

## 16.4 Problem Set IV

1. **Operator methods in quantum mechanics:** The following problem combines the practice of a number different methodologies covered in this course. Here we address the excitation spectrum of a quantum mechanical spin chain. It provides a counterpart to the vibrational modes of the quantum harmonic chain considered in lectures. Here we will address the problem in two different ways.

In strongly correlated solid state systems, the Coulomb interaction can result in electrons becoming localized to the sites of the underlying crystalline lattice – the **Mott transition**. However, in these insulating materials, the spin degrees of freedom carried by the constituent electrons can remain mobile – spin fluctuations can be exchanged between neighbouring electrons without motion of charge. Such systems are described by **quantum magnets**,  $\hat{H} = \sum_{m \neq n} J_{mn} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n$ , where **exchange couplings**  $J_{mn}$  denotes the matrix elements coupling lattice sites  $m$  and  $n$ . Since these matrix elements decay rapidly with distance, it is often legitimate to restrict attention to neighbouring sites. Although these matrix elements are typically positive (leading to an **antiferromagnetic** coupling), in the following we will consider them negative leading to **ferromagnetism** – i.e. neighbouring spins want to lie parallel. Consider then the one-dimensional **spin  $S$  quantum (Heisenberg) ferromagnet**,

$$\hat{H} = -J \sum_m \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1},$$

where  $J > 0$ , and the spins obey the quantum spin algebra,  $[\hat{S}_m^\alpha, \hat{S}_n^\beta] = i\hbar \delta_{mn} \epsilon^{\alpha\beta\gamma} \hat{S}_m^\gamma$ .

- (a) Making use of the spin commutation relations and Ehrenfest's theorem, show that, in the Heisenberg representation, the spins obey the equations of motion,

$$\hbar \frac{d\hat{\mathbf{S}}_m}{dt} = J \hat{\mathbf{S}}_m \times (\hat{\mathbf{S}}_{m+1} + \hat{\mathbf{S}}_{m-1}),$$

where we suppose that the boundary conditions are periodic, i.e.  $\mathbf{S}_{m+N} = \mathbf{S}_m$ .

- (b) For large spin  $S$ , we may take the spin expectation values to be defined by their classical values,  $\langle \hat{\mathbf{S}}_m \rangle = \mathbf{S}_m$ . Moreover, if we are interested in low-energy excitations of the spin chain, only modes of long wavelength contribute (cf. the vibrational modes of the harmonic chain). In this case, we may develop the Taylor series expansion,  $\mathbf{S}_{m+1} = \mathbf{S}_m + \partial \mathbf{S}_m + \frac{1}{2} \partial^2 \mathbf{S}_m + \dots$ , where the lattice spacing is taken as unity. In doing so, show that the leading contribution to the equations of motion in the gradient expansion is given by,

$$\dot{\mathbf{S}} = J \mathbf{S} \times \partial^2 \mathbf{S}.$$

- (c) Show that the solution to this equation is given by  $\mathbf{S}(x, t) = (c \cos(kx - \omega t), c \sin(kx - \omega t), \sqrt{S^2 - c^2})$  and determine the dispersion relation,  $\omega(k)$ . Sketch a “snapshot” configuration of the spins in the chain. These low energy modes of the quantum spin chain are known as a spin waves and mirror the phonon excitations of the quantum harmonic

chain. Notice that the dispersion relation in this case has a quadratic dependence on  $k$  (cf. non-relativistic particles) as opposed to the linear dependence of the phonon spectrum. If you are feeling energetic, you might contemplate the spin wave modes for the antiferromagnetic chain where the dispersion becomes linear. Let us now consider an alternative approach to the spin wave spectrum which follows an operator-based formalism.

- (d) Defining the spin raising and lowering operators,  $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ , show that the ferromagnetic Heisenberg model can be written as

$$\hat{H} = -J \sum_m \left\{ \hat{S}_m^z \hat{S}_{m+1}^z + \frac{1}{2} \left( \hat{S}_m^+ \hat{S}_{m+1}^- + \hat{S}_m^- \hat{S}_{m+1}^+ \right) \right\}.$$

Then, making use of the Holstein–Primakoff spin representation (defined on page 192),  $\hat{S}_m^- = \hbar\sqrt{2S} a_m^\dagger (1 - \frac{a_m^\dagger a_m}{2S})^{1/2}$ ,  $\hat{S}_m^+ = (\hat{S}_m^-)^\dagger$ , and  $\hat{S}_m^z = \hbar(S - a_m^\dagger a_m)$  where  $[a_m, a_n^\dagger] = \delta_{mn}$ , show that the Hamiltonian can be expanded as a bilinear (i.e. to quadratic order) in the raising and lowering operators,

$$\hat{H} = -JNS^2 + S \sum_m (a_{m+1}^\dagger - a_m^\dagger)(a_{m+1} - a_m) + O(S^0).$$

- (e) Being bilinear in operators (i.e. quadratic), the Hamiltonian can be diagonalized by discrete Fourier transformation. With periodic boundary conditions,  $a_{m+N}^\dagger = a_m^\dagger$ , defining

$$a_k^\dagger = \frac{1}{\sqrt{N}} \sum_{m=1}^N e^{ikm} a_m^\dagger, \quad a_m^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikm} a_k^\dagger,$$

where the sum on  $k = 2\pi n/N$ , runs over the  $N$  integers  $n = -N/2 + 1, -N/2 + 2 \dots N/2$ , show that the transformed operators obey the commutation relations,  $[a_k, a_{k'}^\dagger] = \delta_{kk'}$ . In the Fourier representation, show that

$$\hat{H} = -JNS^2 + \sum_k \hbar\omega_k a_k^\dagger a_k + O(S^0)$$

where  $\omega_k = 2JS(1 - \cos k) = 4JS \sin^2(k/2)$  represents the dispersion of the spin excitations.

In the long wavelength limit,  $k \rightarrow 0$ , the energy of the excitations vanishes,  $\omega_k \rightarrow JSk^2$ . These low-energy excitations, known as **spin waves** or **magnons**, describe the elementary spin-wave excitations of the ferromagnet. Taking into account terms at higher order in the parameter  $1/S$ , one finds interactions between the magnons.



2. The following problem involves some revision of time-dependent perturbation theory and then applies the methodology to the problem of an induced transition in a hydrogen atom.

Suppose that a system is prepared in an energy eigenstate  $\psi_0$  at time  $t = 0$  when a weak perturbation  $V(t)$  is applied. Show that the probability of finding the system in state  $\psi_n$  at time  $t$  is given approximately by  $|c_n(t)|^2$  where

$$c_n(t) = \frac{1}{i\hbar} \int_0^t dt' e^{i(E_n - E_0)t'/\hbar} \langle \psi_n | V(t') | \psi_0 \rangle.$$

In lectures, we have discussed the Fourier series expansion,

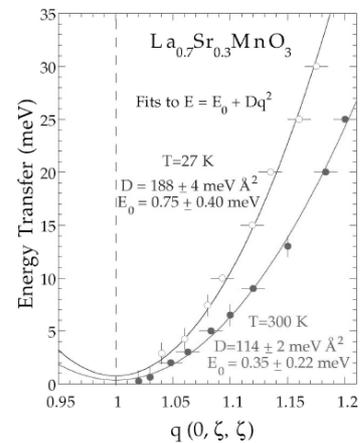
$$f(x) = \frac{1}{\sqrt{L}} \sum_k f_k e^{ikx}$$

$$f_k = \frac{1}{\sqrt{L}} \int_0^L f(x) e^{-ikx}$$

In the following, we are dealing with a discrete lattice where we have to consider the discrete Fourier representation,

$$f_n = \frac{1}{\sqrt{N}} \sum_k f_k e^{ikn}$$

$$f_k = \frac{1}{\sqrt{N}} \sum_n f_n e^{-ikn}.$$



Measurements of the spin-wave dispersion relations for the ferromagnet  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ .

At times  $t > 0$ , an electric field  $\mathcal{E}_z = \mathcal{E}_0 \exp -t/\tau$  is applied to a hydrogen atom, initially prepared in its ground state. Working to first order in the electric field, find the probability that, after a long time,  $t \gg \tau$ , the atom is in (i) the  $2s$  state, and (ii) one of the  $2p$  states (state which one?).



3. This problem addresses the question of spontaneous emission in hydrogen.

Use the formula for the Einstein  $A$ -coefficient derived in class to calculate the lifetime of the  $2p$  state of atomic Hydrogen.

You will need the same matrix elements as you computed in the previous problem.

Without detailed evaluation of the matrix element, explain why the  $3s$  level of hydrogen has a lifetime roughly 100 times longer than the  $2p$  level. And why is the lifetime of the  $2s$  level very much longer than  $2p$ , by a factor  $\sim 10^8$ ?



4. Scattering theory: The following problem revises the derivation of the Born approximation and then applies it to the high energy scattering from an attractive square well potential.

Show that the Born approximation yields the following expression for the elastic scattering of a particle of mass  $m$  and momentum  $\hbar k$  from a spherically symmetric potential  $V(r)$ ,

$$\frac{d\sigma}{d\Omega} = \left( \frac{2m}{\hbar^2 K} \right)^2 \left| \int_0^\infty V(r) r \sin(Kr) dr \right|^2,$$

where  $K = 2k \sin(\theta/2)$  and  $\theta$  is the angle through which the particle is scattered.

Obtain the differential cross-section for scattering from a potential,

$$V(r) = \begin{cases} -V_0 & r \leq a \\ 0 & r > a \end{cases}$$

and verify that the scattering is isotropic when the energy of the incident particle or the size of the scatterer is sufficiently low, so that  $Ka \ll 1$ . Obtain an expression for the total cross-section in this limit.



5. Scattering theory: The following problem involves the application of the partial wave scattering method to a simplified model of a nucleus.

As a crude model for an effective nuclear potential which binds together protons and neutrons, consider a repulsive radial shell potential,  $V(r) = \frac{\hbar^2}{2m} U_0 \delta(r - R)$ .

- Calculate the  $s$ -wave scattering phase shift as a function of  $U_0$ .
- Assuming that  $U_0 \gg 1/R$  and  $U_0 \gg k$ , show that if  $\tan(kR)$  is not close to zero, the phase shift resembles that of a hard sphere.
- Continuing with these assumptions show that, if  $\tan(kR)$  is close (but not equal to) zero, resonance is possible (i.e. the cross section reaches its maximum value). Compare the resonance energy with that of a bound state of the spherical shell with an infinitely impenetrable wall. This is an example of a “scattering resonance”, when the incident energy matches a quasi bound-state.

6. †Relativistic quantum mechanics: The following problem establishes an important relation in the study of relativistic covariance in lectures.

In lectures, it was shown that Lorentz covariance of the Dirac equation relies on the condition  $S(\Lambda)\gamma^\mu S^{-1}(\Lambda) = (\Lambda^{-1})^\mu{}_\nu \gamma^\nu$ . For an infinitesimal proper Lorentz transformation  $\Lambda^\mu{}_\nu = g^\mu{}_\nu + \omega^\mu{}_\nu$ ,  $S(\Lambda) = \mathbb{I} - \frac{i}{4}\Sigma_{\mu\nu}\omega^{\mu\nu} + \dots$ , where  $\omega_{\mu\nu}$  and  $\Sigma_{\mu\nu}$  are antisymmetric. Show that, to leading order in  $\omega$ , this condition translates to

$$[\gamma^\mu, \Sigma_{\alpha\beta}] = 2i \left( g^\mu{}_\alpha \gamma_\beta - g^\mu{}_\beta \gamma_\alpha \right).$$

Show that the following represents a consistent solution,  $\Sigma_{\alpha\beta} = \frac{i}{2}[\gamma_\alpha, \gamma_\beta]$ .

7. Relativistic quantum mechanics: In lectures, we used the relativistic covariance of the Dirac equation to deduce the existence of an intrinsic angular momentum known as spin. In the following problem, we can establish the consistency of this construction by showing that the Dirac Hamiltonian commutes with the total angular momentum,  $\hat{\mathbf{J}}$ .

Verify that the Dirac Hamiltonian  $\hat{H} = \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta m$  commutes with both the helicity operator  $\mathbf{S} \cdot \mathbf{p}/|\mathbf{p}|$ , and the angular momentum  $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \mathbf{S}$  where  $\hat{\mathbf{L}} = \mathbf{x} \times \hat{\mathbf{p}}$ .

8. †Relativistic quantum mechanics: The following problem relates to the vacuum instability and the stimulation of particle/antiparticle pairs.

Following on from the discussion of the potential step in lectures, consider the problem of the transmission through a potential barrier of width  $a$  and height  $eV$ . Apply the boundary conditions at the edge of the barrier, show that the transmission probability is given by

$$|t^2| = \left| \cos(p'a) - i \sin(p'a) \frac{(1 + \zeta^2)}{2\zeta} \right|^{-2},$$

where  $\zeta = \frac{p'(p^0+m)}{p(p^{0'}+m)}$ ,  $E \equiv p^0$ , and  $E' \equiv p^{0'} = E - eV$ . Analyse the transmission probability in the energy ranges  $p^{0'} \equiv E' > m$ ,  $-m < E' < m$ , and  $E' < -m$ . In the third regime, explain why a condition of perfect transmission can be obtained.