van der Waals- und Casimir-Kräfte   Wintersemester 2015/16

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Übungsblatt 2   Ausgabe: Do 29 Okt 15

                                              Eingabe: Do 12 Nov 15

Problem 2.1 – Peel it off (5 Points)

Why is rather easy to peel off Scotch tape (Tesafilm), while it can carry quite heavy weights? Estimate the work necessary to remove a length of tape by peeling it off, and compare to the work necessary to remove the same area at once perpendicularly. The distance between the tape and the surface is approximately 5nm, and the strip could have dimensions 1cm × 5cm.

Web resources: 'adhesion'. Typical values for van der Waals bond lengths = $0.4\ldots 1\,\text{nm}$, Hamaker constants $A \sim 0.1\,\text{eV}$.

Problem 2.2 – Coupled quantum dipoles (8 Points)

(1) Show that for two particles A and B with electric dipole moments, the electrostatic interaction energy is given by

$$V_{dd} = \frac{\mathbf{d}_A \cdot \mathbf{d}_B - 3(\mathbf{d}_A \cdot \hat{\mathbf{r}}_{AB})(\mathbf{d}_B \cdot \hat{\mathbf{r}}_{AB})}{4\pi\epsilon_0 |\mathbf{r}_A - \mathbf{r}_B|^3} \tag{2.1}$$

where $\hat{\mathbf{r}}_{AB}$ is the unit vector along $\mathbf{r}_A - \mathbf{r}_B$. (2) Look up the value of the 'Debye' which gives typical dipole moments of molecules and compare V in order of magnitude with the thermal energy $k_B T$ at room temperature. You may take a distance $|\mathbf{r}_A - \mathbf{r}_B| = 10\,\text{nm}$.

(3) Consider two dipoles with parallel orientation and find a configuration where the interaction energy V_{dd} vanishes.

(4) Consider the following simple quantum version of this interaction

$$V = u(a + a^\dagger)(b + b^\dagger) \tag{2.2}$$

where a and b are lowering operators for two harmonic oscillators. Compare this interaction to V_{dd} and find a reasonable estimate for the energy u.

(5) Work out in first- and second-order perturbation theory the shift in the ground state energy E_0 of the two-oscillator system, assuming a non-perturbed Hamiltonian of the form

$$H_0 = \hbar\omega_A a^\dagger a + \hbar\omega_B b^\dagger b \tag{2.3}$$

In order of magnitude,

$$E_0 \approx \frac{\hbar}{2}\left(\omega_A + \omega_B\right) - (\cdots)\frac{u^2}{\hbar(\omega_A + \omega_B)} \tag{2.4}$$

where $(\cdots)$ is a numerical constant.

Problem 2.3 – Quantum dipole fluctuations (7 Points)

The dipole moment of a one-electron atom is given by the operator $\mathbf{d} = e\mathbf{x}$ where $\mathbf{x}$ is the electron coordinate relative to the nucleus. Consider a ground state whose wave function is the spherically symmetric $\psi_g(\mathbf{x}) = \mathcal{N}^{-1/2}\,\mathrm{e}^{-x/a}$ where a is a length scale, $x = |\mathbf{x}|$, and $\mathcal{N}$ a normalization factor. (Keyword: hydrogen wave functions.)

(1) Show that in the ground state, the average dipole vanishes, $\langle g|\mathbf{d}|g\rangle = \mathbf{0}$.

(2) Argue that the 'correlation matrix' of the dipole is diagonal

$$\langle g|d_i d_j|g\rangle = \delta_{ij}\frac{e^2 a^2}{36} \tag{2.5}$$

and check its nonzero matrix elements.

(3) For the hydrogen ground state 1s, we have $a = 2a_0$ where a_0 is the Bohr radius. Consider the dipole fluctuations along the z-axis and insert a complete set of states to show

$$\langle 1\mathrm{s}|z^2|1\mathrm{s}\rangle = \sum_e |\langle 1\mathrm{s}|z|e\rangle|^2 \tag{2.6}$$

For the particular state $e = 2\mathrm{p}_z$, the matrix element appearing here is

$$\langle 2\mathrm{p}_z|z|1\mathrm{s}\rangle = \frac{128\sqrt{2}}{243}a_0 \tag{2.7}$$

Check that the contribution of this particular excited state relative to the sum (2.6) is larger than 50%.