

# Phys 251A Problem Set 6

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1. In this problem we will compute some prefactors we neglected in lecture and, in the process, understand objects known as “functional determinants.” It is recommended to do the following two problems in order.

(a) Show that

$$\int_{-\infty}^{\infty} dx_1 \cdots dx_n e^{-\frac{1}{2} \mathbf{x}^T A \mathbf{x}} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$

where  $\mathbf{x} = (x_1, \dots, x_n)^T$  and  $A$  is an  $n \times n$  real, symmetric, positive-definite matrix. You should write your answer in terms of the determinant of  $A$ . To do the integral, you should perform a change of variables via an orthogonal matrix that diagonalizes  $A$ . To account for the change in the integration measure, you should use that the determinant of orthogonal matrix is  $\pm 1$ . Finally, you will want to use the fact that the determinant is the product of eigenvalues.

(b) Calculate

$$\int_{-\infty}^{\infty} d^2 z_1 \cdots d^2 z_n e^{-\frac{1}{2} \mathbf{z}^\dagger K \mathbf{z}}$$

in terms of  $\det K$  where  $\mathbf{z} = (z_1, \dots, z_n)^T$  is a vector of complex numbers and  $K = K^\dagger$  is a positive definite Hermitian matrix. You should use a similar argument as in (a), suitably generalized to the complex case.

(c) Recall the propagator that we calculated from the path integral in lecture

$$\langle x_F, T | x_i, 0 \rangle = \langle x_f | e^{-iHT} | x_i \rangle = C(T) \exp\left(\frac{im}{2\hbar} \frac{(x_f - x_i)^2}{T}\right) \quad (1)$$

where

$$C(T) = \int_{y(0)=0}^{y(T)=0} \mathcal{D}y \exp\left(\frac{im}{2\hbar} \int_0^T \dot{y}^2 dt\right) = \int_{y(0)=0}^{y(T)=0} \mathcal{D}y \exp\left(-\frac{m}{2\hbar} \int_0^{\tau_0} (\partial_\tau y)^2 d\tau\right).$$

In the second step we have changed variables to  $\tau = it$  and defined  $\tau_0 = iT$ .

The normalization of  $C(T)$  is subtle, because the path integral measure  $\mathcal{D}y$  is tricky to define in a finite way. It is easier to deduce the correct normalization through comparing with the operator formalism.

Compute  $C(T)$  by starting with

$$1 = \int dx' \langle x' | x \rangle$$

and inserting  $UU^\dagger$  inside the bracket, where  $U = e^{-iHt}$ . Insert a resolution of the identity between  $U$  and  $U^\dagger$ , and identify the two factors as propagators. Use the identity derived in lecture, (1), and perform the gaussian integrals to arrive at an expression for  $C(T)$ . Note that  $C(T) > 0$  when  $\tau_0 = iT$  is real and positive from the path integral definition; this can be used to fix the phase of  $C(T)$ .

If you wish, the integral can be calculated by assuming that  $\tau_0$  is real, and subsequently “analytically continuing” to imaginary  $\tau_0$  and real  $T$ . This simply amounts to substituting  $iT$  for  $\tau_0$  in the final expression and treating  $T$  as ordinary real time. Alternatively you can do the real time integral directly and argue that the rapid oscillations at infinity cancel out with each other, or use contour integral techniques to rotate the contour to be some, arbitrary, diagonal of the complex plane.

2. In this problem we will use one example to illustrate the adiabatic theorem. Consider the Hamiltonian

$$H(\mathbf{B}) = \frac{\hbar\gamma}{2} \mathbf{B} \cdot \boldsymbol{\sigma}$$

where the magnetic field  $\mathbf{B}(t)$  is changing very slowly as  $\mathbf{B}(t) = B_0(\cos \phi(t), \sin \phi(t), 0)$ , where  $\phi(t) = 2\pi t/T$ .

- (a) Find the instantaneous eigenstates  $|\psi_{\pm}(t)\rangle$  and their eigenvalues  $E_{\pm}(t)$  at time  $t$ . Show that the eigenvalues are time-independent.
- (b) For an arbitrary state  $|\alpha, t\rangle = c_+(t)|\psi_+(t)\rangle + c_-(t)|\psi_-(t)\rangle$ , calculate the time derivative of the coefficients  $\dot{c}_{\pm}(t)$  in terms of  $c_{\pm}(t)$ . Express your result as a  $2 \times 2$  matrix transformation:

$$\begin{pmatrix} \dot{c}_+ \\ \dot{c}_- \end{pmatrix} = \mathbf{M}_{2 \times 2} \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

- (c) Write  $\Delta = |E_+ - E_-|$ , show that when  $T \gg \hbar/\Delta$ , that is when the Hamiltonian is changing slowly compared with the intrinsic timescale of the system, we can ignore the off-diagonal terms. This is the adiabatic approximation.
- (d) Calculate the Berry phase of the ground state accumulated from  $t = 0$  to  $T$ , after which the Hamiltonian goes back to the initial values. Comment on your result: does the ground state also return to the initial value?
3. In the problem we will work out of the example of the Berry phase that was briefly discussed in class. Again consider the Hamiltonian

$$H(\mathbf{B}) = \frac{\hbar\gamma}{2} \mathbf{B} \cdot \boldsymbol{\sigma}$$

where the magnetic field  $\mathbf{B}$  is the changing external parameter. Writing  $\mathbf{B} = B(\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ , where  $B = |\mathbf{B}|$

- (a) Write down the Hamiltonian as a  $2 \times 2$  matrix in terms of  $\theta$  and  $\phi$ , and find its ground state.
- (b) Using the definition of Berry connection and Berry curvature,

$$\mathbf{A}_a(\mathbf{R}) = i \langle \psi_n(\mathbf{R}) | \frac{\partial}{\partial R^a} | \psi_n(\mathbf{R}) \rangle$$

$$\mathbf{F}_{ab} = \partial_a \mathbf{A}_b - \partial_b \mathbf{A}_a$$

compute the Berry connection  $\mathbf{A}_{\theta}$  and  $\mathbf{A}_{\phi}$ , and Berry curvature  $\mathbf{F}_{\theta\phi}$  of the ground state.

- (c) To transform the Berry curvature to the Cartesian coordinates, use the coordinate transformation rule  $\tilde{\mathbf{F}}_{\mu\nu} = T_{\mu}^{\lambda} T_{\nu}^{\rho} \mathbf{F}_{\lambda\rho}$ , where  $T_{\nu}^{\mu} = \frac{\partial x^{\mu}}{\partial x^{\nu}}$ , and

$$(|B|, \theta, \phi) = \left( \sqrt{B_x^2 + B_y^2 + B_z^2}, \arccos(B_z / \sqrt{B_x^2 + B_y^2 + B_z^2}), \arctan(B_y / B_x) \right)$$

Show the Berry curvature has the following form in Cartesian coordinates

$$\mathbf{F}_{ij} = \epsilon_{ijk} \frac{B_k}{2|B|^3}$$

You can use Mathematica or other tools for simplification.

- (d) Integrate the Berry curvature over the sphere where  $|B|$  is fixed. Show that the result is an integer multiple of  $2\pi$ . You may find that it is easier to do the integration in  $\theta - \phi$  coordinates.
4. Consider a Dirac particle in a low energy band of a crystal with Hamiltonian

$$H = \hbar v \hat{k}_x \sigma_x + \hbar v \hat{k}_y \sigma_y + \Delta \sigma_z.$$

where the “band gap”  $\Delta$  functions like a “mass.” Here,  $\hat{\mathbf{k}} = -i\nabla$  is the wavevector, or “crystal momentum” operator. In condensed matter physics we often insert a complete set of momentum eigenstates so that

$$H = \sum_{\mathbf{k}} |\mathbf{k}\rangle H(\mathbf{k}) \langle \mathbf{k}|, \quad H(\mathbf{k}) = \langle \mathbf{k}| H |\mathbf{k}\rangle = \hbar v k_x \sigma_x + \hbar v k_y \sigma_y + \Delta \sigma_z.$$

We note that  $H(\mathbf{k})$  is now a  $2 \times 2$  Hamiltonian that depends on the *parameters*, not operators,  $k_x$  and  $k_y$ . Let us denote the positive energy eigenstate of  $H(\mathbf{k})$  as  $|\mathbf{k}+\rangle$  and the negative energy eigenstate as  $|\mathbf{k}-\rangle$ .

- (a) Compute the “Berry connection” for the positive eigenstates:  $\mathbf{A} = i \langle \mathbf{k}+ | \nabla_{\mathbf{k}} | \mathbf{k}+ \rangle$ , where the gradient is taken with respect to  $(k_x, k_y)$ . Note that your answer will depend on your choice of gauge.
- (b) Compute the Berry phase by integrating the Berry connection around a circle of constant  $|\mathbf{k}| = k_F$ ;  $\gamma = \oint_{|\mathbf{k}|=k_F} \mathbf{A}(\mathbf{k}) \cdot d\mathbf{k}$ . Please feel free to use mathematica, but show your work.
- (c) Compute the Berry curvature  $\Omega(\mathbf{k}) = \nabla \times \mathbf{A}(\mathbf{k})$ . Compute the Berry phase again by performing the associated surface integral and show that your answer agrees with the previous part. Again feel free to use mathematica, but show your work.
- (d) Show that the Berry phases are opposite for the negative energy eigenstates (you don’t have to do both methods above, one would suffice). Also note that the Berry phases flip upon  $\Delta \rightarrow -\Delta$ .