

**Assignment 4.** (Due Nov 9, 2005)

- 1 [Sakurai 2.18] A coherent state of a one-dimensional oscillator is defined to be an eigenstate of the (non-Hermitian) annihilation operator  $a$ :

$$a|\lambda\rangle = \lambda|\lambda\rangle \quad (1)$$

where  $\lambda$  is, in general, a complex number.

- a. Prove that

$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle \quad (2)$$

is a normalized coherent state.

- b. Prove the minimum uncertainty relation for such a state.

- c. Write  $|\lambda\rangle$  as,

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle. \quad (3)$$

Show that the distribution of  $|f(n)|^2$  with respect to  $n$  is of the Poisson form. Find the most probable value of  $n$ , and hence of the energy  $E$ .

- d. Show that a coherent state can also be obtained by applying the translation (finite displacement) operator  $e^{-ipl/\hbar}$  (where  $p$  is the momentum operator, and  $l$  is the displacement distance) to the ground state.

2. The transformations from momentum- to position dependent creation and annihilation operators ('field operators') in Fetter and Walecka (FW) Eq.'s (2.1)-(2.4) are just a special case of the general property that in the absence of interactions problems can be solved by transforming the creation- and annihilation operators themselves. In full generality, single particle Hamiltonians become in second quantization (FW Eq. 1.42, 1.60),

$$H = \sum_{p,r} h_{pr} a_p^\dagger a_r \quad (4)$$

with  $h_{pr} = \langle p|H|r\rangle$  and  $a^\dagger, a$  fermionic or bosonic creation/annihilation operators. Let us now transform these operators,

$$\begin{aligned} c_k &= \sum_p U_{kp} a_p \\ c_k^\dagger &= \sum_p a_p^\dagger U_{kp}^\dagger \end{aligned} \quad (5)$$

where  $U_{kp}$  are the elements of a unitary matrix  $\mathbf{U}$ .

- a. Show that the transformed operators obey again the (anti-) commutation relations  $[c_k^\dagger, c_l^\dagger]_\pm = [c_k, c_l]_\pm = 0$  and  $[c_k, c_l^\dagger]_\pm = \delta_{kl}$  where the commutation (-) or anti-commutation (+) property is determined by the statistics of the original ( $a^\dagger, a$ ) particles. Why is this a necessary condition for the transformation to be meaningful? Would this also be the case when the transformation would be non unitary?
  - b. The single particle problem is solved by requiring that the Hamiltonian acquires the form  $H = \sum_k \epsilon_k c_k^\dagger c_k$  in terms of the transformed operators. Demonstrate that this involves the same unitary transformation as the one diagonalizing the problem  $H = \sum_{p,r} |p\rangle h_{pr} \langle r|$ .
  - c. This non-interacting system surely should conserve the total number of particles. Construct the operator  $\hat{N}$  counting all the particles, show that it commutes with the Hamiltonian, and that it is invariant under the unitary transformations  $\mathbf{U}$ .
  - d. Alternatively, the Heisenberg equations of motion can be used to solve the problem. In the Heisenberg picture the time evolution of the creation operators is governed by  $i\hbar \frac{da_p^\dagger}{dt} = [a_p^\dagger, H]$ . The problem is solved when creation operators are found evolving in time according to  $c_k^\dagger(t) = e^{i\epsilon_k t} c_k^\dagger(t=0)$ . Show that this involves the same transformation as in (c). What happens with the annihilation operators?
  - e. Consider a general two-body interaction  $\hat{V} = \frac{1}{2} \sum_{pqrs} V_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$  and add this term to the Hamiltonian. Calculate the equations of motion for  $a_p^\dagger$ , both for fermions and bosons. Is it still possible to diagonalize the problem, using a transformation like  $\mathbf{U}$ ?
3. The two-state problem has a famous extension in the form of a toy model giving a first intuition about the workings of interactions, the 'Hubbard Hydrogen Molecule': the two state problem with two electrons having the simplest imaginable interaction. This can be pictured as two (hydrogen) atoms, each contributing one state (e.g. the 1s atomic state), while electrons can tunnel back and forth with a rate  $t$  between the two atoms. We call the single electron states  $|1\sigma\rangle$  and  $|2\sigma\rangle$  where  $\sigma = \uparrow, \downarrow$  is the spin of the electrons. The single particle Hamiltonian is ( $h.c$  is hermitian conjugate),

$$H = \sum_{i=1,2;\sigma} |i\sigma\rangle \epsilon \langle i\sigma| - t \sum_{\sigma} (|1\sigma\rangle \langle 2\sigma| + h.c.) \quad (6)$$

In this exercise we'll focus on the two-electron states of the non-interacting molecule.

- a. Construct all 2 electron first quantized states (Slater determinants)  $|k\rangle_2 = |i\sigma j\sigma'\rangle$ , in terms of the 'atomic' ( $|1\rangle, |2\rangle$ ) one particle basis. Write the Hamiltonian explicitly in this two-electron basis, in the form  $H = \sum_{kl} |k\rangle_2 h_{kl} \langle l|_2$  and diagonalize this  $6 \times 6$  problem: seek simplifications first, it can be reduced to a  $2 \times 2$  problem! Interpret the outcome in terms of the physics of this toy  $H_2$  molecule.
- b. It is actually more convenient to first diagonalize the single particle Hamiltonian, in terms of the 'molecular orbital' basis  $|\pm, \sigma\rangle = (|1\sigma\rangle \pm |2\sigma\rangle)/\sqrt{2}$ . Construct the two electron states of the molecule from this basis and discuss the correspondence with the states found in (a.).

- c. Introduce operators  $a_{i\sigma}^\dagger, a_{i\sigma}$  creating/annihilating electrons with spin  $\sigma$  on atom  $i$ . Rewrite the Hamiltonian in second quantized form and transform the operators using the recipe of exercise 3. Construct the 2-particle energy eigenstates by acting twice with the creation operators on the vacuum and establish the correspondences with what you found both in (a) and (b).
4. Let us now include the so-called "Hubbard" interaction in the description of the non-interacting molecule of exercise 3. Electrons carry an electrical charge and they surely do not like to be squeezed together in a small space because of the Coulomb repulsion. This is completely ignored in the 'molecular orbital' description of exc. 4, while in reality these Coulomb repulsions are often the largest numbers in the problem.
- a. The main effect of the Coulomb repulsions between the electrons in the molecule is coded into the 'Hubbard interaction'

$$H_1 = U \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow} \quad (7)$$

- where  $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$  is the number operator, counting the number of electrons present in the state of atom  $i = 1, 2$  with spin  $\sigma$ . Explain why this term codes for the main effect of Coulomb repulsion in the molecule. Why can terms like  $n_{i\uparrow} n_{i\uparrow}$  be ignored?
- b. Determine the spectrum of two electron energy eigenvalues for arbitrary  $U$  and  $t$ , and sketch a level diagram both for  $U \gg t$  and  $U \ll t$ . What is the influence of the Hubbard interaction on the stability of the molecule? N.B. the large  $U$  limit is well known in chemistry as the 'Heitler-London theory of chemical binding'.
- c. Consider the 'strong coupling limit',  $U \gg t$ , for the two electron case. Use perturbation theory controlled by the small parameter  $t/U$  to demonstrate that at energies small compared to  $U$  the system is accurately described by a spin Hamiltonian of the form  $H_{eff} = J \vec{S}_1 \cdot \vec{S}_2$ , where  $\vec{S}_i = (S_{x,i}, S_{y,i}, S_{z,i})$  are the spin 1/2 operators keeping track of the spin of the electrons on atom  $i$ . Determine the exchange parameter  $J$  in terms of  $t$  and  $U$ , and discuss why this spin-spin interaction favors anti-ferromagnetism (anti-parallel alignment of the spins). N.B.: this gives away the essence of 'kinetic'- or 'super' exchange, the primary source of spin-spin interactions in magnetic salts.