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Review

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Transformation optics applied to van der Waals interactions

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Abstract The van der Waals force originates from the electromagnetic interaction between quantum fluctuation-induced charges. It is a ubiquitous but subtle force which plays an important role and has a wide range of applications in surface related phenomena like adhesion, friction, and colloidal stability. Calculating the van der Waals force between closely spaced metallic nanoparticles is very challenging due to the strong concentration of electromagnetic fields at the nanometric gap. Especially, at such a small length scale, the macroscopic description of the dielectric properties no longer suffices. The diffuse nonlocal nature of the induced surface electrons which are smeared out near the boundary has to be considered. Here, we review the recent progress on using three-dimensional transformation optics to study the van der Waals forces between closely spaced nanostructures. Through mapping a seemingly asymmetric system to a more symmetric counterpart, transformation optics enables us to look into the behavior of van der Waals forces at extreme length scales, where the effect of nonlocality is found to dramatically weaken the van der Waals interactions.

Keywords van der Waals forces · Transformation optics · Nonlocality · Plasmonics

1 Background and Introduction

All physical systems undergo quantum and thermal fluctuations. A nonpolar molecule like helium consisting of symmetric electron cloud around the nucleus could be temporarily self-polarized due to random fluctuations, which results in attractive forces between neutral atoms. Similarly, the fluctuation of charge density on an electrically neutral surface can randomly generate temporary surface charges. When two surfaces approach each other, the charges on one surface induce the opposite charges on the other. The random fluctuating charges then become correlated and form negative and positive charge pairs. The electromagnetic interactions between these instantaneously fluctuation-induced charges give rise to an attractive force between closely spaced surfaces. Such fluctuation-induced forces have been named differently such as van der Waals forces [1], London dispersion forces [2], Casimir–Polder forces [3], and latterly Casimir [4] (Casimir–Lifshitz [5]) forces. They have the same physical origin at the fundamental level but the latter two usually refer to long-range interactions with the retardation effect (i.e., the speed of light is finite). Since this review focuses on the forces at the nanoscale, we use the term of van der Waals forces.

The van der Waals force exists everywhere and is significant as long as the separation between surfaces is small enough. For instance, the attractive pressure acting on two metallic surfaces of 10 nm separation is comparable with one atmospheric pressure. The van der Waals force is a long-range force acting between particles and plays an

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important role in surface related interactions such as surface adhesion [6], friction [7, 8], colloidal stability and crystallization [9], nanoparticle self-assembly [10], and supramolecular (viruses, proteins, polymers) interactions. Remarkably, this is the mechanism for geckos [11, 12], spiders [13] and flies to stick to walls and climb upside-down on smooth surfaces. The quantitative calculation of van der Waals force is of great importance to guide applications in a broad range of areas such as surface and colloidal science, nanotechnology and macromolecular chemistry.

For a very long time, researchers could only deal with objects with simple geometry such as small molecules and large macroscopic bodies (e.g., parallel surfaces), where the van der Waals forces is calculated by asymptotic equations [1]. For complicated nontrivial geometries, traditional procedures through summing over the contributions from infinitesimal elements, such as Hamaker's method [14] and the proximity force approximation [15], have been widely used to estimate the van der Waals interactions [1]. However, the van der Waals force is inherently a non-additive interaction. This fact makes these "additive" methods not valid for calculating the collective interactions between nontrivial geometries. With the development of the electromagnetic field theories, some geometries such as corrugated plates [16], cylinders [17], spheres [18], edges and tips [19], and gratings [20] can be analytically studied with special boundary conditions. Remarkably, Johnson's team [21, 22] developed a set of numerical techniques which in principle can accurately compute Casimir interactions for arbitrary geometries and materials.

However, for very closely spaced metallic nanostructures with nanometer scale separations, the calculation of van der Waals forces is still very challenging. Metals like gold and silver can support surface plasmons due to the density oscillations of electrons on the surface when excited by an external radiation. Due to the heavy mass of electrons, surface plasmons can have much shorter wavelengths than the corresponding external light. The surface plasmon behavior strongly depends on the profile and the environment of the surface. Geometrical singularities such as sharp edges or touching surfaces can result in enormous field concentrations. When two nanoparticles are brought into close contact, surface plasmonic fields are strongly confined at the nanometric gap [23, 24]. These highly squeezed fields actually dominate the electromagnetic interactions. To exactly calculate the van der Waals forces requires an effective way to describe the highly localized plasmonic fields. In principle, the multipole expansion method [16–20] and numerical techniques [21, 22] can be used to describe the scattering properties of such systems. However, in order to describe the highly localized plasmonic modes, a large number of multipole moments (and hence a large reflection matrix) [18, 25] or extremely fine meshes [26] are required. For instance, in a sphere-plane configuration with a gap-to-radius ratio of 10^{-3}, several thousand spherical harmonics need to be considered [25]. This makes the calculations extremely time-consuming.

Moreover, if the small gaps approach *sub*-nanometer scales, the classical electrodynamics picture which describes the dielectric response in terms of local parameters fails to predict the optical properties of metallic surfaces due to the inherent quantum nature of electrons [27]. The surface electrons induced by an applied electric field are not located precisely on the surface but are smeared across the boundary in a layer whose thickness is comparable to Thomas-Femi wavelength (about 0.1 nm for typical metals). This so-called nonlocal effect [28] will alter the van der Waals forces in the small gap limit. Recently, some researchers gradually recognize the importance of the nonlocality for the van der Waals forces at small separations [29–31]. However, consistent results were not obtained when using different models to describe the nonlocal effect.

Transformation optics offers a feasible route to describing highly localized electromagnetic fields. Hence, it can be used as a powerful tool to calculate van der Waals interactions at the nanometric scale. This review is an overview of the recent progress on transformation optics applied to van der Waals calculations between plasmonic nanostructures which are difficult to handle using traditional methods.

2 Casimir–Lifshitz theory for the van der Waals force calculation

Although the van der Waals force is a quantum phenomenon, the essential part of the calculation turns out to be a classical electromagnetic problem [4, 5]. Intuitively, the van der Waals energy between two objects with a separation of d is calculated by summing over the zero point energy, $\hbar\omega_n/2$, of all the eigenmodes supported by the system,

$$E(d)=\sum_n \frac{1}{2}\hbar\omega_n(d)-\sum_n \frac{1}{2}\hbar\omega_n(d\rightarrow+\infty), \qquad (1)$$

where $\hbar$ is the reduced Planck's constant and ω_n the resonance frequency of each eigenmode. For two parallel perfectly conducting mirrors separated by vacuum, the cavity eigenmodes are given by $\omega_{\boldsymbol{k}_{||},n}=c\sqrt{\boldsymbol{k}_{||}^2+(n\pi/d)^2}$, where $\boldsymbol{k}_{||}$ denotes the parallel component of wave vector and c is the speed of light in vacuum. Inserting in Eq. (1) and changing the summation to an integral, $\sum_{p=\mathrm{TE,TM}}\sum_n \frac{1}{(2\pi)^2}\int \mathrm{d}^2\boldsymbol{k}_{||}$, Casimir [4] obtained the attractive pressure between two conducting mirrors as $P=-\partial E(d)/\partial d=-\hbar c\pi^2/240d^4$. Although Eq. (1) provides an intuitive