Physikalisches Institut
Universität Bonn
Theoretical Physics

Exercise Sheet 13
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Advanced Quantum Theory

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http://www.th.physik.uni-bonn.de/klemm/advancedqm/index.php

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–Exercises–

13.1 (Anti-) Symmetrising Operators $\hat{S}_\pm$

Assume that $\{|i_k\rangle\}$ form a complete basis of orthonormal states in the Hilbert space of single particle states.

a) Show that the (anti-)symmetrising operators $\hat{S}_\pm$ acting on the Hilbert space of N-particle states obey $(S_\pm)^2 = \sqrt{N!}\ \hat{S}_\pm$. *(1 Pt)*

b) Show that the set of (anti-)symmetric states $\{\hat{S}_\pm |i_1, i_2, \cdots, i_N\rangle\}$ yields a complete set of (anti-) symmetric states in the Hilbert space of (anti-) symmetrised N-particle states, i.e., any state $|\psi\rangle_{s/a}$ in this Hilbert space can be expanded in terms of the above defined set. *(1 Pt)*

13.2 Three particle State and S_3

Consider the 3-particle state $|i_1, i_2, i_3\rangle = |i_1\rangle \otimes |i_2\rangle \otimes |i_3\rangle$.

a) Apply the permutation group S_3 on the three-particle state $|i_1, i_2, i_3\rangle$ to construct a six-dimensional Hilbert space of 3-particle states. *(1 Pt)*

b) Compute the totally symmetric and anti-symmetric subspaces for bosonic and fermionic particles, respectively. *(1 Pt)*

13.3 Creation and Annihilation Operators

In the lecture the bosonic Fock space was introduced along with the creation operator $\hat{a}_k^\dagger$ with the property

$$\hat{a}_k^\dagger |n_1, \cdots, n_k, \cdots\rangle = \sqrt{n_k + 1}\, |n_1, \cdots, n_k + 1, \cdots\rangle\,. \tag{1}$$

Here $|n_1, \cdots, n_k, \cdots\rangle$ is a totally symmetric state with occupation numbers $n_1, n_2, \cdots$.

a) Argue that the annihilation operator $\hat{a}_k$ acts as,

$$\hat{a}_k |n_1, \cdots, n_k, \cdots\rangle = \sqrt{n_k}\, |n_1, \cdots, n_k - 1, \cdots\rangle\ \ . \tag{2}$$

(1 Pt)

b) Prove the commutation relation $[\hat{a}_k, \hat{a}_l^\dagger] = \delta_{k,l}$. *(2 Pts)*

c) For the bosonic number operator $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$, compute that

$$\hat{n}_k |n_1, n_2, \cdots, n_k, \cdots\rangle = n_k |n_1, n_2, \cdots, n_k, \cdots\rangle \ . \tag{3}$$

(1 Pt)

Similarly, for the fermionic Fock space with the creation operators $\hat{b}_k^\dagger$, it was stated

$$\hat{b}_k^\dagger |n_1, \cdots, n_k, \cdots\rangle = (1 - n_k)(-1)^{\sum_{j<k} n_j} |n_1, \cdots, n_k + 1, \cdots\rangle \,. \tag{4}$$

Here $|n_1, \cdots, n_k, \cdots\rangle$ is a totally anti-symmetric state.

d) Argue that the annihilation operator $\hat{b}_k$ acts as

$$\hat{b}_k |n_1, \cdots, n_k, \cdots\rangle = (n_k)(-1)^{\sum_{j<k} n_j} |n_1, \cdots, n_k - 1, \cdots\rangle \tag{5}$$

(1 Pt)

e) Prove the anti-commutation relation $\{\hat{b}_k, \hat{b}_l^\dagger\} = \delta_{k,l}$. *(2 Pts)*

f) For the fermionic number operator $\hat{n}_k = \hat{b}_k^\dagger \hat{b}_k$, compute

$$\hat{n}_k |n_1, n_2, \cdots, n_k, \cdots\rangle = n_k |n_1, n_2, \cdots, n_k, \cdots\rangle \ . \tag{6}$$

(1 Pt)

13.4 The Heisenberg XY Model

Consider a one-dimensional chain of L 'sites' which can be in different states. The chain has a Hamiltonian that can be written as[1]

$$\hat{H} = -\frac{J}{2} \sum_{n=1}^{L} \left(\hat{b}_n^\dagger \hat{b}_{n+1} + \hat{b}_{n+1}^\dagger \hat{b}_n \right) \ ; \ J > 0 \ ,$$

where $\hat{b}_n^\dagger$, $\hat{b}_n$ are canonical fermionic creation and annihilation operators at site n and we assume the periodic boundary condition $\hat{b}_{n+L} = \hat{b}_n$.

a) Define

$$\hat{f}_k = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{-ikn} \hat{b}_n \,.$$

Determine the possible values of k such that the operators $\hat{f}_k$ are consistent under the shift $n \mapsto n + L$ of the summation index. Show that the set of allowed $\hat{f}_k$, $\hat{f}_k^\dagger$ satisfy canonical fermionic anticommutation relations. *(2 Pts)*

b) Show that the $\hat{f}_k^\dagger$ create single particle energy eigenstates in the tight-binding chain, *i.e.*, show that $[H, \hat{f}_k^\dagger] = E_k \hat{f}_k^\dagger$, and determine E_k. *(3 Pts)*

[1] Such a model arises for example for a chain of atoms, where each atom provides a slot for a tightly bound electron, and the energy is effectively given by the interatomic matrix element of overlap between neighbouring atoms (*i.e.*, this matrix element defines J).

c) Show that the $\hat{f}_k$ diagonalise the Hamiltonian: $\hat{H} = \sum_k E_k \, \hat{f}_k^\dagger \hat{f}_k$, where the sum runs over a maximal set of k such that the $\hat{f}_k$ are pairwise different. *(3 Pts)*

While negative (positive) energies E_k may be associated to bonding (antibonding) orbitals in the atomic chain, the tight binding model is also used as a simple example of electric band structure. In this case, the ground state is defined as the one in which precisely all states with negative energy are filled:

$$|\psi_0\rangle := \prod_{k:E_k<0} \hat{f}_k^\dagger \, |0\rangle \ ,$$

where $|0\rangle$ denotes the completely unoccupied state in the occupation basis.

d) Verify that this means that the chain is half-filled for large L:

$$\lim_{L\to\infty} \frac{1}{L} \, \langle\psi_0| \, \hat{N} \, |\psi_0\rangle \ = \ \frac{1}{2} \, ,$$

where $\hat{N}$ is the total number operator of fermionic excitations. *(3 Bonus Pts)*

e) In the band structure interpretation, modes which are less than half filled are interpreted as 'hole' excitations. Consider the "physical" ladder operators defined by

$$\hat{s}_k = \begin{cases} \hat{f}_k, & E_k \geq 0, \\ \hat{f}_{-k}^\dagger, & E_k < 0 \, . \end{cases}$$

Which anticommutation relations do the $\hat{s}_k$ and $\hat{s}_k^\dagger$ satisfy, and what is their interpretation? Show that $H = \sum_k |E_k| \hat{s}_k^\dagger \hat{s}_k + H_0$, where H_0 is some constant. Determine the energy density $\hat{H}/L$ of the ground state $|\psi_0\rangle$ in the limit $L \to \infty$. *(4 Bonus Pts)*