Karlsruher Institut für Technologie Institute for Condensed Matter Theory
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Condensed Matter Theory II: Many-Body Theory (TKM II) SoSe 2023

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Homework assignment 3
Deadline: 12 May 2023

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1. Holstein-Primakoff transformation (15 points)

The Holstein–Primakoff transformation, defined as

$$\hat{S}_+ = \hbar\sqrt{2S}\sqrt{1-\frac{\hat{b}^\dagger\hat{b}}{2S}}\,b\,, \qquad \hat{S}_- = \hbar\sqrt{2S}\,\hat{b}^\dagger\sqrt{1-\frac{\hat{b}^\dagger\hat{b}}{2S}}\,, \qquad \hat{S}_z = \hbar\left(S-\hat{b}^\dagger\hat{b}\right)\,,$$

expresses the spin operators $\hat{S}_+$, $\hat{S}_-$, and $\hat{S}_z$ for a spin S through bosonic creation and annihilation operators $\hat{b}^\dagger$ and $\hat{b}$. This transformation is particularly useful when $S \gg 1$: in this case, the square roots can be expanded in Taylor series of powers of $1/S$.

Demonstrate that the operators defined above indeed obey the commutation relations for spin-S operators $\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$, $\hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-)$ and S_z:

$$\left[\hat{S}_x,\hat{S}_x\right]=0, \quad \left[\hat{S}_x,\hat{S}_y\right]=i\hbar\hat{S}_z, \quad \left[\hat{S}_x,\hat{S}_z\right]=-i\hbar\hat{S}_y, \quad \left[\hat{S}_y,\hat{S}_z\right]=i\hbar\hat{S}_x.$$

Solution:

The following identity is very helpful:

$$n_b b = b(n_b - 1). \tag{1}$$

To establish the commutation relations, it is sufficient to compute the following two commutators for the angular momentum ladder operators:

$$\begin{aligned}\left[\hat{S}_+,\hat{S}_-\right] &= \hbar\hat{S}_z\\ \left[\hat{S}_+,\hat{S}_z\right] &= \hbar\hat{S}_+.\end{aligned} \tag{2}$$

The first equation:

$$\begin{aligned}\left[\hat{S}_+,\hat{S}_-\right] &= 2S\hbar^2\left[\sqrt{1-\frac{\hat{n}_b}{2S}}(\hat{n}_b+1)\sqrt{1-\frac{\hat{n}_b}{2S}} - b^\dagger\left(\sqrt{1-\frac{\hat{n}_b}{2S}}\right)^2 b\right]\\ &= 2S\hbar^2\left[\sqrt{1-\frac{\hat{n}_b}{2S}}(\hat{n}_b+1)\sqrt{1-\frac{\hat{n}_b}{2S}} - b^\dagger b\left(\sqrt{1-\frac{\hat{n}_b-1}{2S}}\right)^2\right]\\ &= 2S\hbar^2\left[(\hat{n}_b+1)\left(1-\frac{\hat{n}_b}{2S}\right) - \hat{n}_b\left(1-\frac{\hat{n}_b-1}{2S}\right)\right]\\ &= 2S\hbar^2\left(1-\frac{\hat{n}_b}{S}\right)\\ &= 2\hbar\hat{S}_z\end{aligned} \tag{3}$$

To make this more rigorous, one could define the square root functions with operator arguments by using the Taylor expansion $\sqrt{1+\hat{X}} \equiv \sum_{n=0}^{\infty} \frac{a_n \hat{X}^n}{n!}$, and check that the above manipulations hold.

The second one:

$$\begin{aligned}\left[\hat{S}_+, \hat{S}_z\right] &= \sqrt{2S}\hbar^2 \sqrt{1-\frac{\hat{n}_b}{2S}}\,[b, S-n_b] \\ &= -\sqrt{2S}\hbar^2 \sqrt{1-\frac{\hat{n}_b}{2S}}\,b \\ &= -\hbar \hat{S}_+ \end{aligned} \tag{4}$$

One can also see from the definition that $\hat{S}_+^\dagger = \hat{S}_-$. Thus, a third commutation relation

$$\left[\hat{S}_-, \hat{S}_z\right] = \hbar \hat{S}_- \tag{5}$$

is obtained as the Hermitean conjugate of the second one. The relations for J_x and J_y can be obtained as linear combinations of these three relations.

For example:

$$\left[\hat{S}_x, \hat{S}_z\right] = \frac{1}{2}\left[\hat{S}_+ + \hat{S}_-, \hat{S}_z\right] = -\frac{\hbar}{2}(\hat{S}_+ - \hat{S}_-) = -i\hbar \hat{S}_y. \tag{6}$$

2. Wick's theorem: (10 + 10 points)

The Wick theorem states that a time-ordered product of operators can be rewritten as the normal-ordered product of these operators plus the normal-ordered products with all single contractions among operators plus the normal-ordered products with all double contractions, etc., plus all full contractions (see lecture notes, Sec. 3.8.1).

(a) In the lectures, we assumed that the operators entering the time-ordered (chronological) product are linear in creation/annihilation operators. Is this assumption necessary for the validity of Wick's theorem? Why?

Solution:

Once operators are no longer linear in creators/annihilators a key assumption in the proof breaks down: that contractions are $\mathbb{C}$-numbers that commute with everything.

A consequence is that there is no Wick theorem for spin operators used in Ex. 1:

$$\begin{aligned}\underbrace{S_- S_+} &:= S_- S_+ - \mathcal{N} S_- S_+ \\ &= S_- S_+ - S_+ S_- = -2\hbar S_z \end{aligned} \tag{7}$$

This is an operator which will not commute with ladder operators.

The failure is more apparent if we make an explicit calculation with three operators and use the commutation rules to normal-order the operators to see whether we recover the Wick's theorem. In bosonic case, we have

$$bbb^\dagger = bb^\dagger b + b = b^\dagger bb + 2b \tag{8}$$

which is what Wick's theorem would tell us. The first term is the normal-ordering part and the second term is the sum of all the contractions (there are 2 nonvanishing contractions).

With spin operators we have

$$\begin{aligned} S_-S_-S_+ &= S_-S_+S_- - \hbar S_-S_z && (9)\\ &= S_+S_-S_- - \hbar S_zS_- - \hbar S_zS_- + \hbar^2 S_- && (10)\\ &= S_+S_-S_- - (2S_z - 1)S_-, && (11) \end{aligned}$$

which is not easily interpreted as a sum of contractions in the same sense.

Here we have not considered Wick's theorem for time-dependent (Heisenberg or interaction picture) operators, but for time-independent (Schrödinger) operators. For the relation between the two forms of Wick's theorem, see Molinari's pedagogical paper: `https://doi.org/10.48550/arXiv.1710.09248`.

(b) Would Wick's theorem be valid if we replaced the chronological product in the theorem, as well as in the definition of contraction, by a product that orders the operators according to their coordinate along the x-axis? Substantiate your answer.

Solution: One has to check whether the contractions are $\mathbb{C}$-numbers for path ordering. Then the induction goes through as for time ordering.

A technical complication is that one cannot restrict to creator/annihilator $b_\alpha^\dagger, b_\alpha$ of eigenstates, since path ordering requires the field operator to depend on x.

$$\begin{aligned} \mathcal{P}\psi^\dagger(t_1,x_1)\psi(t_2,x_2) - \mathcal{N}\psi^\dagger(t_1,x_1)\psi(t_2,x_2) &= \begin{cases} 0 & x_1 > x_2 \\ -\{\psi^\dagger(t_1,x_1),\psi(t_2,x_2)\} & x_1 \le x_2 \end{cases}\\ \mathcal{P}\psi(t_1,x_1)\psi(t_2,x_2) - \mathcal{N}\psi(t_1,x_1)\psi(t_2,x_2) &= \begin{cases} 0 & x_1 > x_2 \\ -\{\psi(t_1,x_1),\psi(t_2,x_2)\} & x_1 \le x_2 \end{cases}\\ \mathcal{P}\psi(t_1,x_1)\psi^\dagger(t_2,x_2) - \mathcal{N}\psi(t_1,x_1)\psi^\dagger(t_2,x_2) &= \begin{cases} \{\psi(t_1,x_1),\psi^\dagger(t_2,x_2)\} & x_1 > x_2 \\ 0 & x_1 \le x_2 \end{cases}\\ \mathcal{P}\psi^\dagger(t_1,x_1)\psi^\dagger(t_2,x_2) - \mathcal{N}\psi^\dagger(t_1,x_1)\psi^\dagger(t_2,x_2) &= \begin{cases} 0 & x_1 > x_2 \\ -\{\psi^\dagger(t_1,x_1),\psi^\dagger(t_2,x_2)\} & x_1 \le x_2 \end{cases} \end{aligned} \tag{12}$$

Since the anticommutators of free fields ψ are $\mathbb{C}$ numbers, Wick's theorem for path ordering holds.

3. Spectral weight (15 points)

Demonstrate that the spectral weight in a many-body fermionic system is normalized:

$$\int d\varepsilon \mathcal{A}(\mathbf{p},\varepsilon) = 1.$$

Determine the leading asymptotics of the fermionic Green's functions in the energy-momentum representation for $\varepsilon \to \infty$.

Solution:

According to Eq.(3.102) in the lectures, the spectral weight is given by

$$\begin{aligned}\mathcal{A}(\mathbf{p},\varepsilon_1) = \sum_m \Big\{ &|\langle 0,N,\mathbf{p}=0|\hat{a}_\mathbf{p}|m,N+1,\mathbf{p}\rangle|^2\,\delta(\varepsilon_1-\varepsilon^{(+)}(m,\mathbf{p})+\mu) \\ &+|\langle m,N-1,-\mathbf{p}|\hat{a}_\mathbf{p}|0,N,\mathbf{p}=0\rangle|^2\,\delta(\varepsilon_1-\varepsilon^{(-)}(m,\mathbf{p})+\mu)\Big\},\end{aligned} \tag{13}$$

where $\varepsilon^{(+)}(m,\mathbf{p})+\mu)$ and $\varepsilon^{(-)}(m,\mathbf{p})+\mu)$ are the particle-like and hole-like excitation energies. The states $|m,N+1,\mathbf{p}\rangle$ are the exact eigenstates with $N+1$ particles, and m is the set of quantum numbers characterizing the states.

Integrating over the energy, we obtain

$$\begin{aligned}\int d\varepsilon\mathcal{A}(\mathbf{p},\varepsilon) &= \sum_m \left\{|\langle 0,N,\mathbf{p}=0|\hat{a}_\mathbf{p}|m,N+1,\mathbf{p}\rangle|^2+|\langle m,N-1,-\mathbf{p}|\hat{a}_\mathbf{p}|0,N,\mathbf{p}=0\rangle|^2\right\} \\ &= \sum_m \langle 0,N,\mathbf{p}=0|\hat{a}_\mathbf{p}|m,N+1,\mathbf{p}\rangle\langle m,N+1,\mathbf{p}|\hat{a}^\dagger_\mathbf{p}|0,N,\mathbf{p}=0\rangle \\ &+ \sum_m \langle 0,N,\mathbf{p}=0|\hat{a}^\dagger_\mathbf{p}|m,N-1,\mathbf{p}\rangle\langle m,N-1,\mathbf{p}|\hat{a}_\mathbf{p}|0,N,\mathbf{p}=0\rangle \\ &= \sum_{m,N',\mathbf{p}'} \langle 0,N,\mathbf{p}=0|\hat{a}_\mathbf{p}|m,N',\mathbf{p}'\rangle\langle m,N',\mathbf{p}'|\hat{a}^\dagger_\mathbf{p}|0,N,\mathbf{p}=0\rangle \\ &+ \sum_{m,N',\mathbf{p}'} \langle 0,N,\mathbf{p}=0|\hat{a}^\dagger_\mathbf{p}|m,N',\mathbf{p}'\rangle\langle m,N',\mathbf{p}'|\hat{a}_\mathbf{p}|0,N,\mathbf{p}=0\rangle \\ &= \langle 0,N,\mathbf{p}=0|\underbrace{\hat{a}_\mathbf{p}\hat{a}^\dagger_\mathbf{p}+\hat{a}^\dagger_\mathbf{p}\hat{a}_\mathbf{p}}_{=\delta_{\mathbf{pp}}=1}|0,N,\mathbf{p}=0\rangle = 1.\end{aligned} \tag{14}$$

For a noninteracting system $\hat{a}^\dagger_\mathbf{p}|N,\mathbf{p}=0\rangle = |N+1,\mathbf{p}\rangle$ is an eigenstate and only the term corresponding to it is nonzero:

$$\begin{aligned}\mathcal{A}(\mathbf{p},\varepsilon_1) = &|\langle N,\mathbf{p}=0|\hat{a}_\mathbf{p}|N+1,\mathbf{p}\rangle|^2\,\delta(\varepsilon_1-\varepsilon^{(+)}(\mathbf{p})+\mu) \\ &+|\langle N-1,-\mathbf{p}|\hat{a}_{-\mathbf{p}}|N,\mathbf{p}=0\rangle|^2\,\delta(\varepsilon_1-\varepsilon^{(-)}(\mathbf{p})+\mu).\end{aligned} \tag{15}$$

Now the spectral function is a delta-function at the single-particle energy. This is unlike in the interacting system, where we have the sum over the different m-states, which makes the spectral function to have a finite distribution of energies.

For $\varepsilon\to\infty$:

$$G^X(\mathbf{p},\varepsilon) = \int \mathrm{d}\varepsilon_1 \frac{\mathcal{A}(\mathbf{p},\varepsilon_1)}{\varepsilon-\varepsilon_1\pm i0} \tag{16}$$

$\mathcal{A}(\mathbf{p},\varepsilon_1)$ is only nonzero on a finite range of energies $|\varepsilon_1|<\Lambda$. If $\Lambda<\varepsilon$, we can approximate the denominator by ε and obtain:

$$G(\mathbf{p},\varepsilon)\simeq G^R(\mathbf{p},\varepsilon)\simeq G^A(\mathbf{p},\varepsilon)\simeq \frac{1}{\varepsilon}\int d\varepsilon_1\mathcal{A}(\mathbf{p},\varepsilon_1) = \frac{1}{\varepsilon}. \tag{17}$$