Exercise 11 for Theoretical Solid State Physics in Summer 2021

Prof. Dr. Andreas Klümper
Mathis Giesen (jan.giesen@uni-wuppertal.de G.11.07)

Submission: 02.07.2021, 12:00 in the P.O. Box Giesen on D.10 or by e-mail
Discussion: 05.07.2021, 14:15

1. **BCH formula (10 points)**

   (a) Show for an operator $\mathbf{L}$, linear in the creation and annihilation operators $\mathbf{b}_j^\dagger$ and $\mathbf{b}_j$ of a harmonic oscillator, i.e. $\mathbf{L} = \sum_j \left(c_j \mathbf{b}_j + d_j \mathbf{b}_j^\dagger\right)$, the following relation

   $$\left\langle e^{\mathbf{L}} \right\rangle = e^{\frac{\left\langle \mathbf{L}^2 \right\rangle}{2}},$$

   where the brackets $\langle \cdot \rangle$ describe the expectation value with respect to the canonical density operator of the harmonic oscillator $\mathbf{H} = \sum_j \omega_j \left(\mathbf{b}_j^\dagger \mathbf{b}_j + \frac{1}{2}\right)$.
   Hint: Show the equation first for a single mode, i.e. for $\mathbf{L} = x\mathbf{b} + y\mathbf{b}^\dagger$. By definition, the LHS as well as the RHS of

   $$\left\langle e^{\mathbf{L}} \right\rangle = e^{\frac{\left\langle \mathbf{L}^2 \right\rangle}{2}},$$

   are functions of the two arguments x, y. In fact, both sides of the equation are functions only of a single variable, namely of the product $z := x \cdot y$. Why? As an illustration evaluate $\langle \mathbf{L}^2 \rangle$ explicitly. A similar explicit evaluation of the LHS is difficult.

   Instead of a direct evaluation of the LHS we can derive a simple functional equation. Denote the density operator by

   $$\rho := \frac{e^{-\beta\omega \mathbf{b}^\dagger \mathbf{b}}}{Z}$$

   Because of the identity

   $$\mathbf{b}\rho = e^{-\beta\omega} \rho \mathbf{b}$$

we find

$$\langle e^{y\mathbf{b}^\dagger} e^{x\mathbf{b}} \rangle = \mathrm{Tr}\left[e^{y\mathbf{b}^\dagger} e^{x\mathbf{b}} \rho \right] = \mathrm{Tr}\left[e^{y\mathbf{b}^\dagger} \rho \, e^{\tilde{x}\mathbf{b}} \right] = \mathrm{Tr}\left[e^{\tilde{x}\mathbf{b}} e^{y\mathbf{b}^\dagger} \rho \right] = \langle e^{\tilde{x}\mathbf{b}} e^{y\mathbf{b}^\dagger} \rangle$$

with $\tilde{x} := e^{-\beta\omega} x$. From this you obtain the relation

$$e^{-\frac{1}{2}xy} \left\langle e^{\mathbf{L}} \right\rangle = e^{\frac{1}{2}\tilde{x}y} \left\langle e^{\tilde{\mathbf{L}}} \right\rangle,$$

where $\tilde{\mathbf{L}}$ is similar to $\mathbf{L}$ with x replaced by $\tilde{x}$ (and same y). This equation can be written with $l(z) := \log\left(\langle e^{\mathbf{L}} \rangle\right)$ as

$$-\frac{1}{2}z + l(z) = \frac{1}{2} z e^{-\beta\omega} + l(e^{-\beta\omega} z),$$

where z is a variable and $e^{-\beta\omega}$ is a constant. Solve this functional equation for $l(z)$ and find the identity.

Last you can treat the general case with $\mathbf{L}$ being a sum over several modes by reducing the expectation values to products over single mode expressions.

(b) Show for operators $\mathbf{A}$ and $\mathbf{B}$, which are linear in the creation and annihilation operators $\mathbf{b}_j^\dagger$ and $\mathbf{b}_j$, the relation

$$\left\langle e^{\mathbf{A}} e^{\mathbf{B}} \right\rangle = e^{\frac{1}{2}\left\langle \mathbf{A}^2 + 2\mathbf{A}\mathbf{B} + \mathbf{B}^2 \right\rangle}.$$

2. **Debye-Waller factor (6 points)**

The Debye-Waller factor for a sc-lattice is given by

$$W(q) = \frac{\hbar q^2}{4M} \int_0^\infty \frac{\mathrm{d}\omega}{\omega} D(\omega) \coth \frac{\hbar\beta\omega}{2}.$$

(a) Compute $W(q)$ for the Debye model and consider the behavior for $T \ll \hbar\omega_D$ and for $T \gg \hbar\omega_D$.

(b) Compute $W(q)$ for the Einstein model and consider the behavior for $T \ll \hbar\omega_0$ and for $T \gg \hbar\omega_0$.