle x, a \;\middle|\; x^2 = -1, a^3 = -1, xax^{-1} = a^{-1} \right\rangle \tag{8}$$

Here we presume that a corresponds to a 1/3 counter-clockwise turn. (We will not write out the whole multiplication table.)

(d) *View the defect in Fig. 9(a) as three* 1/3 *counterclockwise turns. What is the homotopy group element in* Dic_3 *for the defect? How did lifting to* Dic_3 *fix the problem we had in part (c)?*

The rotation of the molecular orientation by 2π gives a net minus sign, just as for an electron spin.

Now we still need to understand how the two defects in Fig. 8, with different group elements (in both D_3 and Dic_3), can be the same defect. Mermin tells us that defects with non-abelian homotopy groups are not classified by their homotopy group elements, but by the *conjugacy classes* of the group. The conjugacy classes are subsets of the group whose elements are related by conjugation. Two group elements g and h are said to be conjugate if there exists a group element γ such that $h = \gamma g \gamma^{-1}$.

(e) *Show in complete generality that the identity element* $g = 1$ *of a homotopy group is the only element in its conjugacy class. Interpret this physically: can there be two different ways of having no defect?* One can check that -1 commutes with all other group elements, implying that it too is the only element in its class.

Do the two defects in Fig. 8 indeed lie in the same conjugacy class?

(f) *What is the homotopy group element* $\beta \in \mathrm{Dic}_3$ *for the defect in Fig. 8(a)?* The two defects in that figure combine to form no defect, so the defect in Fig. 8(b) must have homotopy group element $\widehat{\beta} = \beta^{-1}$. *Find a group element* γ *that shows* $\widehat{\beta} = \gamma \beta \gamma^{-1}$.

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[13] Mermin tells us [3] that the order parameter space of our dihedral liquid crystal is $\mathrm{SO}(3)/D_3$ (the continuous broken symmetry modulo the residual symmetry group). The first homotopy group of a simply–connected group modulo a discrete subgroup is the discrete subgroup – but SO(3) is not simply connected. He prescribes using the simply-connected universal cover SU(2), and the corresponding discrete group Dic_3. Thus $\Pi_1\left(SO(3)/D_3\right) \cong \Pi_1\left(SU(2)/\mathrm{Dic}_3\right) \cong \mathrm{Dic}_3$.

Is there a physical reason for this peculiar conjugacy class[14] criterion? Indeed: it is precisely the transformation of the defect β when it *braids* around another defect γ.

Braiding[15] in three dimensions is associated with hair-styling: you take two or more strings of hair or string and weave them over and under one another to form a kind of rope. If we move a point defect with strength β in two dimensions around another defect α (with the necessary continuous readjustments of the order parameter fields), we can view the process as braiding in space-time.

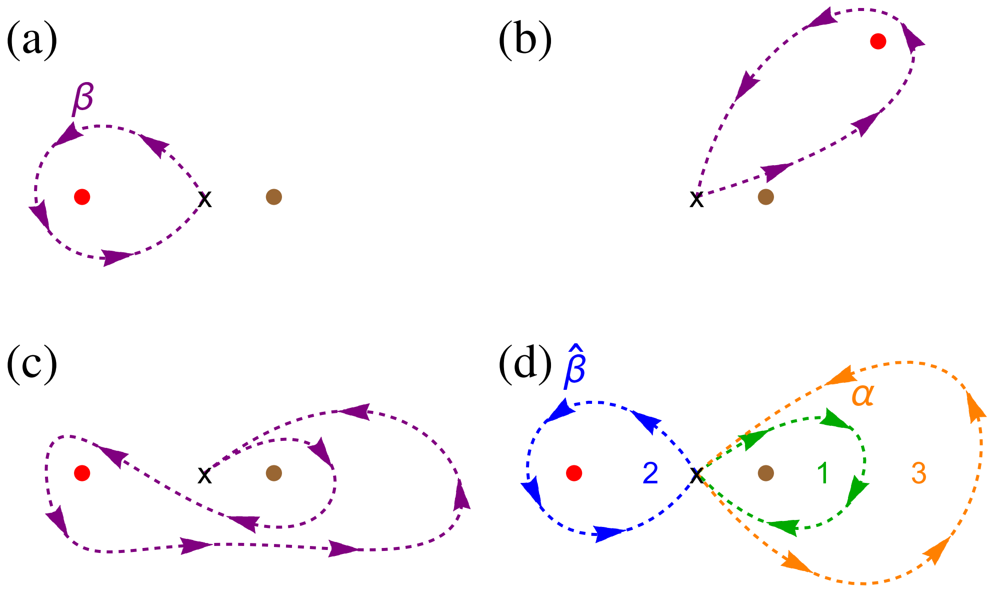

Fig. 10 Braiding two defects. (a-d) can represent the motion of a red two-dimensional point defect around a brown defect in time, or a red line defect curling around a brown line defect in three dimensions. (a) The red defect has strength β, measured by the path beginning and ending at **X**. (The connection to **X** makes this a *based* homotopy class, which is important for the argument but not crucial here.) (b-c) The defect is continuously dragged around the brown defect of strength α. The measured strength cannot change, either as the red defect continuously is dragged, or as the path anchored at **X** is continuously modified to surround β without touching α. (d) When the red defect returns to its original position, the original path 2 may measure a different strength $\widehat{\beta}$ than β measured by the deformed path ($1 \to 2 \to 3$).

Figure 10 visually argues that a defect β encircling a defect α indeed changes its ho-

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[14] The conjugacy classes of Dic_3 are as follows:

$$\begin{gathered} C_0 = \{1\}\,,\ \ \overline{C_0} = \{-1\}\,,\ \ C_1 = \left\{a, -a^2\right\}\,,\ \ C_2 = \left\{a^2, -a\right\}\,, \\ C_{\text{even}} = \left\{x, xa^2, -xa\right\}\,,\ \ C_{\text{odd}} = \left\{xa, -x, -xa^2\right\}\,. \end{gathered} \tag{9}$$

[15] Braiding is important for the study of anyons. Nonabelian braiding is important for topological quantum computing.

motopy group element.[16] It argues that the original path β deforms into another path (in the same homotopy class) as the defect circumnavigates α. This path becomes the product of three simpler loops.

(g) *In Fig. 10(d), what homotopy group elements g_1, g_2, and g_3 correspond to the three segments of the path?* (The labels $\widehat{\beta}$ and α suggest the answers for two of the three.) *What is β, in terms of g_1, g_2, and g_3?*[17] *What is $\widehat{\beta}$ in terms of β and α?*

The schematic of braiding in Figure 10 is translated into a real configuration of our order parameter with two defects in Figure 11.

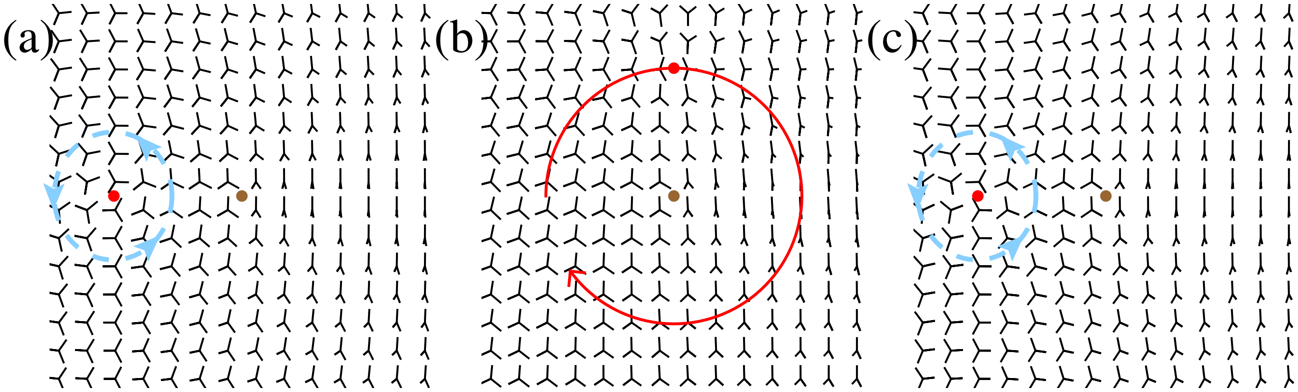

Fig. 11 Braiding in practice. (a) The order parameter field in the vicinity of two defects. (b) The order parameter field after one defect has been pulled a quarter-way around the other. (c) The resulting order parameter field after the braiding process. Also, view the evolution of the order parameter in time at the course Web site [6].

(h) *What is the homotopy group element $\beta \in \mathrm{Dic}_3$ of the left defect in Fig. 11(a)? What is the element α for the defect in the center of the figure?*[18] The central brown defect does not change during the braiding process, just as in Figure 11. *What is the homotopy group element $\widehat{\beta}$ for the left defect in frame (c)? Use the group multiplication rules (eqn 8) to verify that your prediction in part (g) for $\widehat{\beta}$ is correct.*

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[16] We found in Fingerprints (Exercise 9.17) that moving a dislocation around a disclination can change the sign of its Burger's vector. This too is due to a non-abelian homotopy group, discussed by Poenaru et al. [4] in one of the founding papers in this field. They find that the combined order parameter space of rotations and translations relevant for fingerprints is the Klein bottle. Its first homotopy group is nonabelian, which provides an explanation for the dislocation annihilation in Fig. 9.36.

[17] It turns out that there is ambiguity in whether a concatenation of two loops (traveling along 1 and then 2) with homotopy elements g_1 and g_2 corresponds to a single combined loop with homotopy element $g_1 g_2$ or $g_2 g_1$. However, once a convention is chosen, the element assigned to the concatenation of several loops $g_1, \ldots, g_n$ is fixed. You are free to choose this convention.

[18] The element assigned to this defect also depends on multiple conventions, including whether the molecules in Fig. 11 rotate up or down in the third dimension. Your choice of convention will affect the element α, but not the result of the braiding $\widehat{\beta}$.

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