

**Problem 4.1** – A quantum crystal made of Helium (5 Points)

For the van der Waals interaction between Helium atoms, we have seen a plot in the paper by London (“Zur Theorie und Systematik der Molekularkräfte”, *Z. Phys.* **63** (1930) 245), with a discussion of the quantum states in the interaction potential (also known as molecular bound states). Find on the web numbers and experimental evidence: how can one tell that liquid (or solid) Helium is a ‘truly quantum’ system? What would you expect for a ‘classical’ material?

**Problem 4.2** – ‘Round molecules have an isotropic polarizability’ (5 Points)

For a molecule in the state  $|g\rangle$ , the (dynamical) polarizability is the tensor

$$\alpha_{ij}^g(\omega) = \sum_e \frac{2(\omega_{eg}/\hbar)\langle g|d_i|e\rangle\langle e|d_j|g\rangle}{\omega_{eg}^2 - \omega^2} \quad (4.1)$$

where the sum is over other states  $|e\rangle$  and  $\omega_{eg} = (E_e - E_g)/\hbar$  are the Bohr frequencies. If  $|g\rangle$  has angular momentum  $J_g$ , then by a so-called selection rule, the sum is running only over states with  $J_e = J_g, |J_g \pm 1|$ .

(1) Take  $|g\rangle$  as s-state, and three p-states for  $|e\rangle$ . In the ‘chemists’ basis’  $\{|p_x\rangle, |p_y\rangle, |p_z\rangle\}$ , the dipole matrix elements have the form

$$\langle p_i|\mathbf{d}|g\rangle = D \mathbf{e}_i, \quad i = x, y, z \quad (4.2)$$

where  $D$  is a scalar number and  $\mathbf{e}_i$  the unit vector along the  $i$ -axis. Show that the polarizability (4.1) is proportional to  $\delta_{ij}$  and compute the prefactor  $\alpha(\omega)$ .

(2) The Kramers-Kronig relations apply to response functions that are analytic (holomorphic) in the upper half-plane of complex frequencies. Check that this is the case for the polarizability and show from Cauchy’s theorem that for imaginary frequencies, we have

$$\alpha_{ij}(i\xi) = \delta_{ij} \frac{2}{\pi} \int_0^\infty d\omega \frac{\omega \operatorname{Im} \alpha(\omega + i0)}{\omega^2 + \xi^2} \quad (4.3)$$

(3) In the lecture, we have briefly discussed the autocorrelation function  $\langle d_i(t)d_j(t') \rangle$  of the dipole operator and its spectral expansion:

$$\langle g|d_i(t)d_j(t')|g \rangle = \int \frac{d\omega}{2\pi} S_d^{ij}(\omega) e^{-i\omega(t-t')} \quad (4.4)$$

$$S_d^{ij}(\omega) = (\dots) \text{Im } \alpha_{ij}(\omega + i0), \quad \text{if } \omega \geq 0 \quad (4.5)$$

To complete the prefactor  $(\dots)$  missing in the second relation, check the weights of the  $\delta$ -peaks in the two expressions. This is the so-called fluctuation–dissipation relation for the dipole in the ground state.

**Problem 4.3 – Mirror reflexions (5 Points)**

In electrostatics, you have learned that at the surface of a good conductor, the electric field lines are perpendicular and ‘terminate there’. This can be used to construct the electric field generated by charged objects near a conducting surface. We take a planar surface for simplicity.

(1) Argue that the electric field of a point charge is given by the sum of the Coulomb field in free space, plus the field of a fictitious charge of opposite sign, placed at the mirror position of the charge below the surface. Make a sketch of the electric potential and of the field lines. What kind of interaction between the charge and the surface would you expect? (Keyword for the web: the pseudo-atom ‘mirium’.)

(2) Generalize to an electric dipole that you may build from two nearby charges. How does the image dipole look when the dipole is oriented parallel or perpendicular to the surface? What about the sign of the interaction in the two cases?

(3) Consider finally a magnetic dipole built from a charge distribution flowing in a small ring (suitably neutralized to have no net charge). What do the magnetic dipole and its image tell you about the force near the surface? Hold it: can this work with a good (non-magnetic) conductor like copper? Try to make an estimation for a typical toy magnet.