van der Waals- und Casimir-Kräfte

Wintersemester 2015/16

Carsten Henkel

Übungsblatt 3

Hand out: 19 Nov 2015
hand in: 26 Nov 2015

Problem 3.1 – Factorizing integral (5 Points)

In Eisenschitz and London's calculation, we find in the denominator sums of energy differences (or Bohr frequencies)

$$\frac{1}{E_{k'} + E_{l'} - (E_k + E_l)} = \frac{1/\hbar}{\omega_A + \omega_B} = \frac{2}{\pi\hbar} \int\limits_0^\infty \mathrm{d}x \frac{\omega_A}{\omega_A^2 + x^2} \frac{\omega_B}{\omega_B^2 + x^2} \tag{3.1}$$

Show that this integral formula is correct.

Problem 3.2 – Correlated atoms (5 Points)

Check from your lecture on perturbation theory that to first order in the perturbation W, the state changes to

$$|\Psi^{(0)}\rangle \mapsto |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle = |\Psi^{(0)}\rangle - (H^{(0)} - E^{(0)})^{-1} W |\Psi^{(0)}\rangle \tag{3.2}$$

For the dipole-dipole interaction between two hydrogen atoms in the 1s state, try to find out whether this is a 'correlated' state of the two atoms. You are allowed to choose the distance vector $\hat{\mathbf{r}}$ along the z-axis. As a simple approximation, take into account only transitions between the 1s and $2\mathrm{p}_{x,y,z}$ states.

Problem 3.3 – Polarizability and Kubo formula (10 Points)

The Japanese physicist R. Kubo has developed the theory of the 'linear response' of quantum mechanical systems to a perturbation. This is an example of time-dependent perturbation analysis. One key result is the formula for the dynamic polarizability of an atom or molecule in an electric field $\mathbf{E}(t)$: the particle responds with an average dipole moment given by

$$\langle d_i(t) \rangle = \int\limits_{-\infty}^{\infty} \mathrm{d}t' \sum_j \alpha_{ij}(t - t') E_j(t') \tag{3.3}$$

where the polarizability is given by

$$\alpha_{ij}(t - t') = \frac{\mathrm{i}}{\hbar} \langle [d_i(t), d_j(t')] \rangle \Theta(t - t') \tag{3.4}$$

where $\Theta(t - t') = 1$ $(= 0)$ for $t > t'$ $(t < t')$ is the unit step function and $\mathbf{d}(t)$ is the dipole operator of the atom in the Heisenberg picture.

(1) Why does the step function appear here?

(2) The expectation value in Eq.(3.4) is taken in the non-perturbed state of the particle. Take the ground state, check that α_{ij} depends indeed only on the time difference $t - t'$ and show that the polarizability in Fourier space is

$$\alpha_{ij}(\omega) = \sum_e \frac{2(\omega_{eg}/\hbar)\langle g|d_i|e\rangle\langle e|d_j|g\rangle}{\omega_{eg}^2 - \omega^2} \tag{3.5}$$

where d_i is the dipole operator in the Schrödinger picture and the $|e\rangle$'s are excited states. Setting $\omega = \omega' + \mathrm{i}\epsilon$ with $\epsilon > 0$, make a sketch of the real and imaginary part of α. You may use the fact that the dipole matrix elements are real.

(3) Look up the information that retarded response functions are analytic functions for complex frequencies in the upper half plane and show that along the upper imaginary axis, we have

$$\alpha_{ij}(\mathrm{i}\xi) = \sum_e \frac{2(\omega_{eg}/\hbar)\langle g|d_i|e\rangle\langle e|d_j|g\rangle}{\omega_{eg}^2 + \xi^2} \tag{3.6}$$

which is a real and positive tensor. (What is a positive tensor?)