

**Problem Set 2: Quantum Dynamics, Path Integrals, and Aharonov Bohm
Graduate Quantum I**

Physics 6572

James Sethna

Due Monday September 10

Last correction at September 22, 2012, 9:20 am

Reading

Sakurai and Napolitano, sections 1.6, chapter 2

2.1 **Commutation of functions of x and p :** Sakurai and Napolitano, exercise 1.29.

2.2 **Dirac δ -functions.** (Math) ③

Quantum bound-state wavefunctions are unit vectors in a complex Hilbert space. If there are N particles in 3 dimensions, the Hilbert space is the space of complex-valued functions $\psi(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^{3N}$ whose absolute squares are integrable: $\int d\mathbf{x} |\psi(\mathbf{x})|^2 < \infty$.

But what about unbound states? For example, the propagating plane-wave states¹ $\psi(x) = |k\rangle \propto \exp(ikx)$ for a free particle in one dimension? Because unbound states are spread out over an infinite volume, their probability density at any given point is zero – but we surely don't want to normalize $|k\rangle$ by multiplying it by zero.

Mathematicians incorporate continuum states by extending the space into a *rigged Hilbert space*. The trick is that the unbound states form a *continuum*, rather than a discrete spectrum – so instead of summing over states to decompose wavefunctions $|\phi\rangle = \mathbb{1}\phi = \sum_n |n\rangle\langle n|\phi\rangle$ we integrate over states $\phi = \mathbb{1}\phi = \int dk |k\rangle\langle k|\phi\rangle$. This tells us how we must normalize our continuum wavefunctions: instead of the Kronecker- δ function $\langle m|n\rangle = \delta_{mn}$ enforcing orthonormal states, we demand $|k'\rangle = \mathbb{1}|k'\rangle = \int dk |k\rangle\langle k|k'\rangle = |k'\rangle = \int dk |k\rangle\delta(k - k')$ telling us that $\langle k|k'\rangle = \delta(k - k')$ is needed to ensure the useful decomposition $\mathbb{1} = \int dk |k\rangle\langle k|$.

Let's work out how this works as physicists, by starting with the particles in a box, and then taking the box size to infinity. For convenience, let us work in a one dimensional box $0 \leq x < L$, and use *periodic boundary conditions*, so $\psi(0) = \psi(L)$. This choice allows us to continue to work with plane-wave states $|n\rangle \propto \exp(ik_n x)$ in the box. (We could have used a square well with infinite sides, but then we'd need to fiddle with wave-functions $\propto \sin(kx)$.)

(a) *What values of k_n are allowed by the periodic boundary conditions? What is the separation Δk between successive wavevectors? Does it go to zero as $L \rightarrow \infty$, leading to a continuum of states?*

¹Here mathematically $\psi(x) = \langle x|k\rangle$; $|k\rangle$ is an abstract vector, and $\psi(x)$ are its coordinates in a particular basis. But physicists often abuse notation: this is equivalent to writing $\vec{F} = (3.0, 4.0, 2.0)$.

To figure out how to normalize our continuum wavefunctions, we now start with the relation $\langle m|n\rangle = \delta_{mn}$ and take the continuum limit. We want the normalization N_k of the continuum wavefunctions to give $\langle k|k'\rangle = \int_{-\infty}^{\infty} N_k N_{k'} \exp(i(k' - k)x) dx = \delta(k - k')$.

(b) What is the normalization $\langle x|n\rangle = N_n \exp(ik_n x)$ for the discrete wave-functions in the periodic box, to make $\langle m|n\rangle = \int_0^L N_m N_n \exp(i(k_n - k_m)x) dx = \delta_{mn}$? Write $\mathbb{1} = \sum_n |n\rangle\langle n|$, and change the sum to an integral in the usual way ($\int dk |k\rangle\langle k| \approx \sum_n |n\rangle\langle n| \Delta k$). Show that the normalization of the continuum wavefunctions must be $N_k = 1/\sqrt{2\pi}$, so $\psi_k(x) = \langle x|k\rangle = \exp(ikx)/\sqrt{2\pi}$. (Hint: If working with operators is confusing, ensure that $\langle x|\mathbb{1}|x'\rangle$ for $0 < x, x' < L$ is the same for $\mathbb{1} = \sum_n |n\rangle\langle n|$ (valid in the periodic box) and for $\mathbb{1} = \int dk |k\rangle\langle k|$ (valid for all x).

Notice some interesting ramifications:

I. The fact that our continuum plane waves have normalization $1/\sqrt{2\pi}$ incidentally tells us one form of the δ function:

$$\delta(k - k') = \langle k|k'\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(i(k' - k)x) dx. \quad (1)$$

Also, $\delta(x - x') = 1/(2\pi) \int_{-\infty}^{\infty} dk \exp(-ik(x' - x))$.

II. The same normalization is used for ‘position eigenstates’ $|x\rangle$, so $\langle x'|x\rangle = \delta(x' - x)$ and $\mathbb{1} = \int dx |x\rangle\langle x|$.

III. The Fourier transform can be viewed as a change of variables from the basis $|x\rangle$ to the basis $|k\rangle$:

$$\tilde{\phi}(k) = \langle k|\phi\rangle = \langle k|\mathbb{1}|\phi\rangle = \int dx \langle k|x\rangle \langle x|\phi\rangle = 1/\sqrt{2\pi} \int dx \exp(-ikx) \phi(x) \quad (2)$$

Note that this definition is different from that I used in the appendix of my book (Statistical Mechanics: Entropy, Order Parameters, and Complexity, <http://pages.physics.cornell.edu/~sethna/StatMech/EntropyOrderParametersComplexity.pdf>); there the 2π is placed entirely on the inverse Fourier transform, which here it is split symmetrically between the two, so the inverse Fourier transform is

$$\phi(x) = \langle x|\phi\rangle = \langle x|\mathbb{1}|\phi\rangle = \int dk \langle x|k\rangle \langle k|\phi\rangle = 1/\sqrt{2\pi} \int dk \exp(ikx) \tilde{\phi}(k). \quad (3)$$

IV. The Dirac δ -function can be written in many different ways. It is basically the limit² as $\epsilon \rightarrow 0$ of sharply-peaked, integral-one functions of width ϵ and height $1/\epsilon$ centered at zero. Let’s use this to derive the useful relation:

$$\lim_{\epsilon \rightarrow 0^+} \frac{1}{x - i\epsilon} = p.v. \frac{1}{x} + i\pi\delta(x). \quad (4)$$

²Clearly this is not a limit in the ordinary sense: the difference between functions does not go to zero as ϵ goes to zero, but rather (within ϵ of the origin) has large positive and negative values that cancel. It is a *weak limit* – when integrated against any smooth functions, the differences go to zero.

Here all these expressions are meant to be inside integrals, and p.v. is the Cauchy principal value of the integral:³

$$p.v. \int_{-\infty}^{\infty} = \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty}. \quad (5)$$

(c) Note that $\epsilon/(x^2 + \epsilon^2)$ has half-width ϵ at half-maximum, height ϵ , and integrates to π , so basically (i.e., in the weak limit) $\lim_{\epsilon \rightarrow 0} \epsilon/(x^2 + \epsilon^2) = \pi\delta(x)$. Argue that $\lim_{\epsilon \rightarrow 0} \int f(x)/(x - i\epsilon) dx = p.v. \int f(x)/x dx + i\pi f(0)$. (Hints: The integral of $1/(1+y^2)$ is $\arctan(y)$, which becomes $\pm\pi/2$ at $y = \pm\infty$. Multiply numerator and denominator by $x + i\epsilon$.)

2.3 Entangled Spins. (Spins) ③

In class, we studied the entanglement of the singlet spin state $|\mathcal{S}\rangle = (1/\sqrt{2})(|\uparrow\rangle_\ell|\downarrow\rangle_r - |\downarrow\rangle_\ell|\uparrow\rangle_r)$ of electrons of a diatomic molecule as the atoms L and R are separated;⁴ the spins on the two atoms are in opposite directions, but the system is in a superposition of the two choices. Here we discuss another such superposition, but with a different relative phase for the two choices:

$$|\chi\rangle = (1/\sqrt{2})(|\uparrow\rangle_\ell|\downarrow\rangle_r + |\downarrow\rangle_\ell|\uparrow\rangle_r) \quad (6)$$

You should know from angular momentum addition rules that the space of product wavefunctions of two spin $1/2$ states can be decomposed into a spin 1 and a spin 0 piece: $1/2 \otimes 1/2 = 1 \oplus 0$. So there are two orthogonal eigenstates of S_z with eigenvalue zero: one of total spin zero and one of total spin one.

(a) **Total spin.** Which state is which? (If you don't know from previous work, calculate!) Why do we call $|\mathcal{S}\rangle$ a singlet?

Now, is the spin wavefunction compatible with what we know about electron wavefunctions?

(b) **Symmetry.** When the two spins are exchanged, how does $|\chi\rangle$ change? If the total wavefunction $\Psi(x_L, s_L, x_R, s_R)$ is a product of this spin wavefunction $\chi(s_L, s_R)$ and a two-particle spatial wavefunction $\psi(x_L, x_R)$, what symmetry must ψ have under interchange of electrons?

We noted in class that two other spin-1 product states, $|\uparrow\rangle_\ell|\uparrow\rangle_r$ and $|\downarrow\rangle_\ell|\downarrow\rangle_r$ do not form entangled states when L and R separate. Is $|\chi\rangle$ like these spin-1 states, or is it entangled like $|\mathcal{S}\rangle$ is?

³If $f(x)$ is positive at zero, $\int f(x)/x dx$ is the sum of minus infinity for $x < 0$ and positive infinity for $x > 0$; taking the principal value tells us to find the sum of these two canceling infinities by chopping them symmetrically about zero.

⁴We assumed that, when separated, one electron is localized basically on each of the two atoms, and the spin kets are labeled based on the primary locale of the corresponding spatial wavefunction for that electron.

(c) **Entanglement.** Give the Schmidt decomposition of $|\chi\rangle$. What are the singular values? What is the entanglement entropy? (Hint: The steps should be very familiar from class.)

(d) **Singular Value Decomposition (SVD).** Let M be the matrix which gives $|\chi\rangle$ as a product of left and right spin states:

$$|\chi\rangle = (|\uparrow\rangle_\ell \ |\downarrow\rangle_\ell) M \begin{pmatrix} |\uparrow\rangle_r \\ |\downarrow\rangle_r \end{pmatrix}. \quad (7)$$

What is M ? Give an explicit singular value decomposition⁵ $M = U\Sigma V^T$ of the matrix M . Explain how the SVD gives us the Schmidt decomposition of part (c).

2.4 Aharonov-Bohm Wire. (ParallelTransport) ③

What happens to the electronic states in a thin metal loop as a magnetic flux Φ_B is threaded through it? This was a big topic in the mid-1980's, with experiments suggesting that the loops would develop a spontaneous current, that depended on the flux Φ_B/Φ_0 , with $\Phi_0 = hc/e$ the 'quantum of flux' familiar from the Bohm-Aharonov effect. In particular, Nandini Trivedi worked on the question while she was a graduate student here:

Nandini Trivedi and Dana Browne, 'Mesoscopic ring in a magnetic field: Reactive and dissipative response', *Phys. Rev. B* **38**, 9581-9593 (1988);

she's now a faculty member at Ohio State.

Some of the experiments clearly indicated that the periodicity in the current went as $\Phi_0/2 = hc/2e$ – half the period demanded by Bohm and Aharonov from fundamental principles. (This is OK; having a *greater* period would cause one to wonder about fractional charges.) Others found (noisier) periods of Φ_0 . Can we do a free-particle-on-a-ring calculation to see if for some reason we get half the period too?

Consider a thin wire of radius R along $x^2 + y^2 = R^2$. Let a solenoid containing magnetic flux Φ_B , thin compared to R , lie along the \hat{z} axis. Let ϕ be the angle around the circle with respect to the positive x -axis. (Don't confuse the flux Φ_B with the angle ϕ !) We'll assume the wire confines the electron to lie along the circle, so we're solving a one-dimensional Schrödinger's equation along the coordinate $s = R\phi$ around the circle. Assume the electrons experience a random potential $V(s)$ along the circumference $C = 2\pi R$ of the wire.

(a) Choose a gauge for \vec{A} so that it points along $\hat{\phi}$. What is the one-dimensional time-independent Schrödinger equation giving the eigenenergies for electrons on this ring? What is the boundary conditions for the electron wavefunction ψ at $s = 0$ and $s = C$?

⁵Remember that the SVD guarantees that U and V have orthonormal columns, and Σ is a diagonal matrix whose diagonal elements σ_i are all positive and decreasing (so $\sigma_i \geq \sigma_{i+1} \geq 0$). There is some flexibility in the singular vectors (i.e., matched pairs can both have their signs changed), but the singular values are unique and hence a property of the matrix.

(Hint: the wire is a circle; nothing fancy yet. I'm not asking you to solve the equation – only to write it down.)

Deriving the Bohm-Aharonov effect using Schrödinger's equation is easiest done using a singular gauge transformation.

(b) Consider the gauge transformation $\Lambda(r, \phi) = -\phi\Phi_B/(2\pi)$. Show that $\vec{A}' = \vec{A} + \nabla\Lambda$ is zero along the wire for $0 < s < C$, so that we are left with a zero-field Schrödinger equation. What happens at the endpoint C ? What is the new boundary condition for the electron wave function ψ' after this gauge transformation? Does the effect vanish for $\Phi_B = n\Phi_0$ for integer n , as the Bohm-Aharonov effect says it should?

Realistically, the electrons in a large, room-temperature wire get scattered by phonons or electron-hole pairs (effectively, a quantum measurement of sorts) long before they propagate around the whole wire, so these effects were only seen experimentally when the wires were cold (to reduce phonons and electron-hole pairs) and 'mesoscopic' (tiny, so the scattering length is comparable to or larger than the circumference).

Finally, let's assume free electrons, so $V(s) = 0$. What's more, to make things simpler, let's imagine that there is only one electron in the wire.

(c) Ignoring the energy needed to confine the electrons into the thin wire, solve the one-dimensional Schrödinger equation to give the ground state of the electron as a function of Φ_B . Plot the current in the wire as a function of Φ_B . Is it periodic with period Φ_0 , or periodic with period $\Phi_0/2$?

In the end, it was determined that there were two classes of experiments. Those that measured many rings at once (measuring an average current, an easier experiment) got periodicity of $hc/2e$, while those that attempted the challenge of measuring one mesoscopic ring at a time find hc/e .

2.5 Superfluid order and vortices. (Quantum, Condensed matter) ③

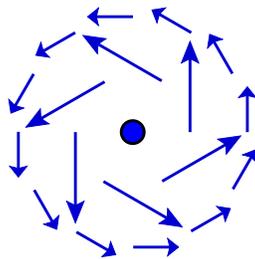


Fig. 1 Superfluid vortex line. Velocity flow $\mathbf{v}(\mathbf{x})$ around a superfluid vortex line.

Superfluidity in helium is closely related to Bose condensation of an ideal gas; the strong interactions between the helium atoms quantitatively change things, but many properties are shared. In particular, we describe the superfluid in terms of a complex number $\psi(\mathbf{r})$, which we think of as a wavefunction which is occupied by a large fraction of all the atoms in the fluid.

(a) If N non-interacting bosons all reside in the same single-particle state with wavefunction $\zeta(\mathbf{r})$, write an expression for the net current density $J(\mathbf{r})$.⁶ Write the complex field $\zeta(\mathbf{r})$ in terms of an amplitude and a phase, $\zeta(\mathbf{r}) = |\zeta(\mathbf{r})| \exp(i\phi(\mathbf{r}))$. We write the superfluid density as $n_s = N|\zeta|^2$. Give the current J in terms of ϕ and n_s . What is the resulting superfluid velocity, $v = J/n_s$? (It should be independent of n_s .)

The Landau order parameter in superfluids $\psi(\mathbf{r})$ is traditionally normalized so that the amplitude is the square root of the superfluid density; in part (a), $\psi(\mathbf{r}) = \sqrt{N}\zeta(\mathbf{r})$.

In equilibrium statistical mechanics, the macroscopically occupied state is always the ground state, which is real and hence has no current. We can form non-equilibrium states, however, which macroscopically occupy other quantum states. For example, an experimentalist might cool a container filled with helium while it is moving; the ground state in the moving reference frame has a current in the unmoving laboratory frame. More commonly, the helium is prepared in a rotating state.

(b) Consider a torus filled with an ideal Bose gas at $T = 0$ with the hole along the vertical axis; the superfluid is condensed into a state which is rotating around the hole. Using your formula from part (a) and the fact that $\phi + 2n\pi$ is indistinguishable from ϕ for any integer n , show that the circulation $\oint v \cdot d\mathbf{r}$ around the hole is quantized. What is the quantum of circulation?

Superfluid helium cannot swirl except in quantized units! Notice that you have now explained why superfluids have no viscosity. The velocity around the torus is quantized, and hence it cannot decay continuously to zero; if it starts swirling with non-zero n around the torus, it must swirl forever.⁷ This is why we call them superfluids.

In bulk helium this winding number labels line defects called *vortex lines*.

2.6 Parallel Transport, Frustration, and the Blue Phase. (Liquid Crystals) ③

“Relieving Cholesteric Frustration: The Blue Phase in a Curved Space,” J. P. Sethna, D. C. Wright and N. D. Mermin, *Phys. Rev. Lett.* **51**, 467 (1983).

“Frustration, Curvature, and Defect Lines in Metallic Glasses and the Cholesteric Blue Phases,” James P. Sethna, *Phys. Rev. B* **31**, 6278 (1985).

“Frustration and Curvature: the Orange Peel Carpet”, <http://www.lassp.cornell.edu/sethna/FrustrationCurvature/>

“The Blue Phases, Frustrated Liquid Crystals and Differential Geometry”, <http://www.lassp.cornell.edu/sethna/LiquidCrystals/BluePhase/BluePhases.html>.

⁶You can use the standard quantum mechanics single-particle expression $J = (\hbar/2m)(\zeta\nabla\zeta^* - \zeta^*\nabla\zeta)$ and multiply by the number of particles, or you can use the many-particle formula $J(\mathbf{r}) = (\hbar/2m) \int d^3\mathbf{r}_1 \cdots d^3\mathbf{r}_N \sum_\ell \delta(\mathbf{r}_\ell - \mathbf{r})(\Psi\nabla_\ell\Psi^* - \Psi^*\nabla_\ell\Psi)$ and substitute in the condensate wavefunction $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_n \zeta(\mathbf{r}_n)$.

⁷Or at least until a dramatic event occurs which changes n , like a vortex line passing across the torus, demanding an activation energy proportional to the width of the torus. See also Exercise (7.9) in my book.

(Optional: for those wanting a challenge.) Both the Aharonov Bohm effect and Berry's phase (later) are generalizations of the idea of *parallel transport*. Parallel transport, from differential geometry, tells one how to drag tangent vectors around on smooth surfaces. Just as we discovered that dragging the phase of a wavefunction around a closed loop in space gave it a net rotation due to the magnetic field (Aharonov-Bohm), the phase can rotate also when the Hamiltonian is changed around a closed curve in Hamiltonian space (Berry's phase). Here we discuss how vectors rotate as one drags them around closed loops, leading us to the *curvature tensor*.

(a) **Parallel transport on the sphere.** *Imagine you're in St. Louis (longitude 90° W, latitude ~ 40° N), pointing north. You walk around a triangle, first to the North Pole, then take a right-angle turn, walk down through Greenwich, England and Madrid, Spain (longitude ~ 0° W) down to the equator, turn right, walk back to longitude 90° W along the equator, turn north, and walk back to St. Louis. All during the walk, you keep pointing your finger in the same direction as far as feasible (i.e., straight ahead on the first leg, off to the left on the second, and so on). What angle does the vector formed by your final pointing finger make with respect to your original finger? If you turned west in Madrid and walked along that latitude (~ 40° N) to St. Louis (yes, it's just as far north), would the angle be the same? (Hint: what about transport around a tiny quarter circle centered at the north pole?)*

Lightning Intro to Differential Geometry. Parallel transport of vectors on surfaces is described using a *covariant derivative* $(D_i v)^j = \partial_i v^j + \Gamma_{ik}^j v^k$ involving the Christoffel symbol Γ_{ik}^j . The amount a vector v^i changes when taken around a tiny loop $\Delta s \Delta t (-\Delta s) (-\Delta t)$ is given by the Riemannian curvature tensor and the area of the loop

$$v^i - v^i = R_{jkl}^i v^j \Delta s^k \Delta t^l. \quad (8)$$

The algebra gets messy on the sphere, though (spherical coordinates are pretty ugly).

Instead, we'll work with a twisty kind of parallel transport, that my advisor and I figured out describe how molecules of the Blue Phase like to locally align. These long, thin molecules locally line up with their axes in a direction $\mathbf{n}(\mathbf{r})$, and are happiest when that axis twists so as to make zero the covariant derivative

$$(D_i n)^j = \partial_i n^j - q \epsilon_{ijk} n_k, \quad (9)$$

where ϵ_{ijk} is the totally antisymmetric tensor⁸ with three indices (Fig. 2 and 3). Since the Blue Phases are in flat space, you don't need to worry about the difference between upper and lower indices.

⁸Hence $\Gamma_{ik}^j = -q \epsilon_{ijk}$. Warning: this connection has *torsion*: it's not symmetric under interchange of the two bottom indices. This is what allows it to have a non-zero curvature even when the liquid crystal lives in flat space. But it will make some of the traditional differential geometry formulas incorrect, which usually presume zero torsion.

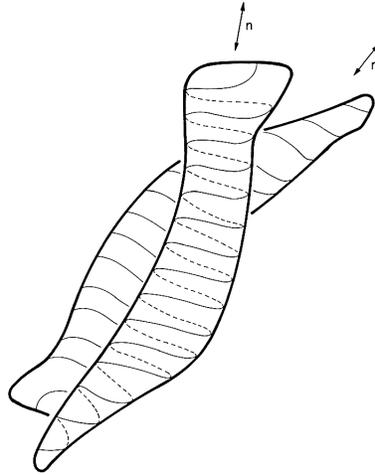


Fig. 2 Blue Phase Molecules, long thin molecules aligned along an axis $\hat{\mathbf{n}}(\mathbf{r})$, like to sit at a slight angle with respect to their neighbors. To align the threads and grooves on the touching surface between the molecules demands a slight twist. This happens because, like threaded bolts or screws, these molecules are *chiral*.

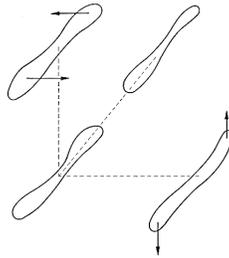


Fig. 3 Twisted Parallel Transport. The natural parallel transport, $D_i n_j = \partial_i n_j - q\epsilon_{ijk} n_k$, twists perpendicular to the long axis, but doesn't twist when moving along the axis.

(b) What direction will a molecule with $\mathbf{n} = \hat{x}$ like to twist as one moves along the x -direction? The y -direction? The z -direction? Is the local low energy structure more like that of Fig. 4(a) (the low-temperature state of this system), or that of Fig. 4(b)?

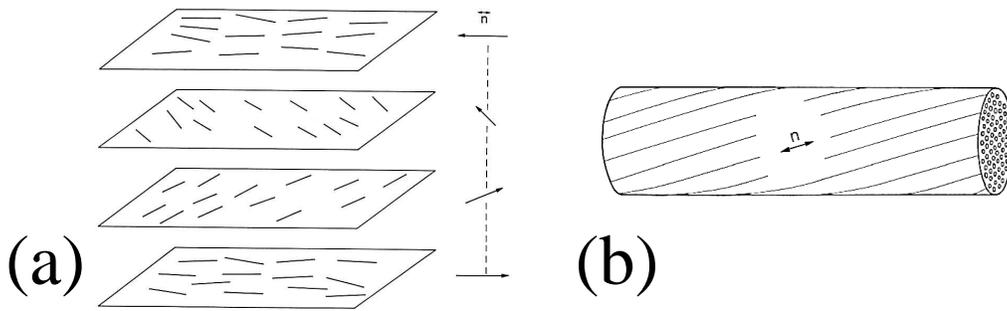


Fig. 4 Local structures of cholesteric liquid crystals. (a) Helical. (b) Tube.

So, what's the curvature tensor (eqn 8) for the blue phase? I figured out at the time that it came out to be

$$R_{ijkl} = q^2(\delta_{il}\delta_{kj} - \delta_{ik}\delta_{lj}). \quad (10)$$

This curvature means that the blue phases are *frustrated*; you can't fill space everywhere with material that's 'happy', with $D\mathbf{n} = \mathbf{0}$.

(c) If \mathbf{n} starts at \hat{x} , and we transport along the tiny loop $\{\Delta x, \Delta y, -\Delta x, -\Delta y\}$, calculate the vector \mathbf{n}' as it returns to the origin using the curvature tensor (eqns 8 and 10). according to eqn (8) Is the shift in \mathbf{n} along the same direction we observe for the larger loop in Fig 5?

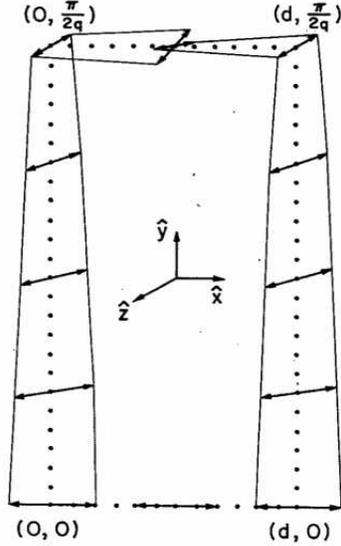


Fig. 5 Parallel transport frustration. We can check your answer to part (c) qualitatively by thinking about a larger loop (Fig. 5). Consider starting from two places separated $\Delta x = d$ apart along the axis of a double-twisting region (the center of the tube in Fig. 4(b)). If we move a distance $\Delta y = \pi/(2q)$ radially outward, the orientation of both will now point along \hat{z} . Transporting them each inward by $d/2$ then will cause a further twist.

We can use the curvature tensor of the Blue Phase to calculate a scalar curvature $R_{ijij} = -6q^2$. Thus the blue phases are negatively curved, even though they live in flat space. We looked to see what would happen if we put the blue phases into a positively curved space. Picking the sphere in four dimensions with the correct radius, we could make the curvature (and the frustration) go away, and find the ideal template for the blue phases. We think of the real blue phase as pieces of this ideal template, cut, flattened, and sewn together to fill space, like an orange-peel carpet (Fig. 6).

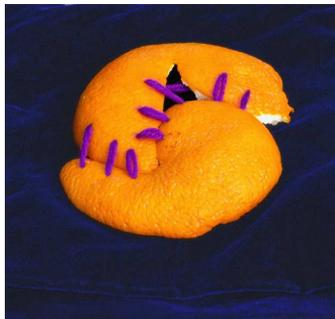


Fig. 6 Orange-peel carpet. (Copyright Pamela Davis Kivelson)