M.Phys Option in Theoretical Physics: C6. Problem Sheet 1

Problems marked as (optional) will not be discussed in the problem classes, but written solutions will be provided.

Question 1. Consider paths $\mathbf{X} = \mathbf{X}(\tau)$, where τ is a parameter, and the functional

$$l[\mathbf{X}] = \int_{\tau_0}^{\tau_1} d\tau\, n(\mathbf{X}) \sqrt{\frac{d\mathbf{X}}{d\tau} \cdot \frac{d\mathbf{X}}{d\tau}}\ ,$$

where $n = n(\mathbf{X})$ is a function. (The minima of this functional can be interpreted as light rays propagating in a medium with refractive index n.)

a) Vary the above functional and derive the differential equation which has to be satisfied by minimal paths $\mathbf{X}$.

b) Consider a two-dimensional situation with paths $\mathbf{X}(\tau) = (X(\tau), Y(\tau))$ in the x, y plane and a function $n = n_0 + (n_1 - n_0)\,\theta(x)$. (The Heaviside function $\theta(x)$ is defined to be 0 for $x < 0$ and 1 for $x \geq 0$. Recall that $\theta'(x) = \delta(x)$.) Solve the differential equation in a) for this situation, using the coordinate x as parameter τ along the path.

c) Show that the solution in b) leads to the standard law for refraction at the boundary between two media with refractive indices n_0 and n_1.

Question 2. (optional)

a) Evaluate the Gaussian integral

$$\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}zx^2} \tag{1}$$

for a complex constant z. What is the requirement on z for the integral to exist?

b) The gamma function Γ is defined by

$$\Gamma(s+1) = \int_0^{\infty} dx\, x^s e^{-x}\ .$$

c) Show that $\Gamma(1) = 1$ and $\Gamma(s+1) = s\Gamma(s)$. (Hence $\Gamma(n+1) = n!$)

d) Take s to be real and positive. Evaluate $\Gamma(s+1)$ in the *steepest descent approximation*: write the integrand in the form $e^{f(x)}$ and argue that for large $s \gg 1$ the dominant contribution to the integral arises from the minima of $f(x)$. Expand the function to quadratic order around the minimum, argue that you may extend the integration boundaries to $\pm\infty$, and then carry out the resulting integral. Your result is known as *Stirling's approximation*: it tells what $n!$ is when n becomes large.

e)* The following extension is for complex analysis afficionados, so simply omit it if you haven't taken the short option. Take s to be complex with positive real part. Deform the contour in a suitable way, so that you can again apply a steepest descent approximation. Ponder the name of the method. What is Stirling's approximation for complex s?

Question 3. (optional) Consider a free QM particle moving in one dimension. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\ . \tag{2}$$

We have shown in the lecture that the propagator can be represented in the form

$$\langle x_N | e^{-\frac{i}{\hbar}tH} | x_0 \rangle \;=\; \lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} \int dx_1 \dots dx_{N-1} \exp\left(\frac{i\epsilon}{\hbar}\sum_{n=0}^{N-1} \frac{m}{2}\left(\frac{x_{n+1}-x_n}{\epsilon}\right)^2\right)\ . \tag{3}$$

a) Change variables from x_j to $y_j = x_j - x_N$ to bring it to the form

$$\langle x_N | e^{-\frac{i}{\hbar}tH} | x_0 \rangle \;=\; \lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar\epsilon}\right]^{\frac{N}{2}} \int d\mathbf{y} \exp\left(-\frac{1}{2}\mathbf{y}^T\mathbf{A}\mathbf{y} + \mathbf{J}^T \cdot \mathbf{y}\right) e^{\frac{im}{2\hbar\epsilon}(x_0 - x_N)^2}. \tag{4}$$

Give expressions for $\mathbf{J}$ and $\mathbf{A}$.

b) Carry out the integrals over y_j to get an expression for the propagator in terms of $\mathbf{A}$ and $\mathbf{J}$.

c) Work out the eigenvalues λ_n and eigenvectors $\mathbf{a}_n$ of the matrix $\mathbf{A}$. You may find helpful hints in the lecture notes.
d) What is $\det(\mathbf{A})$? A useful identity you may use is

$$\prod_{j=1}^{N-1} 2\sin(\pi j/2N) = \sqrt{N}. \tag{5}$$

Now work out $\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J}$ by working in the eigenbasis of $\mathbf{A}^{-1}$ (Hint: write this as $\mathbf{J}^T\mathbf{A}^{-1}\mathbf{J} = \mathbf{J}^T\mathbf{O}^T\mathbf{O}\mathbf{A}^{-1}\mathbf{O}^T\mathbf{O}\mathbf{J}$, where $\mathbf{O}^T\mathbf{O} = 1$ and $\mathbf{O}\mathbf{A}^{-1}\mathbf{O}^T$ is a diagonal matrix you have already calculated above.). A useful identity you may use is

$$\sum_{j=1}^{N-1} \cos^2(\pi j/2N) = \frac{N-1}{2}. \tag{6}$$

e) Use the result you have obtained to write an explicit expression for the propagator.

Question 4. Denote the propagator by

$$K(t,x;t'x') = \langle x|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle. \tag{7}$$

Show that the wave function $\psi(t,x) = \langle x|\Psi(t)\rangle$, where $|\Psi(t)\rangle$ is a solution to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle, \tag{8}$$

fulfils the integral equation

$$\psi(t,x) = \int_{-\infty}^{\infty} dx'\ K(t,x;t'x')\ \psi(t',x'). \tag{9}$$

Question 5. Diffraction through a slit. A free particle starting at $x=0$ when $t=0$ is determined to pass between $x_0 - b$ and $x_0 + b$ at time T. We wish to calculate the probabilty of finding the particle at position x at time $t = T + \tau$.
a) Argue on the basis of Qu 5. that the (un-normalized) wave function can be written in the form

$$\psi(T+\tau,x) = \int_{-b}^{b} dy\ K(T+\tau,x;T,x_0+y)\ K(T,x_0+y;0,0)\ , \tag{10}$$

where

$$K(t,x;t'x') = \langle x|e^{-\frac{i}{\hbar}H(t-t')}|x'\rangle. \tag{11}$$

b) Using that the propagation for $0 \le t < T$ and $T \le t < T+\tau$ is that of a free particle, obtain an explicit integral representation for the wave function.
c) Show that the wave function can be expressed in terms of the *Fresnel integrals*

$$C(x) = \int_0^x dy\ \cos(\pi y^2/2)\ , \quad S(x) = \int_0^x dy\ \sin(\pi y^2/2)\ . \tag{12}$$

Hint: make a substitution $z = \alpha y + \beta$ with suitably chosen α and β.

Derive an expression for the ratio $P(T+\tau,x)/P(T+\tau,x_0)$, where $P(T+\tau,x)dx$ is the probability of finding the particle in the interval $[x, x+dx]$ at time $T+\tau$.
d) (optional) If you can get hold of *Mathematica* (the default assumption is that you will not), plot the result as a function of the dimensionless parameter $x/[b(1+\tau/T)]$ for $x_0 = 0$ and different values of the ratio

$$\gamma = \frac{mb^2(1+\tau/T)}{\hbar\tau}\ . \tag{13}$$

Discuss your findings.

Question 6. In this question the objective is to evaluate the Feynman path integral in one of the relatively few cases, besides those treated in lectures, for which exact results can be obtained. The system we consider consists of a particle of mass m moving on a circle of circumference L. The quantum Hamiltonian is

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

and wavefunctions obey $\psi(x+L)=\psi(x)$. We want to determine the imaginary time propagator

$$\langle x_1|\exp(-\beta H)|x_2\rangle\,.$$

a) What are the eigenstates and eigenvalues of H? As we are dealing with a free particle, we can determine the propagator as in the lectures in a simple way by inserting resolutions of the identity in terms of the eigenstates of H. Show that this leads to the following result

$$\langle x_1|\exp(-\beta H)|x_2\rangle=\sum_{n=-\infty}^{\infty}\frac{1}{L}\exp\left(-\frac{\beta(2\pi n)^2\hbar^2}{2mL^2}+2\pi\mathrm{i}n\frac{[x_1-x_2]}{L}\right)\,. \tag{14}$$

b) Next, approach this using a path integral in which paths $x(\tau)$ for $0\le\tau\le\beta\hbar$ satisfy the boundary conditions $x(0)=x_1$ and $x(\beta\hbar)=x_2$. The special feature of a particle moving on a circle is that such paths may wind any integer number l times around the circle. To build in this feature, write

$$x(\tau)=x_1+\frac{\tau}{\beta\hbar}[(x_2-x_1)+lL]+s(\tau),$$

where the contribution $s(\tau)$ obeys the simpler boundary conditions $s(0)=s(\beta\hbar)=0$ and does *not* wrap around the circle. Show that the Euclidean action for the system on such a path is

$$S[x(\tau)]=S_l+S[s(\tau)]\qquad\text{where}\qquad S_l=\frac{m}{2\beta\hbar}[(x_2-x_1)+lL]^2\qquad\text{and}\qquad S[s(\tau)]=\int_0^{\beta\hbar}\mathrm{d}\tau\frac{m}{2}\left(\frac{\mathrm{d}s}{\mathrm{d}\tau}\right)^2.$$

c) using the results of b) show that

$$\langle x_1|\exp(-\beta H)|x_2\rangle\;=\mathcal{Z}_0\sum_{l=-\infty}^{\infty}\exp\left(-\frac{m}{2\beta\hbar^2}[(x_1-x_2)+lL]^2\right), \tag{15}$$

where $\mathcal{Z}_0$ is the diagonal matrix element $\langle x|\mathrm{e}^{-\beta H}|x\rangle$ for a *free* particle (i.e. without periodic boundary conditions) moving in one dimension.
d) Argue on the basis of the result you obtained in Qu 3. for the propagator of a free particle that

$$\mathcal{Z}_0=\left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2}. \tag{16}$$

e) Show that the expressions in Eq. (14) and Eq. (15) are indeed equal. To do so, you should use the *Poisson summation formula*

$$\sum_{l=-\infty}^{\infty}\delta(y-l)=\sum_{n=-\infty}^{\infty}\mathrm{e}^{-2\pi\mathrm{i}ny}$$

(think about how to justify this). Introduce the left hand side of this expression into Eq. (15) by using the relation, valid for any smooth function $f(y)$,

$$\sum_{l=-\infty}^{\infty}f(l)=\int_{-\infty}^{\infty}\mathrm{d}y\sum_{l=-\infty}^{\infty}\delta(y-l)f(y)\,,$$

substitute the right hand side of the summation formula, carry out the (Gaussian) integral on y, and hence establish the required equality.

Question 7. Anharmonic Oscillator. Consider the anharmonic oscillator

$$H(\lambda_1,\lambda_2)=\frac{\hat{p}^2}{2m}+\frac{\kappa}{2}\hat{x}^2+\frac{\lambda_1}{3!}\hat{x}^3+\frac{\lambda_2}{4!}\hat{x}^4. \tag{17}$$

where $\kappa,\lambda_{1,2}>0$ and $\lambda_1^2-3\kappa\lambda_2<0$. Define a generating functional by

$$W_{\lambda_1,\lambda_2}[J]=\mathcal{N}\int\mathcal{D}x(\tau)\;e^{\left\{\int_0^{\hbar\beta}d\tau\left[-\frac{1}{2}x(\tau)\hat{D}x(\tau)+J(\tau)x(\tau)\right]+U\left(x(\tau)\right)\right\}}\,, \tag{18}$$

where

$$U\big(x(\tau)\big) = -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[\frac{\lambda_1}{3!}x^3(\tau) + \frac{\lambda_2}{4!}x^4(\tau)\right], \quad \hat{D} = -\frac{m}{\hbar}\frac{d^2}{d\tau^2} + \frac{\kappa}{\hbar}. \tag{19}$$

a) Show that the partition function is equal to

$$Z_{\lambda_1,\lambda_2}(\beta) = W_{\lambda_1,\lambda_2}[0]. \tag{20}$$

b) Show that the generating functional can be expressed in the form

$$W_{\lambda_1,\lambda_2}[J] = \exp\left(U\Big(\frac{\delta}{\delta J(\tau)}\Big)\right) W_{0,0}[J]. \tag{21}$$

c) Determine the first order perturbative corrections in λ_1 and λ_2 to the partition function. Draw the corresponding Feynman diagrams.
d) Determine the perturbative correction to the partition function proportional to λ_1^2. Draw the corresponding Feynman diagrams. Are there corrections of order $\lambda_1\lambda_2$?
e) (optional) Determine the first order corrections to the two-point function

$$\langle T_\tau \bar{x}(\tau_1)\bar{x}(\tau_2)\rangle_\beta. \tag{22}$$

Draw the corresponding Feynman diagrams. What diagrams to you get in second order in perturbation theory?
Question 8. A lattice model for non-ideal gas is defined as follows. The sites i of a lattice may be empty or occupied by at most one atom, and the variable n_i takes the values $n_i = 0$ and $n_i = 1$ in the two cases. There is an attractive interaction energy J between atoms that occupy neighbouring sites, and a chemical potential μ. The model Hamiltonian is

$$\mathcal{H} = -J\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i\,, \tag{23}$$

where $\sum_{\langle ij\rangle}$ is a sum over neighbouring pairs of sites.
a) Describe briefly how the *transfer matrix method* may be used to calculate the statistical-mechanical properties of one-dimensional lattice models with short range interactions. Illustrate your answer by explaining how the partition function for a one-dimensional version of the lattice gas, Eq. (1), defined on a lattice of N sites with periodic boundary conditions, may be evaluated using the matrix

$$\mathbf{T} = \begin{pmatrix} 1 & e^{\beta\mu/2} \\ e^{\beta\mu/2} & e^{\beta(J+\mu)} \end{pmatrix}.$$

b) Derive an expression for $\langle n_i\rangle$ in the limit $N\to\infty$, in terms of elements of the eigenvectors of this matrix.
c) Show that

$$\langle n_i\rangle = \frac{1}{1+e^{-2\theta}}\,,$$

where

$$\sinh(\theta) = \exp(\beta J/2)\sinh(\beta[J+\mu]/2)\,.$$

Sketch $\langle n_i\rangle$ as a function of μ for $\beta J \gg 1$, and comment on the physical significance of your result.

Question 9. (optional) The one-dimensional 3-state Potts model is defined as follows. At lattice sites $i = 0, 1, \ldots, L$ "spin" variables σ_i take integer values $\sigma_i = 1, 2, 3$. The Hamiltonian is then given by

$$H = -J\sum_{i=0}^{L-1} \delta_{\sigma_i,\sigma_{i+1}}, \tag{24}$$

where $\delta_{a,b}$ is the Kronecker delta, $J > 0$.
a) What are the ground states and first excited states for this model?
b) Write down the transfer matrix for (24). Derive an expression for the free energy per site f in the limit of large L in terms of the transfer matrix eigenvalues. Show that vectors of the form $(1, z, z^2)$ with $z^3 = 1$ are eigenvectors,

and hence find the corresponding eigenvalues. Show that at temperature T (with $\beta = 1/k_B T$) and in the limit $L \to \infty$

$$f = -k_B T \ln \left(3 + e^{\beta J} - 1\right). \tag{25}$$

c) The boundary variable σ_0 is fixed in the state $\sigma_0 = 1$. Derive an expression (for large L), that the variable at site $\ell \gg 1$ is in the same state, in terms of the transfer matrix eigenvalues and eigenvectors. Show that your result has the form

$$\langle \delta_{\sigma_\ell,1} \rangle = \frac{1}{3} + \frac{2}{3} e^{-\ell/\xi}. \tag{26}$$

How does ξ behave in the low and high temperature limits?

Question 10. Consider a one dimensional Ising model on an open chain with N sites, where N is odd. On all even sites a magnetic field $2h$ is applied, see Fig. 1. The energy is

$$E = -J \sum_{j=1}^{N-1} \sigma_j \sigma_{j+1} + 2h \sum_{j=1}^{(N-1)/2} \sigma_{2j}. \tag{27}$$

a) Show that the partition function can be written in the form

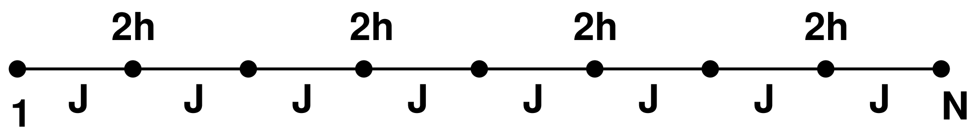

Figure 1: Open Ising chain with magnetic field applied to all even sites.

$$Z = \langle u | T^{(N-1)/2} | v \rangle , \tag{28}$$

where T is an appropriately constructed transfer matrix, and $|u\rangle$ and $|v\rangle$ two dimensional vectors. Give explicit expressions for T, $|u\rangle$ and $|v\rangle$.

b) Calculate Z for the case $h = 0$.