M.Phys C6 Theoretical Physics Option
M.Math.Phys. Advanced Quantum Theory
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

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

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

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

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

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

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

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

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

Question 4. Denote the propagator by

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

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

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

fulfils the integral equation

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

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

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

where

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

b) Using that the propagation for $0 \leq t < T$ and $T \leq t < T + \tau$ 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 $0 \leq \tau \leq \beta\hbar$ 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*

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

(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

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

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

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

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

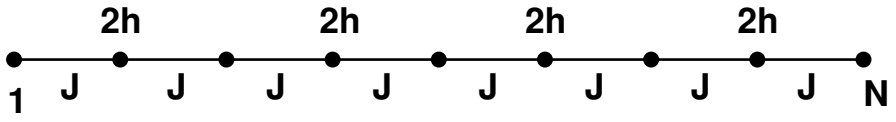


Figure 1: Open Ising chain with magnetic field applied to all even sites.

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

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 $h = 0$.

M.Phys C6 Theoretical Physics Option
M.Math.Phys. Advanced Quantum Theory
Problem Sheet 2

Question 11. Consider a fermion 'system' with just one single-particle orbital, so that the only states of the system are $|0\rangle$ (unoccupied) and $|1\rangle$ (occupied). Show that we can represent the operators a and $a^\dagger$ by the matrices

$$a^\dagger = \begin{pmatrix} 0 & 0 \\ C & 0 \end{pmatrix}, \quad a = \begin{pmatrix} 0 & C^* \\ 0 & 0 \end{pmatrix}.$$

You can do this by checking the values of aa, $a^\dagger a^\dagger$ and $a^\dagger a + a a^\dagger$. What values may the constant C take?

Question 12. A quantum-mechanical Hamiltonian for a system of an even number N of point unit masses interacting by nearest-neighbour forces in one dimension is given by

$$H = \frac{1}{2}\sum_{r=1}^{N} \left(p_r^2 + (q_{r+1} - q_r)^2\right),$$

where the Hermitian operators q_r, p_r satisfy the commutation relations $[q_r, q_s] = [p_r, p_s] = 0$, $[q_r, p_s] = \mathrm{i}\delta_{rs}$, and where $q_{r+N} = q_r$. New operators Q_k, P_k are defined by

$$q_r = \frac{1}{\sqrt{N}}\sum_k Q_k \mathrm{e}^{\mathrm{i}kr} \qquad \text{and} \qquad p_r = \frac{1}{\sqrt{N}}\sum_k P_k \mathrm{e}^{-\mathrm{i}kr},$$

where $k = 2\pi n/N$ with $n = -N/2+1, \ldots, 0, \ldots, N/2$.

Show that:

(a) $Q_k = \dfrac{1}{\sqrt{N}}\displaystyle\sum_{s=1}^{N} q_s \mathrm{e}^{-\mathrm{i}ks}$ and $P_k = \frac{1}{\sqrt{N}}\sum_{s=1}^{N} p_s \mathrm{e}^{\mathrm{i}ks}$

(b) $[Q_k, P_{k'}] = \mathrm{i}\delta_{kk'}$

(c) $H = \frac{1}{2}\left(\sum_k P_k P_{-k} + \omega^2 Q_k Q_{-k}\right)$, where $\omega^2 = 2(1-\cos k)$.

Similarly to the treatment of the simple harmonic oscillator in QM I we then define annihilation operators a_k by

$$a_k = \frac{1}{(2\omega_k)^{1/2}}(\omega_k Q_k + \mathrm{i}P_{-k}).$$

Show that the Hermitian conjugate operators are

$$a_k^\dagger = \frac{1}{(2\omega_k)^{1/2}}(\omega_k Q_{-k} - \mathrm{i}P_k),$$

and determine the canonical commutation relations for a_k and $a_p^\dagger$. Construct the Fock space of states and determine the eigenstates and eigenvalues of H.

Question 13. Bosonic creation operators are defined through their action on basis states in the occupation number representation as

$$c_l^\dagger |n_1 n_2 \ldots\rangle = \sqrt{n_l + 1}\,|n_1 n_2 \ldots n_l + 1 \ldots\rangle\ , \tag{1}$$

a) Deduce from this how bosonic annihilation operators act.
b) Show that the creation and annihilation operators fulfil *canonical commutation relations*

$$[c_l, c_m] = 0 = [c_l^\dagger, c_m^\dagger] \ , \quad [c_l, c_m^\dagger] = \delta_{l,m}. \tag{2}$$

Question 14. Consider the N-particle interaction potential

$$\hat{V} = \sum_{i<j}^{N} V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j),$$

where $V(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) = V(\hat{\mathbf{r}}_j, \hat{\mathbf{r}}_i)$. Show that in second quantization it is expressed as

$$\hat{V} = \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \ V(\mathbf{r}, \mathbf{r}') \ c^\dagger(\mathbf{r}) c^\dagger(\mathbf{r}') c(\mathbf{r}') c(\mathbf{r}).$$

To do so consider the action of $\hat{V}$ on a basis of N-particle position eigenstates

$$|\mathbf{r}_1 \dots \mathbf{r}_N\rangle = \frac{1}{\sqrt{N! n_1! n_2! \dots}} \sum_P (\pm 1)^{|P|} |\mathbf{r}_1\rangle \otimes |\mathbf{r}_2\rangle \otimes |\mathbf{r}_N\rangle = \frac{1}{\sqrt{n_1! n_2! \dots}} \prod_{j=1}^{N} c^\dagger(\mathbf{r}_j)|0\rangle \ ,$$

where n_j is the occupation number of the j^{th} single-particle state. Argue that in an arbitrary basis of single-particle eigenstates $|l\rangle$ $\hat{V}$ can be expressed in the form

$$\hat{V} = \sum_{ll'mm'} \langle ll'|\hat{V}|mm'\rangle c_l^\dagger c_{l'}^\dagger c_{m'} c_m. \tag{3}$$

Question 15. Consider a system of fermions moving freely on a one-dimensional ring of length L, i.e. periodic boundary conditions are applied between $x = 0$ and $x = L$. The fermions are all in the same spin state, so that spin quantum numbers may be omitted. Fermion creation and annihilation operators at the point x are denoted by $\psi^\dagger(x)$ and $\psi(x)$.
a) Write down the complete set of anticommutation relation satisfied by $\psi^\dagger(x_1)$ and $\psi(x_2)$.
b) Write down the wave-functions of single-particle momentum eigenstates (make sure to take the boundary conditions into account!). What are the allowed values of momentum? Using this result, derive an expression for the momentum space creation and annihilation operators $\Psi_p^\dagger$ and Ψ_p in terms of $\psi^\dagger(x)$ and $\psi(x)$ (hint: use the general result for basis transformation obtained in the lecture notes).
c) Starting with your expression for the anticommutator $\{\psi^\dagger(x_1), \psi(x_2)\}$, evaluate $\{\Psi_p^\dagger, \Psi_q\}$.
d) Derive an expression for $\psi(x)$ in terms of Ψ_k.
e) The density operator $\rho(x)$ is defined by $\rho(x) = \psi^\dagger(x)\,\psi(x)$. The number operator is

$$N = \int_0^L dx\, \rho(x)\,.$$

Express $\rho(x)$ in terms of $\Psi_p^\dagger$ and Ψ_q, and show from this that

$$N = \sum_k \Psi_k^\dagger \Psi_k\,.$$

Let $|0\rangle$ be the vacuum state (containing no particles) and define $|\phi\rangle$ by

$$|\phi\rangle = A \prod_k (u_k + v_k \Psi_k^\dagger)|0\rangle,$$

where u_k and v_k are complex numbers depending on the label k, and A is a normalisation constant.

Evaluate (i) $|A|^2$, (ii) $\langle\phi|N|\phi\rangle$, and (iii) $\langle\phi|N^2|\phi\rangle$. Under what conditions is $|\phi\rangle$ an eigenstate of particle number?

Question 16. Consider a system of fermions in which the functions $\varphi_\ell(x)$, $\ell = 1, 2 \ldots N$, form a complete orthonormal basis for single particle wavefunctions.
a) Explain how Slater determinants may be used to construct a complete orthonormal basis for n-particle states with $n = 2, 3 \ldots N$. Calculate the normalisation constant for such a Slater determinant at a general value of n. How many independent n-particle states are there for each n?
b) Let $C_\ell^\dagger$ and C_ℓ be fermion creation and destruction operators which satisfy the usual anti-commutation relations. The quantities a_k are defined by

$$a_k = \sum_{\ell=1}^{N} U_{k\ell} C_\ell,$$

where $U_{k\ell}$ are elements of an $N \times N$ matrix, U. Write down an expression for $a_k^\dagger$. Find the condition which must be satisfied by the matrix U in order that the operators $a_k^\dagger$ and a_k also satisfy fermion anticommutation relations.
c) Non-interacting spinless fermions move in one dimension in an infinite square-well potential, with position coordinate $0 \le x \le L$. The normalised single particle energy eigenstates are

$$\varphi_\ell(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\ell\pi x}{L}\right) ,$$

and the corresponding fermion creation operator is $C_\ell^\dagger$.

Write down expressions for $C^\dagger(x)$, the fermion creation operator at the point x, and for $\rho(x)$, the particle density operator, in terms of $C_\ell^\dagger$, C_ℓ and $\varphi_\ell(x)$.
d) What is the ground state expectation value $\langle\rho(x)\rangle$ in a system of n fermions?

In the limit $n \to \infty$, $L \to \infty$, taken at fixed average density $\rho_0 = n/L$, show that

$$\langle\rho(x)\rangle = \rho_0 \left[1 - \frac{\sin 2\pi\rho_0 x}{2\pi\rho_0 x}\right] .$$

Sketch this function and comment briefly on its behaviour for $x \to 0$ and $x \to \infty$.

Question 17. (optional) Consider the ideal Fermi gas at finite density N/V in a periodic 3-dimensional box of length L.
(a) Give an expression of the ground state in terms of creation operators for momentum eigenstates.
(b) Calculate the **single-particle Green's function**

$$\begin{aligned} G_{\sigma\tau}(\omega, \mathbf{q}) &= \int dt\; e^{i\omega(t-t')} \int d^3\mathbf{r}\; e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}') \;, \\ G_{\sigma\tau}(t, \mathbf{r}; t', \mathbf{r}') &= -i\langle GS|T c_\sigma(\mathbf{r}, t)\; c_\tau^\dagger(\mathbf{r}', t')|GS\rangle, \end{aligned} \tag{4}$$

where T denotes time-ordering (i.e. $T\mathcal{O}(t_1)\mathcal{O}(t_2) = \theta(t_1 - t_2)\mathcal{O}(t_1)\mathcal{O}(t_2) - \theta(t_2 - t_1)\mathcal{O}(t_2)\mathcal{O}(t_1)$ for fermionic operators), and

$$c_\sigma(\mathbf{r}, t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{r}) e^{-\frac{i}{\hbar}Ht}. \tag{5}$$

First express the creation/annihilation operators $c^\dagger_\sigma(\mathbf{r},t)$, $c_\sigma(\mathbf{r},t)$ in terms of creation/annihilation operators in momentum space $c^\dagger_\sigma(\mathbf{p},t)$, $c_\sigma(\mathbf{p},t)$. Then show that for annihilation operators in momentum space we have

$$c_\sigma(\mathbf{p},t) \equiv e^{\frac{i}{\hbar}Ht} c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}Ht} = c_\sigma(\mathbf{p}) e^{-\frac{i}{\hbar}t\epsilon(\mathbf{p})} \ , \tag{6}$$

where $\epsilon(\mathbf{p}) = \mathbf{p}^2/2m - \mu$. Use this to show that

$$c_\sigma(\mathbf{r},t) = \frac{1}{L^{3/2}} \sum_{\mathbf{p}} e^{-\frac{i}{\hbar}t\epsilon(\mathbf{p}) + i\mathbf{p}\cdot\mathbf{r}} \ c_\sigma(\mathbf{p}). \tag{7}$$

Now insert (7) into (4) and evaluate the ground state expectation value to obtain an integral representation for $G_{\sigma\tau}(t,\mathbf{r};t',\mathbf{r}')$. Why does the Green's function only depend on $t-t'$ and $\mathbf{r}-\mathbf{r}'$? Finally, calculate $G_{\sigma\tau}(\omega,\mathbf{q})$.

Note: the imaginary part of the single-particle Green's function is (approximately) measured by angle resolved photoemission (ARPES) experiments.

M.Phys C6 Theoretical Physics Option
M.Math.Phys. Advanced Quantum Theory
Problem Sheet 3

Question 18. A magnetic system consists of two types of Heisenberg spin $\mathbf{S}^A$ and $\mathbf{S}^B$ located respectively on the two inter-penetrating sublattices of an NaCl crystal structure (i.e. a simple cubic structure with alternate A and B in any Cartesian direction). Its Hamiltonian is

$$H = J \sum_{i,j} \mathbf{S}_i^A \cdot \mathbf{S}_j^B$$

where the i, j are nearest neighbours, respectively on the A and B sublattices. J is positive. Show that the classical ground state has all the A spins ferromagnetically aligned in one direction and all the B spins ferromagnetically aligned in the opposite direction. Assume the quantum mechanical ground state is well approximated by the classical one. To a first approximation the spin operators are given in terms of boson operators a, b by

A sublattice	B sublattice
$S_i^z = S^A - a_i^\dagger a_i$	$S_j^z = -S^B + b_j^\dagger b_j$
$S_i^+ \equiv S_i^x + \mathrm{i}S_i^y \simeq (2S^A)^{1/2} a_i$	$S_j^+ \equiv S_j^x + \mathrm{i}S_j^y \simeq (2S^B)^{1/2} b_j^\dagger$
$S_i^- \equiv S_i^x - \mathrm{i}S_i^y \simeq (2S^A)^{1/2} a_i^\dagger$	$S_j^- \equiv S_j^x - \mathrm{i}S_j^y \simeq (2S^B)^{1/2} b_j$

Discuss the validity of this approximation. Use these relations to express the Hamiltonian in terms of the boson operators to quadratic order.

Transforming to crystal momentum space using (with N the number of sites on one sublattice)

$$a_i = N^{-1/2} \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} a_{\mathbf{k}}, \quad b_j = N^{-1/2} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j} b_{\mathbf{k}}$$

show that your result can be expressed in the form

$$H = E_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + B_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + C_{\mathbf{k}} (a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger + b_{\mathbf{k}} a_{\mathbf{k}}) \right]$$

and determine the coefficients. Hence calculate the spectrum of excitations at low momenta. Consider both the cases with $S^A = S^B$ and $S^A \neq S^B$ and comment on your results.

Question 19. Consider a Landau expansion of the free energy of the form

$$F = \frac{a}{2} m^2 + \frac{b}{4} m^4 + \frac{c}{6} m^6$$

with $c > 0$. Examine the phase diagram in the $a - b$ plane, and show that there is a line of critical transitions $a = 0$, $b > 0$ which joins a line of first order transitions $b = -4(ca/3)^{1/2}$ at a point $a = b = 0$ known as a tricritical point.

Supposing that a varies linearly with temperature and that b is independent of temperature, compare the value of the exponent β at the tricritical point with its value on the critical line.

From Yeomans, *Statistical Mechanics of Phase Transitions*

Question 20.
(a) Discuss how an order parameter may be used to characterise symmetry breaking at a phase transition.
(b) Argue that the uniaxial ferromagnet-paramagnet transition can be described by by a Landau free energy of the form

$$F = \int d^3\mathbf{r} \left[\frac{1}{2}|\nabla\phi(\mathbf{r})|^2 - h\phi(\mathbf{r}) + \alpha_2\phi^2(\mathbf{r}) + \alpha_3\phi^3(\mathbf{r}) + \alpha_4\phi^4(\mathbf{r}) \right]. \tag{1}$$

What can you say about α_4?
(c) What is the nature of the transition for $h = 0$ if $\alpha_3 \neq 0$? Explain your answer.
(d) Now assume that $\alpha_3 = h = 0$. Argue that close to the critical point

$$\alpha_2 = At \ , \quad t = \frac{T - T_c}{T_c} \text{ and } A > 0. \tag{2}$$

(e) Derive the equation characterizing the saddle point solution for $\alpha_3 = h = 0$. What are the configurations ϕ with the lowest free energy for $h = 0$, at $T > T_c$ and at $T < T_c$? Why are these $\mathbf{r}$ independent?
(f) Now consider more general solutions to the saddle point equation in the low-temperature phase. With suitable boundary conditions the saddle point solutions for the order parameter are functions of x only, i.e. $\phi = \phi(x)$. Show that in this case

$$E = \frac{1}{2}\left[\frac{d\phi(x)}{dx}\right]^2 - \alpha_2\phi^2 - \alpha_4\phi^4 \tag{3}$$

is independent of x. Construct a solution $\phi(x)$ such that

$$\lim_{x\to\infty} \phi(x) = \phi_1 \ , \quad \lim_{x\to-\infty} \phi(x) = \phi_2, \tag{4}$$

where $\phi_{1,2}$ are the solutions found in (d). Hint: determine E for such solutions first.

Question 21. A system with a real, two-component order parameter $(\phi_1(\mathbf{r}), \phi_2(\mathbf{r}))$ has a free energy

$$F = \int \mathrm{d}^d\mathbf{r} \left[\frac{1}{2}|\nabla\phi_1(\mathbf{r})|^2 + \frac{1}{2}|\nabla\phi_2(\mathbf{r})|^2 - \frac{1}{2}\left(\phi_1^2(\mathbf{r}) + \phi_2^2(\mathbf{r})\right) + \frac{1}{4}\left(\phi_1^2(\mathbf{r}) + \phi_2^2(\mathbf{r})\right)^2 \right] .$$

Find the order-parameter values Φ_1, Φ_2 that minimise this free energy. Consider small fluctuations around such state, with $(\phi_1(\mathbf{r}), \phi_2(\mathbf{r})) = (\Phi_1 + \varphi_1(\mathbf{r}), \Phi_2 + \varphi_2(\mathbf{r}))$ and expand F to second order in φ.

Assuming that the statistical weight of thermal fluctuations is proportional to $\exp(-F)$, calculate approximately the correlation function

$$\langle \varphi_1(\mathbf{r})\varphi_1(\mathbf{0}) + \varphi_2(\mathbf{r})\varphi_2(\mathbf{0}) \rangle$$

by evaluating a Gaussian functional integral. How does your result depend on the dimensionality d of the system?

M.Phys C6 Theoretical Physics Option
M.Math.Phys. Advanced Quantum Theory
Problem Sheet 3

Question 22. This question is concerned with the central limit theorem.
(i) Show explicitly that for $N \gg 1, pN \gg 1$ the binomial distribution

$$P_N(n) = \frac{N!}{n!(N-n)!} p^n q^{N-n}, \qquad p+q=1$$

becomes

$$P_N(n) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(n- < n >)^2}{2\sigma^2}\right)$$

where $\sigma^2 = Npq$. Check that the same result follows from the central limit theorem.
(ii) Consider a random walk in one dimension, for which the probability of taking a step of length $x \to x + dx$ is

$$f(x)dx = \frac{1}{\pi} \frac{\gamma}{x^2+\gamma^2} dx.$$

Find the probability distribution for the total displacement after N steps. Does it satisfy the central limit theorem? Should it? What are the cumulants of this distribution?

Question 23. Let $y = \pm 1$. Show that

$$P_{1|1}(y,t \mid y',t') = \frac{1}{2}\left\{1 + e^{-2\gamma(t-t')}\right\}\delta_{y,y'} + \frac{1}{2}\left\{1 - e^{-2\gamma(t-t')}\right\}\delta_{y,-y'} \tag{1}$$

obeys the Chapman-Kolmogorov equation.

Show that

$$P_1(y,t) = \frac{1}{2}(\delta_{y,1} + \delta_{y,-1}) \tag{2}$$

is a stationary solution. Write $P_{1|1}$ as a 2×2 matrix and formulate the Chapman-Kolmogarov equation as a property of that matrix.

Question 24. This question is about a continuous random walk, also known as a Wiener process. Show that for $-\infty < y < \infty$ and $t_2 > t_1$ the Chapman-Kolmogarov equation is satisfied for

$$P_{1|1}(y_2,t_2 \mid y_1,t_1) = \frac{1}{\sqrt{2\pi(t_2-t_1)}} \exp - \left\{\frac{(y_2-y_1)^2}{2(t_2-t_1)}\right\}. \tag{3}$$

Choose $P_1(y_1,0) = \delta(y_1)$. Show that for $t > 0$

$$P_1(y,t) = \frac{1}{\sqrt{2\pi t}} \exp\left\{\frac{-y^2}{2t}\right\}. \tag{4}$$

Show that $P_1(y,t)$ obeys the diffusion equation

$$\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial y^2} \tag{5}$$

for $D = \frac{1}{2}$. What is the solution for arbitrary $D > 0$?

Question 25. A particle suspended in a fluid undergoes Brownian motion in one dimension with position $x(t)$ and velocity $v(t)$. This motion is modelled by the Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \eta(t),$$

where $\eta(t)$ is a Gaussian random variable characterised completely by the averages $\langle \eta(t) \rangle = 0$ and $\langle \eta(t_1)\eta(t_2) \rangle = \Gamma \delta(t_1 - t_2)$. Discuss the physical origin of each of the terms in the Langevin equation.

What is meant by the term *Markov process*? Illustrate your answer by discussing which of the following are Markov processes: (a) $v(t)$ alone; (b) $x(t)$ alone; (c) $v(t)$ and $x(t)$ together.

Show that for $t > 0$

$$x(t) = \frac{v(0)}{\gamma}\left(1 - \mathrm{e}^{-\gamma t}\right) + \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \; \mathrm{e}^{-\gamma(t_1 - t_2)}\, \eta(t_2)$$

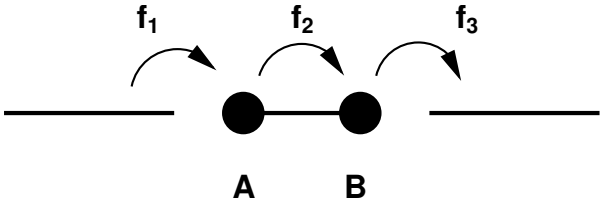
is a solution of the Langevin equation with initial condition $x(0) = 0$. Calculate the average $\langle x(t)\, v(t) \rangle$ and discuss its limiting behaviour at short and long times.

Question 26. The time evolution of a stochastic system is represented by a master equation of the form

$$\frac{\mathrm{d}p_n(t)}{\mathrm{d}t} = \sum_m W_{nm} p_m(t)\,.$$

Explain briefly the meaning of this equation and discuss the assumptions on which it is based. What general conditions should the matrix elements W_{nm} satisfy?

A molecule lies between two atomic-scale contacts and conducts charge between them. A simple model of this situation is illustrated below. The model has three states: the molecule may be uncharged, or may carry a single charge at either site A or site B but not both. Charges hop between these sites, and between the sites and the contacts, at the rates indicated in the figure. (For example, a charge at site A has probability f_2 per unit time of hopping to site B.)



Write down a master equation for this model. For the system in equilibrium, calculate the occupation probabilities of the three states, and show that the average number of charges flowing through the molecule per unit time is

$$\frac{f_1 f_2 f_3}{f_1 f_2 + f_1 f_3 + f_2 f_3}\,.$$

Consider the case $f_1 = f_2 = f_3 \equiv f$. The molecule is uncharged at time $t = 0$. Show that the probability $p(t)$ for it to be uncharged at a later time t is

$$p(t) = \frac{1}{3} + \frac{2}{3}\exp\left(-\frac{3}{2}ft\right)\cos\left(\frac{\sqrt{3}}{2}ft\right)\,.$$

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

Question 1. Anharmonic Oscillator. Consider the anharmonic oscillator

$$H(\lambda) = \frac{\hat{p}^2}{2m} + \frac{\kappa}{2}\hat{x}^2 + \frac{\lambda}{4!}\hat{x}^4, \tag{1}$$

where $\kappa, \lambda > 0$.
(a) Discuss how the partition function $Z_\lambda(\beta)$ can be represented as a path integral. What kinds of paths are integrated over?
(b) What is the definition of the imaginary time Green's function of the harmonic oscillator ($\lambda = 0$)? How can it be expressed as a path integral (for $0 < \tau < \hbar\beta$)?
(c) Define a generating functional by

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

where

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

Show that the partition function is equal to

$$Z_\lambda(\beta) = W_\lambda[0]. \tag{4}$$

(d) Show that the generating functional can be expressed in the form

$$W_\lambda[J] = \exp\left(U\Big(\frac{\delta}{\delta J(\tau)}\Big)\right) W_0[J]. \tag{5}$$

(e) Draw the Feynman diagrams for the first and second order perturbative corrections in λ to the partition function. Determine the first order corrections to the partition function.
(f) Determine the first order corrections to the two-point function

$$\langle T_\tau \bar{x}(\tau_1)\bar{x}(\tau_2)\rangle_\beta. \tag{6}$$

Draw the corresponding Feynman diagrams.

Question 2. The Hamiltonian for a one-dimensional ferromagnetic Ising model is

$$H = -J\sum_{n=1}^{L} S_n S_{n+1}\,,$$

where $J > 0$, S_n take the values $-2, -1, 0, 1, 2$, and where we have imposed periodic boundary conditions $S_{L+1} = S_1$. Write down the transfer matrix for this model. Give an exact express of the free energy per site in terms of the transfer matrix eigenvalues (do not attempt to calculate the eigenvalues explicitly). How does the answer simplify in the limit $L \to \infty$?

Derive an expression for the probability $\langle \delta_{S_1,1}\delta_{S_\ell,-1}\rangle$ that the spins at sites 1 and ℓ take the respective values 1 and -1 in terms of the transfer matrix eigenvalues λ_j and eigenvectors $|j\rangle$ (without calculating them).

Question 3. Consider the quantum spin-S chain

$$H = -\sum_{j=1}^{L} J^x S_j^x S_{j+1}^x + J^y S_j^y S_{j+1}^y\,, \tag{7}$$

where $J^x, J^y > 0$, $S_{L+1}^\alpha = S_1^\alpha$ and

$$\big(S_j^x\big)^2 + \big(S_j^y\big)^2 + \big(S_j^z\big)^2 = S(S+1). \tag{8}$$

(a) What are the classical ground states of this model (take the spins to be classical vectors of length S)? Consider the cases $J^x \neq J^y$ and $J^x = J^y$ separately.

(b) Explain the idea of spontaneous symmetry breaking for the cases $J^x > J^y$ and $J^x = J^y$ in this model. Which symmetries are broken?
(c) We now want to solve the model for $J^x > J^y$ in the linear spinwave approximation. To that end, we first carry out a rotation of spin quantization axis such that the classical ground state maps onto the ferromagnetic state, where all spins point along the z-axis in spin space. Show that this transformation is of the form

$$\tilde{S}_j^z = S_j^x \ , \quad \tilde{S}_j^y = S_j^y \ , \quad \tilde{S}_j^x = -S_j^z. \tag{9}$$

Express the Hamiltonian in terms of the rotated spin operators.

Then use the Holstein-Primakoff representation

$$\tilde{S}_j^z = S - a_j^\dagger a_j \ , \quad \tilde{S}_j^+ = \tilde{S}_j^x + i\tilde{S}_j^y = \sqrt{2S - a_j^\dagger a_j}\ a_j \ , \quad [a_j, a_k^\dagger] = \delta_{j,k} \ , \quad [a_j, a_k] = 0 \tag{10}$$

to carry out an expansion of H in inverse powers of S. Ignore the constant contribution and keep only the terms proportional to S. Give an explicit representation of the resulting Hamiltonian $H_{\rm LSW}$, in terms of creation and annihilation operators in momentum space.
(d) What is a Bogoliubov transformation (BT), and what is its use? Diagonalize $H_{\rm LSW}$ by means of a BT (you may drop the constant contribution).

Question 4. A particle undergoes Brownian motion in one dimension. Its speed $v(t)$ satises the Langevin equation

$$\frac{dv(t)}{dt} = -\gamma v(t) + \eta(t), \tag{11}$$

where $\eta(t)$ is a Gaussian random variable, characterised by the averages

$$\langle \eta(t) \rangle = 0 \ , \quad \langle \eta(t_1)\eta(t_2) \rangle = \Gamma\, \delta(t_1 - t_2). \tag{12}$$

(a) Discuss the physical origin of each term in this equation.
(b) Show that, with initial condition $v(0) = 0$, the function

$$v_0(t) = \int_0^t dt'\ e^{-\gamma(t-t')}\eta(t') \tag{13}$$

is a solution to the Langevin equation for $t > 0$.
(c) Evaluate

$$\langle v_0(t_0)v_0(t_0 + t) \rangle \tag{14}$$

for $t_0 \to \infty$. Consider both cases $t < 0$ and $t > 0$. Explain how the result enables one to express Γ in terms of temperature and other parameters characterising the system.
(d) In the presence of an additional force on the particle, the Langevin equation has the modified form

$$\frac{dv(t)}{dt} = f - \gamma v(t) + \eta(t). \tag{15}$$

Show for constant f that the solution to this modified equation may be written in the form $v(t) = v_0(t) + u(t)$, and find $u(t)$.

Question 5. (a) Argue that the Landau free energy for a rotationally invariant system with a real, N-component order parameter $\vec{\phi}(\mathbf{r}) = (\phi_1(\mathbf{r}), \phi_2(\mathbf{r}), \ldots, \phi_N(\mathbf{r}))$ is of the form

$$F = \int \mathrm{d}^d\mathbf{r} \left[\frac{1}{2}|\nabla\vec{\phi}(\mathbf{r})|^2 + \alpha_2\vec{\phi}(\mathbf{r}) \cdot \vec{\phi}(\mathbf{r}) + \alpha_4 \left(\vec{\phi}(\mathbf{r}) \cdot \vec{\phi}(\mathbf{r}) \right)^2 \right] \ . \tag{16}$$

(b) What can you say about the values of α_2 and α_4?
(c) Discuss the different phases and the nature of the phase transitions between them.
(d) Are there gapless Goldstone modes in the ordered phase (justify your answer)?