Ap 295b **Problem Set 3** **Due: Thursday, October 31st, 2002**

Problem 1

The anisotropic Heisenberg model is defined by the Hamiltonian

$$\mathcal{H} = -\sum_{ij} [J'_{ij}\ S_i^z\ S_j^z\ + \frac{1}{2} J_{ij} (S_i^+\ S_j^- + S_i^- S_j^+)]$$

Consider a one-dimensional system with nearest-neighbor interactions and ferromagnetic coupling $J > 0, J' > 0$

a) Show that for $J' > J$ the ferromagnetically ordered state with magnetization aligned in the z direction is the ground state of the Hamiltonian.

b) Show that for $J' > J$ the magnon wavefunctions are similar to the isotropic Heisenberg model solutions, but they have a nonzero energy at $k = 0$

c) Show that for $J' < J$ the ferromagnetically ordered state with magnetization aligned in the z direction is <u>not</u> the ground state of the Hamiltonian.

Problem 2

A simple model that exhibits some of the magnetic properties of an atom, which has more than one shell occupied, consists of an equilateral triangle of sites 1, 2 and 3 with hopping between them and on site interactions only.

$$\mathcal{H} = -t \sum_{\delta} [C^+_{1\delta} C_{2\delta} + C^+_{2\delta} C_{3\delta} + C^+_{3\delta} C_{1\delta} + h.c.] + U \sum_j n_{j\uparrow} n_{j\downarrow}$$

We are interested in the case with 4 electrons

a) For $U = 0$ find the one-electron states. What are the lowest energy four electron states? How many of these are there? Use a basis in which the three one-electron states are labelled by their "orbital angular momentum, " $m = -1, 0, 1$.

b) To lowest order in $\frac{U}{t} <<$, find an effective Hamiltonian for the space of low energy 4 electron states from (a) and find the resulting low energy states, their energies, and their degeneracies.

c) Is the atom ferromagnetic or antiferromagnetic?

Problem 3

Consider neutral bosonic atoms with effecitve spin 1/2 ($\sigma = \uparrow\downarrow$) in a peridic potential created by laser beams (optical lattice). When the potential is sufficiently strong we can project the kinetic energy of bosons into the lowest Bloch band and consider interaction between particles only when they occupy the same well (see Figure). In this limit the Hamiltonian of the system is given by (see e.g. Phys.Rev.Lett. **81**, 3108 (1998))

$$\mathcal{H} = -\sum_{\langle ij\rangle\sigma} t_\sigma b^\dagger_{i\sigma} b_{j\sigma} + \sum_{i\sigma} U_{\sigma\sigma} n_{i\sigma}(n_{i\sigma} - 1) + U_{\uparrow\downarrow} \sum_i n_{i\uparrow} n_{i\downarrow}$$

Here t_σ is the tunneling amplitude for atoms with spin σ between the near-neighbor sites $\langle ij\rangle$. Let the density of particles be such that there is one particle per well on the average. When repulsion between particles is strong, we have small fluctuations in the number of particles in each well, so the system is in the insulating regime (for spinless bosons such insulating phase has been observed by Greiner *et.al.*, see Nature **415**, 39 (2002)). Then the only degree of freedom left is the spin orienation of atoms in individual wells.

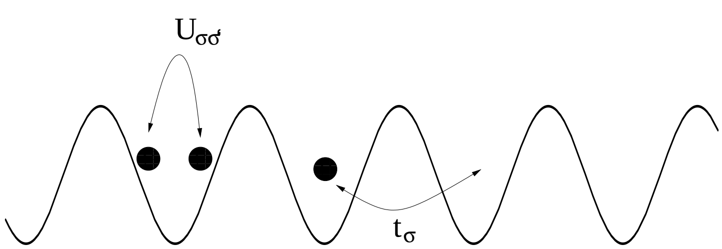

FIG. 1: Problem 3

a) By doing perturbative calculations in t/U derive an effective spin Hamiltonian of the form

$$\mathcal{H} = J_z \sum_{\langle ij\rangle} S^z_i S^z_j + J_\perp \sum_{\langle ij\rangle} (S^x_i S^x_j + S^y_i S^y_j) + H \sum_i S^z_i \tag{1}$$

Obtain explicit expressions for $J_\perp$, J_z, and H in the leading order in t/U.

b) By changing parameters of the optical lattice we can change J_z, $J_\perp$, and H independently. Assuming that $J_\perp$ is fixed, discuss the phase diagram of (1) as a function of J_z, and H on a cubic lattice.

Problem 4

Consider the SDW ground state of positive - U Hubbard model at half-filling with magnetic order in the z-direction (see lecture notes pp. 73 - 76).

a) Transform the density and spin operators $\rho(q)$ and $S^i(q)$ into the γ- representation (i.e. write them in terms of $\gamma^{C,V}_{k\delta}$ operators).

b) Consider the correlation functions for charge and spin in the presence of SDW background

$$\overline{\chi}^{\,\circ\circ}(q,q',t) = \frac{i\theta(t)}{N}\langle\Omega|\rho(q,t)\rho(-q',t=0)|\Omega\rangle + \frac{i\theta(-t)}{N}\langle\Omega|\rho(-q',t=0)\rho(q,t)|\Omega\rangle$$

$$\overline{\chi}^{\,ij}(q,q',t) = \frac{i\theta(t)}{N}\langle\Omega|S^i(q,t)S^j(-q',t=0)|\Omega\rangle + \frac{i\theta(-t)}{N}\langle\Omega|S^j(-q',t=0)S^i(q,t)|\Omega\rangle$$

The time dependence of the γ operators is given simply by

$$\gamma^C_{k,\alpha}(t) = e^{-itE_k}\gamma^C_{k,\alpha}(0)$$

$$\gamma^V_{k,\alpha}(t) = e^{itE_k}\gamma^V_{k,\alpha}(0)$$

In evaluating the average, the only non-vanishing terms arise from the combinations such as

$$<\ \gamma^{V\dagger}_{k\alpha}\ \ \gamma^{C}_{p\beta}\ \ \gamma^{C\dagger}_{p'\beta'}\ \ \gamma^{V}_{k'\alpha'}\ >= \delta_{kk'}\delta_{pp'}\delta_{\alpha\alpha'}\delta_{\beta\beta'}$$

Show that

$$\begin{aligned}
\overline{\chi}^{\circ\circ}\ (q,q',\omega) &= \delta(q-q')\,\overline{\chi}^{\circ\circ}_{\circ}(q,\omega) \\
\overline{\chi}^{+-}(q,q',\omega) &= \delta(q-q')\ \overline{\chi}^{+-}_{\circ}(q,\omega) + \delta(q-q'+Q)\ \overline{\chi}^{+-}_{Q}(q,\omega)
\end{aligned} \tag{2}$$

where

$$
\begin{aligned}
\overline{\chi}_{\circ}^{\circ\circ}(q,\omega) &= \frac{1}{N}\sum_{k\epsilon BZ'}\left[1-\frac{\varepsilon_k\varepsilon_{k+q}+\Delta^2}{E_kE_{k+q}}\right]\left\{\frac{1}{(\omega-E_{k+q}-E_k+i\delta)}-\frac{1}{(\omega+E_{k+q}+E_k-i\delta)}\right\}\\
\overline{\chi}_{\circ}^{+-}(q,\omega) &= \frac{1}{N}\sum_{k\epsilon BZ'}\left[1-\frac{\varepsilon_k\varepsilon_{k+q}-\Delta^2}{E_kE_{k+q}}\right]\left\{\frac{1}{(\omega-E_{k+q}-E_k+i\delta)}-\frac{1}{(\omega+E_{k+q}+E_k-i\delta)}\right\}\\
\overline{\chi}_{Q}^{+-}(q,\omega) &= -\frac{1}{N}\sum_{k\epsilon BZ'}\frac{4\Delta}{E_k}\left\{\frac{1}{(\omega-E_{k+q}-E_k+i\delta)}-\frac{1}{(\omega+E_{k+q}+E_k-i\delta)}\right\} \qquad (3)
\end{aligned}
$$

c*) Equations (2), (3) give the response functions in the absence of interactions. The GRPA response functions can be obtained by solving

$$
\overline{\chi}_{GRPA}^{+-}(q,q',\omega)=\sum_{q_1}\overline{\chi}_{\circ}^{+-}(q,q_1,\omega)\left[1+U\overline{\chi}_{\circ}^{+-}(q_1,q',\omega)\right]^{-1}
$$

where $[1+U\overline{\chi}_{\circ}^{+-}(q_1,q\prime,\omega)]^{-1}$ is a matrix inverse in momentum space. Show that $\overline{\chi}_{GRPA}^{+-}$ contains a gapless pole, as predicted by the Goldstone theorem.

Hint: Use the self-consistency condition

$$
\frac{1}{N}\sum_{k\epsilon BZ\prime}\frac{1}{(\varepsilon_k^2+\Delta^2)^{\frac{1}{2}}}=\frac{1}{U}
$$

d*) Show that in the large U limit the spin-wave velocity is $v=\frac{1}{\sqrt{2}}J$, where $J=\frac{4t^2}{U}$. This agrees exactly with the result for the Heisenberg model.