Assignments to Condensed Matter Theory I
Sheet 3

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sheet online: `http://www-MCG.uni-R.de/teaching/`

Problem set: Second quantization (bosonic gymnastic)

3.1. Bosonic commutation relations

Refresh the physics of the simple harmonic oscillator

$$\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2},$$

which can be written in "second quantized" form, by expressing x and p in terms of *boson* creation and annihilation operators:

$$\hat{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \quad a^\dagger = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}\,\hat{x} - \mathrm{i}\frac{\hat{p}}{\sqrt{m\omega}}\right).$$

(a) Show that the following basis commutation relations hold

$$[a, a^\dagger] = 1, \quad [a, a] = 0, \quad a\,|0\rangle = 0$$

where $[A, B] = AB - BA$, $|0\rangle$ the vacuum, and $\dagger$ indicates the Hilbert space adjoint. From these, determine all normalized eigenstates $|n\rangle$ ($\langle n, m\rangle = \delta_{nm}$) of $a^\dagger a$, and show that they have the following properties,

$$\begin{aligned} a^\dagger a\,|n\rangle &= n\,|n\rangle\,, \quad n = 0, 1, 2, \ldots \\ a\,|n\rangle &= \sqrt{n}\,|n-1\rangle\,, \\ a^\dagger\,|n\rangle &= \sqrt{n+1}\,|n+1\rangle\,. \end{aligned}$$

(b) Compute $F = -k_{\mathrm{B}}T \ln Z$ with

$$Z = \mathrm{Tr}\left\{\exp\left[-\frac{\hbar\omega}{k_{\mathrm{B}}T}\left(a^\dagger a + \frac{1}{2}\right)\right]\right\} = \sum_n \left\langle n \left| \exp\left[-\frac{\hbar\omega}{k_{\mathrm{B}}T}\left(a^\dagger a + \frac{1}{2}\right)\right]\right| n \right\rangle$$

(c) Plot F against temperature for different values of $\hbar\omega$.

3.2. Calculating with bosonic operators

(a) Show that for two non commuting bosonic operators A, and B it holds

$$[A, B^n] = \sum_{k=0}^{n-1} B^k \, [A, B] \, B^{n-1-k}.$$

(b) Prove —using (a)— that for bosonic operators b, $b^\dagger$

$$\begin{aligned}
\left[b, (b^\dagger)^n\right] &= n(b^\dagger)^{n-1} = \frac{\partial (b^\dagger)^n}{\partial b^\dagger}, \\
\left[b^\dagger, b^n\right] &= -nb^{n-1} = -\frac{\partial b^n}{\partial b}, \\
\left[b, f(b^\dagger)\right] &= \frac{\partial f(b^\dagger)}{\partial b^\dagger}, \\
\left[b^\dagger, f(b)\right] &= -\frac{\partial f(b)}{\partial b},
\end{aligned}$$

where the functions $f(b^\dagger)$ and $f(b)$ are representable as a power series ($[b, b^\dagger] = 1$).

(c) Using the previous arguments (Ex 3.2 b)) show that the following relations hold

$$g_1(\alpha; b, b^\dagger) = \mathrm{e}^{-\alpha b^\dagger} b \mathrm{e}^{\alpha b^\dagger} = b + \alpha, \qquad h_1(\alpha; b, b^\dagger) = \mathrm{e}^{-\alpha b} b^\dagger \mathrm{e}^{\alpha b} = b^\dagger - \alpha.$$

In a similar fashion, simplify the following expressions

$$g_2(\alpha; b, b^\dagger) = \mathrm{e}^{-(\alpha^* b^\dagger - \alpha b)} b \mathrm{e}^{(\alpha^* b^\dagger - \alpha b)}, \quad h_2(\alpha; b, b^\dagger) = \mathrm{e}^{-(\alpha^* b^\dagger - \alpha b)} b^\dagger \mathrm{e}^{(\alpha^* b^\dagger - \alpha b)},$$
$$g_3(\alpha; b, b^\dagger) = \mathrm{e}^{-\alpha b^\dagger b} b \mathrm{e}^{\alpha b^\dagger b}, \qquad h_3(\alpha; b, b^\dagger) = \mathrm{e}^{-\alpha b^\dagger b} b^\dagger \mathrm{e}^{\alpha b^\dagger b}.$$

`Hint:` Introduce a dummy variable λ as in

$$g_i(\lambda, \alpha; b, b^\dagger) = \mathrm{e}^{-\lambda f(\alpha; b, b^\dagger)} b \mathrm{e}^{\lambda f(\alpha; b, b^\dagger)}$$

and calculate the derivative $\partial g_i(\lambda, \alpha; b, b^\dagger)/\partial \lambda$. Same thing for $h_i(\lambda, \alpha; b, b^\dagger)$.

(d) Prove the identity

$$\mathrm{e}^{\alpha b^\dagger} \mathrm{e}^{\beta b} = \exp\left(\alpha b^\dagger + \beta b - \frac{\alpha\beta}{2}\right)$$

`Hint:` Show first that the quantity

$$f(\lambda) = \mathrm{e}^{\lambda \alpha b^\dagger} \mathrm{e}^{\lambda \beta b} \mathrm{e}^{\lambda^2 \frac{\alpha\beta}{2}}$$

satisfies the following relation

$$\frac{\partial f(\lambda)}{\partial \lambda} = \left(\alpha b^\dagger + \beta b\right) f(\lambda).$$

3.3. Cubic correction to the q-harmonic oscillator (Kür)

Calculate the correction to the frequency of an oscillator in its ground state due to a cubic anharmonicity. It arises by expanding the adiabatic potential beyond the harmonic terms. This corresponds to an oscillator problem with the Hamiltonian

$$H = \hbar\omega_0 \left(a^\dagger a + \frac{1}{2} \right) + \Delta (a^\dagger + a)^3 \ .$$

`Note:` In order to have a bounded Hamiltonian (with converging wave functions at large distances) one would need fourth order corrections in the spring energy. Still, the cubic correction presented in this exercise provides, for low energies, a *relatively* straight forward insight into the physics of the quantum anharmonic oscillator. You might want to read the original paper "C. M. Bender and T. T. Wu, Phys. Rev. **184**, 1231 (1969)" to learn more on this fundamental issue. It is available online (when logged in the `uni-r.de` domain) under `http://prola.aps.org/abstract/PR/v184/i5/p1231_1`

(a) Treat the anharmonicity by bringing the third order terms in the phonon operators first into normal order and reduce them by replacing the number operator whenever possible by the thermal expectation value $n(T)$.

`Hint:` The cubic anharmonicity $\Delta(a^\dagger + a)^3$ is first written in normal order

$$(a^\dagger + a)^3 = a^{\dagger 3} + 3a^{\dagger 2}a + 3(a^\dagger + a) + 3a^\dagger a^2 + a^3$$

and then truncated by replacing $a^\dagger a \to \langle a^\dagger a \rangle = n(T)$ and omitting the terms $a^{\dagger 3}$ and a^3. Thus the hamiltonian reduces to

$$H = \hbar\omega_0 \left(a^\dagger a + \frac{1}{2} \right) + \Delta(T)(a^\dagger + a) \ , \quad \text{with} \quad \Delta(T) = 3\Delta\big(n(T) + 1\big) \ .$$

(b) Solve the resulting Hamiltonian by means of the Brillouin-Wigner perturbation theory [1].

`Hint:` This is obtained by calculating now the second order corrections to the oscillator ground state $|n\rangle$ with $n = 0$ due to the anharmonicity, which by making use of $\langle 0|a|1\rangle\langle 1|a^\dagger|0\rangle = 1$ reads in Brillouin-Wigner perturbation theory

$$\varepsilon = E_0 - \frac{\hbar\omega_0}{2} = \frac{\Delta^2(T)}{\varepsilon - \hbar\omega_0} \ .$$

Alternatively, you can exactly solve the problem by using one expansion of Ex.3.2(c).

[1] W. Nolting Grundkurs Theoretische Physik 5/2, page 182 3^{rd} edition, Springer (2001).

(c) Find the lowest eigenvalue and show that the smaller solution of the quadratic equation in ε

$$E_0 = \frac{1}{2}\hbar\omega_0 - \frac{\Delta^2(T)}{\hbar\omega_0}$$

expresses a zero-point energy which decreases as $\Delta(T)$ increases due to thermal phonon excitation with the temperature. This is the behavior of a soft mode.