

Mechanisms of Electrostatic Interactions between Two Charged Dielectric Spheres inside a Polarizable Medium: An Effective-dipole Analysis

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Abstract: The mechanisms of electrostatic interactions between two charged dielectric spheres inside a polarizable medium have been investigated, in terms of **hypothetical effective dipoles** that depict how the positive and negative charge in each particle are separated. Our findings, which revealed that it is possible for polarization-induced **opposite-charge repulsion** to occur at short interparticle separations if the **dielectric constant of the medium is greater than the dielectric constants of both spheres**, provide insights into the physics of charge separation in each sphere and of polarization in the medium behind such counterintuitive behavior.

Introduction

Coulomb's Law is to describe the electrostatic force between **point charges** in vacuum, as shown in Fig.1. It **does not** necessarily describe the electrostatic interaction between two charged **dielectric particles**.

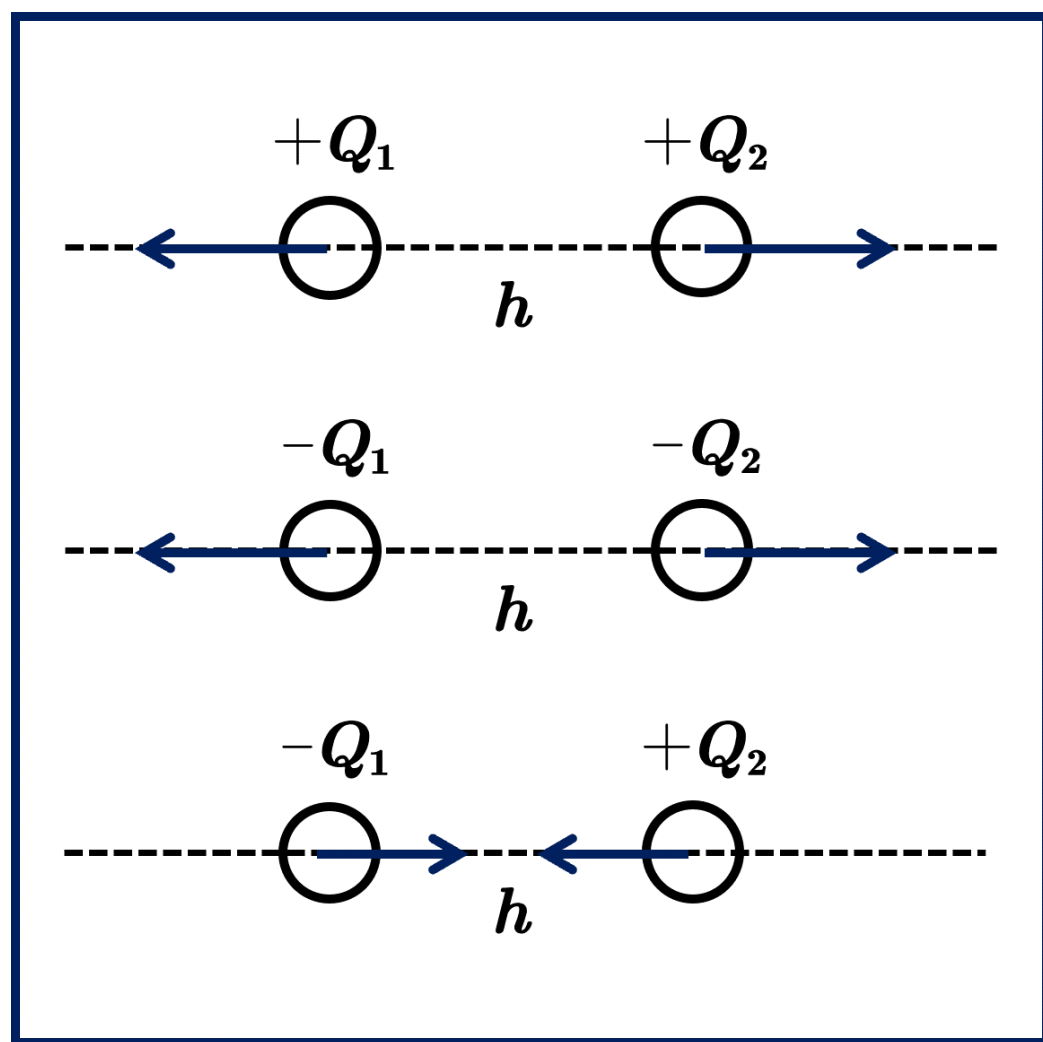


Figure 1. Coulomb's Law

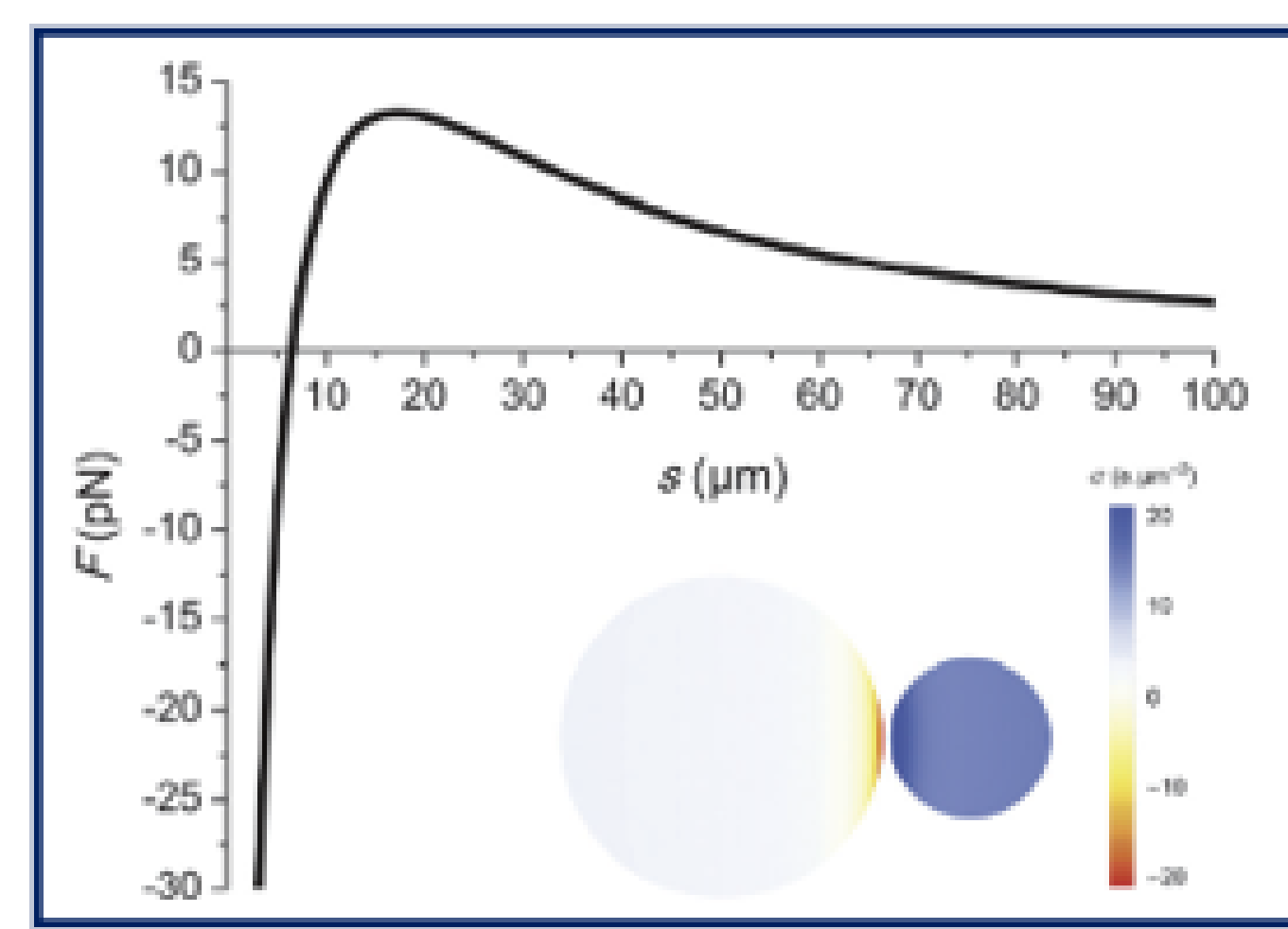


Figure 2. Like-charge attraction [1]

In some cases, there could be a **significant deviation** from the Coulomb force **at small separations**, resulting in the occurrence of polarization-driven **like-charge attraction**, as illustrated in Fig.2.

Model & Methodology

Consider two dielectric spheres immersed in a polarizable medium (see Fig.3) and separated by a center-to-center separation h . For sphere $i \in \{1,2\}$ with a radius a_i , its free charge q_i is concentrated at the particle's center $\mathbf{z}_i = [0, 0, z_i]$, and its bound charge spans the particle's surface.

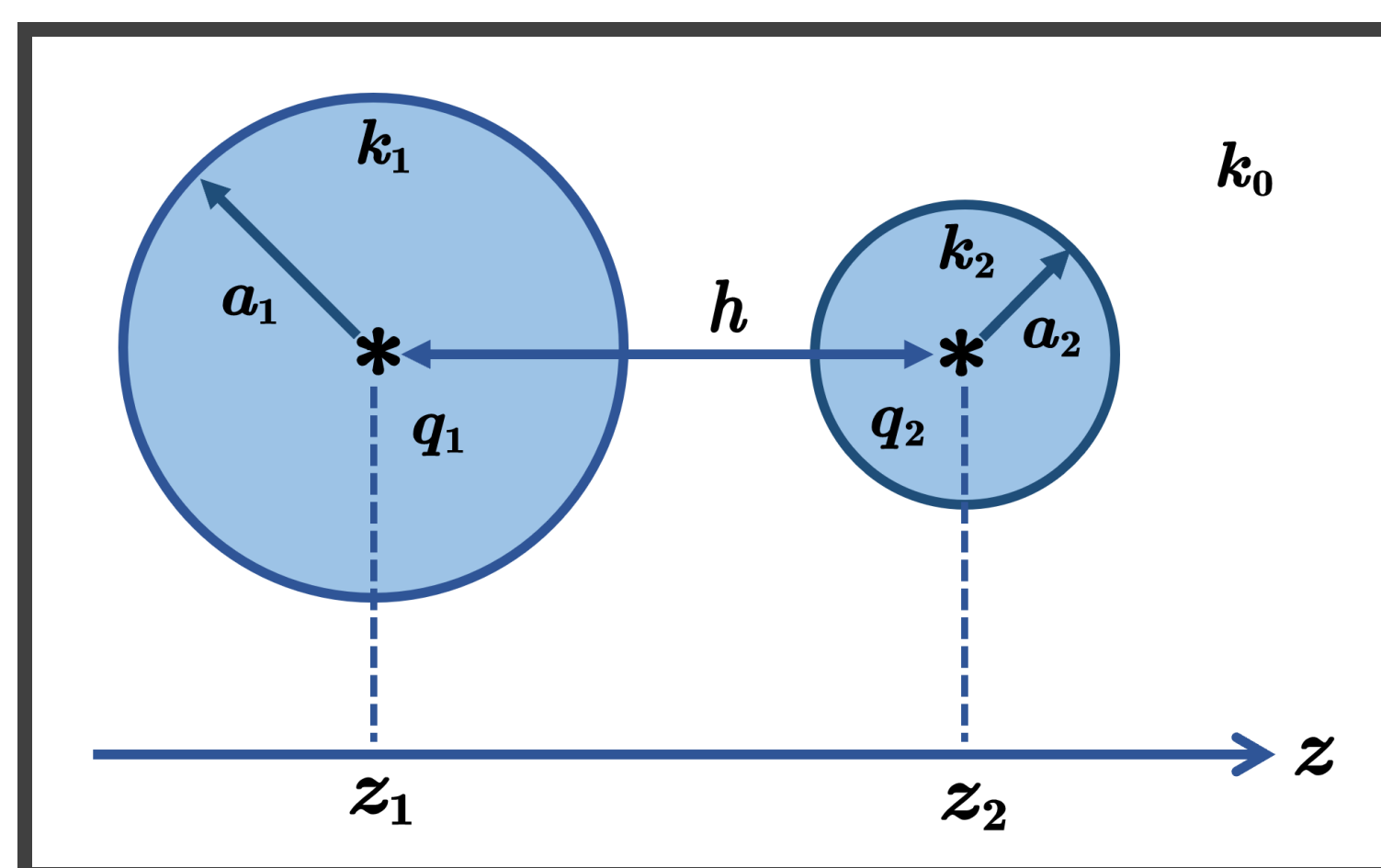


Figure 3. Schematic illustration of two charged dielectric spheres immersed in a polarizable medium.

Our **effective-dipole approach** [2] averages over not only the first-order dipole contributions but also all quadrupole and higher-order contributions, which can be evaluated by Hybrid Method [3].

$$\begin{aligned}\tilde{q}_i^+ &= \int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_P(\sigma_{b,i}(\mathbf{r})) dS_i \\ \tilde{\mathbf{r}}_i^+ &= \frac{\int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_P(\sigma_{b,i}(\mathbf{r})) \mathbf{r} dS_i}{\int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_P(\sigma_{b,i}(\mathbf{r})) dS_i} \\ \tilde{q}_i^- &= \int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_N(\sigma_{b,i}(\mathbf{r})) dS_i \\ \tilde{\mathbf{r}}_i^- &= \frac{\int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_N(\sigma_{b,i}(\mathbf{r})) \mathbf{r} dS_i}{\int \sigma_{b,i}(\mathbf{r}) \mathbb{I}_N(\sigma_{b,i}(\mathbf{r})) dS_i}\end{aligned}$$

Polarization Effects

- **Equal-sized spheres** with different dielectric constants and charges (shown in Fig. 4).
- **Unequal-sized spheres** sharing the same dielectric constants and charge magnitudes (shown in Fig.5).

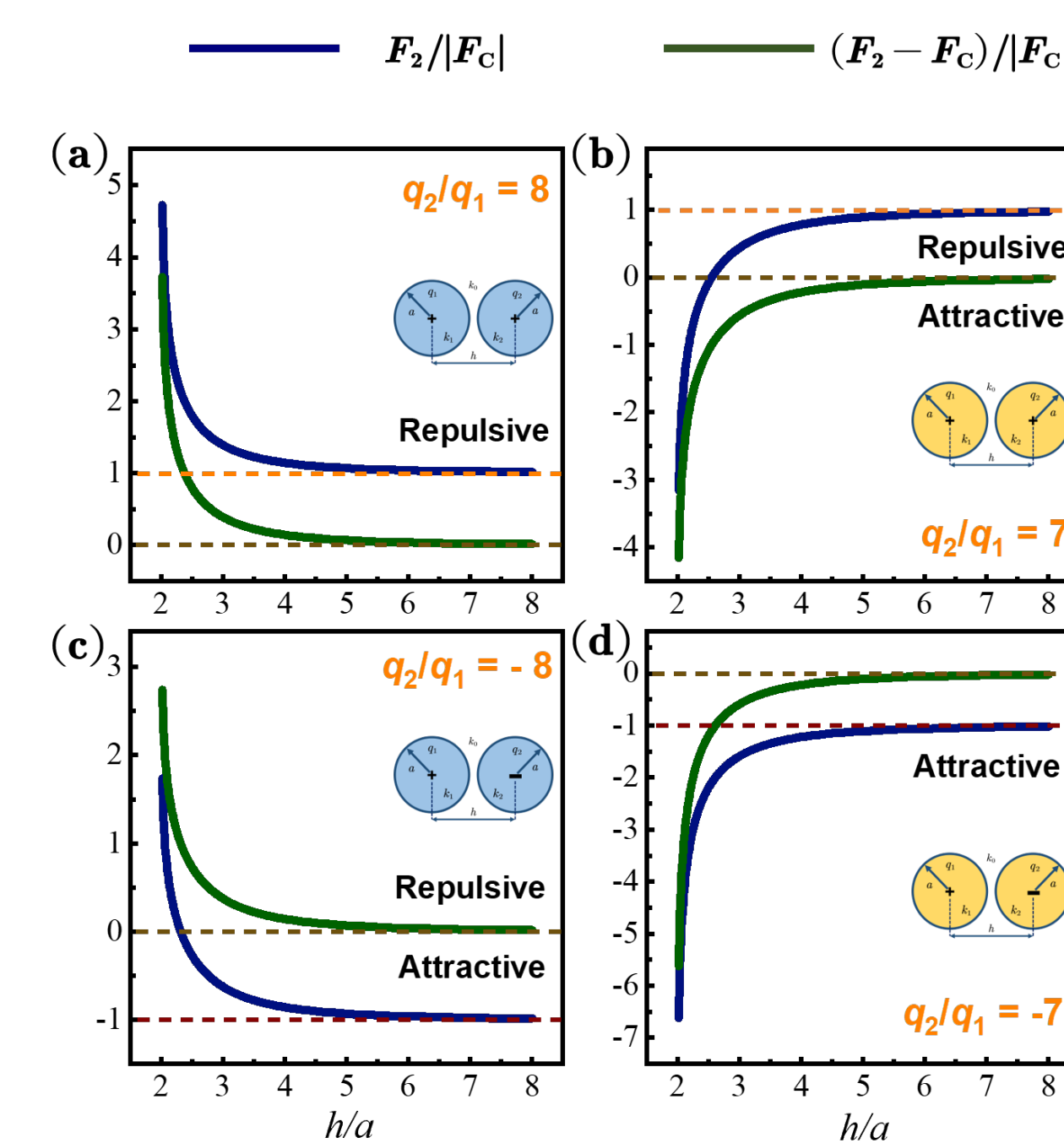


Figure 4. Rescaled electrostatic force and rescaled polarization force for equal-sized spheres : (a) $k_1/k_0 = 0.001$, $k_2/k_0 = 0.08$ and $q_2/q_1=8$; (b) $k_1/k_0 = 30$, $k_2/k_0 = 4$ and $q_2/q_1=7$; (c) $k_1/k_0 = 0.001$, $k_2/k_0 = 0.08$ and $q_2/q_1=-8$; (d) $k_1/k_0 = 30$, $k_2/k_0 = 4$ and $q_2/q_1=-7$.

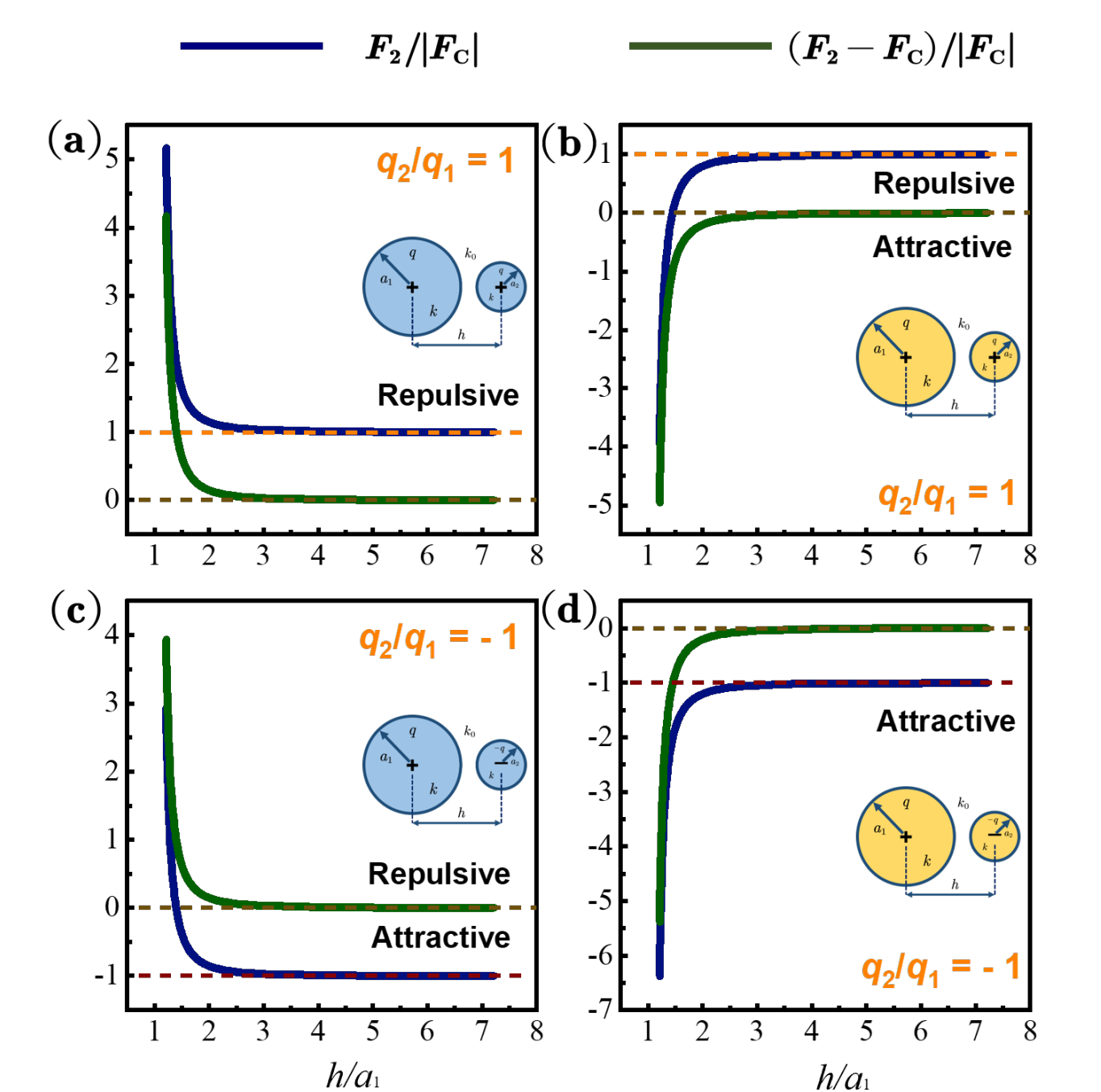


Figure 5. Rescaled electrostatic force and rescaled polarization force for unequal-sized spheres with $k_1/k_0 = k_2/k_0 = k$ and $a_2/a_1 = 0.2$: (a) $q_2/q_1 = 1$, $k=0.25$; (b) $q_2/q_1 = 1$, $k=4$; (c) $q_2/q_1 = -1$, $k=0.25$; (d) $q_2/q_1 = -1$, $k=4$;

Mechanisms in Different Scenarios

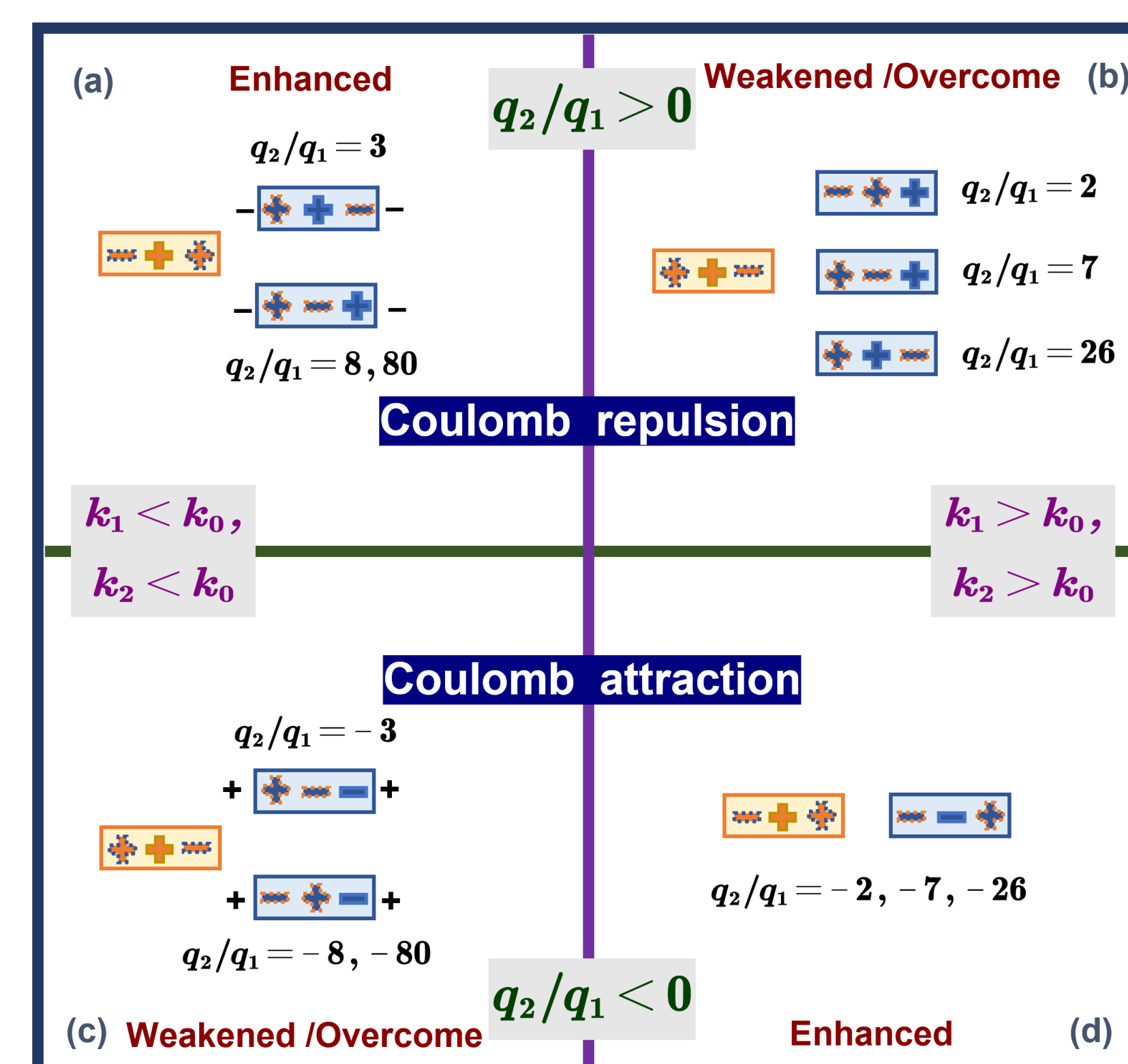


Figure 6. **Mechanisms** in different scenarios for equal-sized spheres [4]. The permittivities are defined as $k_1/k_0 = 0.001$, $k_2/k_0 = 0.08$ for (a), (c), and) $k_1/k_0 = 30$, $k_2/k_0 = 4$ for (b), (d).

Schematic illustration of the **4 scenarios** and **corresponding mechanisms** in close center-to-center distance of electrostatic interactions under consideration:
(a) $k_1 < k_0$, $k_2 < k_0$ and $q_2/q_1 > 0$;
(b) $k_1 > k_0$, $k_2 > k_0$ and $q_2/q_1 > 0$;
(c) $k_1 < k_0$, $k_2 < k_0$ and $q_2/q_1 < 0$;
(d) $k_1 > k_0$, $k_2 > k_0$ and $q_2/q_1 < 0$.

References

- [1] Lindgren E B, Chan H K, Stace A J, et al., *Phys. Chem. Chem. Phys.*, 2016, 18(8): 5883-5895.
- [2] Lindgren E B, Derbenev I N, Khachatourian A, et al., *J. Chem. Theory Comput.*, 2018, 14(2): 905-915.
- [3] Gan Z, Wang Z, Jiang S, et al., *J. Chem. Phys.*, 2019, 151(2).
- [4] Duan Y, Gan Z, Chan H K, *Soft Matter*, 2025, 21, 1860-1872.

Conclusions

This study revealed a **significant deviation** of the interparticle force from that described by **Coulomb's law** and an intriguing correlation of **the nature** of interparticle interaction with the **polarizability of the medium**.