

Crucial role of long-range interactions in the ultracold regime

Standard multipolar long-range expansion $V(R) = \frac{1}{4\pi\epsilon_0} \sum_{\ell_A \ell_B m} \frac{f_{\ell_A \ell_B m}}{R^{1+\ell_A+\ell_B}} Q_{\ell_A}^m Q_{\ell_B}^{-m}$

Multipolar moments $Q_{\ell_A}^m = \sqrt{\frac{4\pi}{2\ell_A+1}} \sum_{i \in A} r_i^{\ell_A} Y_{\ell_A}^m(\theta_i, \phi_i), A \rightarrow B, i \rightarrow j$

See for instance:

B. Bussery-Honvault, et al, J. Chem. Phys. **129**, 234302 (2008).

D. V. M. R. Flannery and V. N. Ostrovsky, J. Phys. B **38**, S279 (2005).

G. C. Groenenboom, et al, J. Chem. Phys. **126**, 204306 (2007).

$$f_{\ell_A \ell_B m} = \frac{(-1)^{\ell_B} (\ell_A + \ell_B)!}{\sqrt{(\ell_A + m)! (\ell_A - m)! (\ell_B + m)! (\ell_B - m)!}}$$

Long-range interaction between vibrating-rotating dipolar ground state molecules

No permanent dipole moment in the lab frame in free space

2nd order induced dipole-dipole interaction in R⁻⁶ (Van de Waals)

$$C_6(\nu) = \frac{3}{\pi} \int_0^\infty \alpha_\nu^A(i\omega) \alpha_\nu^B(i\omega) d\omega$$

C₆ deduced from the polarizability computed at imaginary frequencies: $\alpha_\nu(i\omega)$

$\alpha_\nu(i\omega)$: Sum over all transitions including all transitions within the ground state and with excited electronic states

$$\alpha_I(i\omega) = \frac{2}{3} \sum_{p \neq 0} \frac{\Delta E_{p0}}{(\Delta E_{p0})^2 + \omega^2} \left(\left| \langle \Psi_p | \hat{q}_1^0(I) | \Psi_0 \rangle \right|^2 + 2 \left| \langle \Psi_p | \hat{q}_1^1(I) | \Psi_0 \rangle \right|^2 \right)$$

$$C_6(\nu) = \frac{3}{\pi} \int_0^\infty (\alpha_\nu^g(i\omega) + \alpha_\nu^e(i\omega))^2 d\omega = C_6^g(\nu) + C_6^e(\nu) + C_6^{g-e}(\nu)$$

[More results in:](#) M. Lepers, R. Vexiau, M. Aymar, N. Bouloufa-Maafa, O. Dulieu, *Long-range interactions between polar alkali-metal diatoms in external electric fields*, Phys. Rev. A **88**, 032709 (2013)