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# Charge-dipole and dipole-dipole interactions in two-dimensional materials

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We derive the explicit analytical form for the charge-dipole and dipole-dipole interactions in two-dimensional (2D) configuration space. We demonstrate that the reduction of dimensionality can alter the charge-dipole and dipole-dipole interactions in the 2D case. The asymptotics of these interactions at long distances coincide to the charge-dipole and dipole-dipole interactions in three-dimensional configuration space. The obtained charge-dipole and dipole-dipole interactions will find wide application and contribute to the advancement of research on novel two-dimensional materials.

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In classical electrodynamics for description of the field produced by a system of electric charges at long distances the concepts of dipoles and multipole moments are very important and well developed [1,2]. This approach is based on the potential of a single charge in three-dimensional (3D) configuration space. Ordinary matter is more or less uncharged, but it is reach in pair of charges called dipoles. Dipoles are building blocks of bulk dielectric and magnetic materials. Not surprisingly, it turns out to be efficient mathematically to deal with the dipole not as just a pair of individual positive and negative charges.

In the past two decades, discoveries and studies of two-dimensional (2D) materials have attracted a considerable interest. Atomically thin materials, such as graphene and monolayer transition-metal dichalcogenides (TMDCs), phosphorene, and Xenes (silicene, germanine, and stanene), exhibit remarkable physical properties resulting from their reduced dimensionality and crystal symmetry. The family of semiconducting transition-metal dichalcogenides is an especially promising platform for fundamental studies of two-dimensional systems with potential applications in optoelectronics and valleytronics due to their direct band gap in the monolayer. The exciton is the simplest bound complex formed by an electron in a conduction band and hole in a valence band. The description of excitons, trions, and biexcitons in 2D material requires knowledge of electrostatic interaction in reduced dimensionality.

The interaction of two charge particles in two-dimensional space is studied in detail, and the analytical expression for two-charged particle interaction is well known [3,4] and widely used for the description of excitonic complexes in 2D materials (see reviews: Refs. [5–7]). In 3D configuration space when charged particles interact via the Coulomb potential the corresponding charge-dipole and dipole-dipole potentials are well known. In contrast, the influence of the reduction of dimensionality on the charge-dipole and dipole-dipole interactions in 2D configuration space has not yet been investigated. We still lack the analytical expression for the charge-dipole and dipole-dipole 2D interactions. Below we derive the explicit analytical form for the charge-dipole and dipole-dipole interactions in 2D space.

## I. CHARGE-CHARGE INTERACTION IN 2D CONFIGURATION SPACE

An interaction of two charged particles in the context of thin semiconductor films was derived analytically by Rytova [3] and a decade later by Keldysh [4], and it was shown that the electron-hole interaction potential in a thin semiconductor layer is not Coulombic. This potential describes the interaction between two particles in a film of finite thickness $d$ and dielectric constant $\varepsilon$ and implies the intrinsic assumption that the screening can be quantified by the dielectric constant. Three decades later a strict 2D derivation of the macroscopic screening derived by Keldysh as a limiting case of a thin film was provided in Ref. [8]. This potential has the same functional form as Refs. [3,4] but the macroscopic screening in this case is quantified by the 2D polarizability. Over the course of a decade the effective 2D potential has been widely used to describe the electrostatic interaction of few-body complexes, such as excitons, trions, and biexcitons in monolayer transition-metal dichalcogenides, phosphorene, and Xenes [7]. When a monolayer is encapsulated by dielectrics, the effective electron-hole potential, which takes into account screening due to the reduction of dimensionality is given by [8,9]

$$V(R) = -\frac{\pi k e^2}{2\kappa \rho_0}\left[H_0\left(\frac{R}{\rho_0}\right) - Y_0\left(\frac{R}{\rho_0}\right)\right]. \tag{1}$$

In Eq. (1), $k = 9\times 10^9\ \mathrm{N\,m^2/C^2}$, $R = |\mathbf{R}|$ is the magnitude of the relative electron-hole separation, $\kappa = (\epsilon_1 + \epsilon_2)/2$ describes the surrounding dielectric environment, where $\epsilon_1$ and $\epsilon_2$ correspond to the dielectric constants of the materials above

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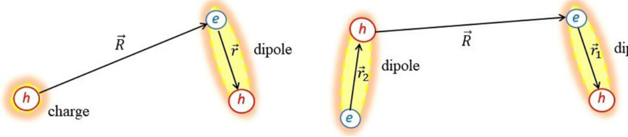

FIG. 1. Schematics for the charge-dipole and dipole-dipole interactions in 2D configuration space.

and below the monolayer, $H_0$ and $Y_0$ are the Struve and Bessel functions of the second kind, respectively, and $\rho_0$ is the screening length, which has a different physical meaning than in Ref. [4] even it has the dimension of a length. In the case of atomically thin 2D materials encapsulated by dielectrics with $\epsilon_1$ and $\epsilon_2$ the screening length is given by Refs. [8,9],

$$\rho_0 = \frac{2\pi\chi_{2D}}{\kappa}, \tag{2}$$

where $\chi_{2D}$ is the 2D polarizability, which can be calculated via *ab initio* methods or considered as a phenomenological parameter. In the strictly 2D limit of a polarizable semiconductor in vacuum ($\epsilon_1 = \epsilon_2 = 1$), $\rho_0 = 2\pi\chi_{2D}$, which is determined by the polarizability $\chi_{2D}$ of the dielectric layer [8]. The inclusion of finite thickness effects in a 2D dielectric requires a microscopic treatment of the screening (see, for example, Ref. [10]). The screening length typically ranges from roughly 30 to 80 Å [6]. The effective interaction potential (1) has an asymptotic behavior $\sim 1/R$ only at long distances between the particles, that follows from Refs. [11,12]. This limiting case corresponds to the Coulomb interaction unaffected by the dielectric polarization of a 2D layer as most of the electric-field lines between two distant charges go outside of the 2D semiconductor. Interestingly enough, in this limiting case two charges are interacting the same way as in vacuum. At shorter distances the potential deviates strongly from the usual $1/R$ form, and the dependence has a logarithmic behavior $\sim\ln(2/r) - \gamma$ [8,11,12], where $\gamma = 0.5772\cdots$ is Euler's constant.

Below we derive the explicit analytical form for the charge-dipole and dipole-dipole interactions in 2D configuration space. The starting point is the functional form (1) that does not depend by the microscopic treatments of screening.

## II. CHARGE-DIPOLE INTERACTION IN 2D CONFIGURATION SPACE

Consider two opposite closely spaced charges in a monolayer that form a dipole with the dipole moment $\mathbf{d} = e\mathbf{r}$ and a single charge placed at a distance $R$ as shown in Fig. 1. The point charge interacts with the dipole via the potential in the functional form (1). In this case following notations in Fig. 1 for the charge-dipole interaction we have

$$\begin{aligned} V_{\rm cd}(\mathbf{R}) &\equiv V_{\rm eh}(R) + V_{\rm hh}(|\mathbf{R}+\mathbf{r}|) \\ &= -\frac{\pi ke^2}{2\kappa\rho_0}\left[H_0\left(\frac{R}{\rho_0}\right) - Y_0\left(\frac{R}{\rho_0}\right)\right] \\ &\quad + \frac{\pi ke^2}{2\kappa\rho_0}\left[H_0\left(\frac{|\mathbf{R}+\mathbf{r}|}{\rho_0}\right) - Y_0\left(\frac{|\mathbf{R}+\mathbf{r}|}{\rho_0}\right)\right], \end{aligned} \tag{3}$$

where

$$|\mathbf{R}+\mathbf{r}| = R\sqrt{1 + \frac{2\mathbf{R}\cdot\mathbf{r}}{R^2} + \frac{r^2}{R^2}}. \tag{4}$$

For $R \gg r$ $(1 + \frac{2\mathbf{R}\cdot\mathbf{r}}{R^2} + \frac{r^2}{R^2})^{1/2} \simeq 1 + \frac{1}{2}(\frac{2\mathbf{R}\cdot\mathbf{r}}{R^2} + \frac{r^2}{R^2})$. Considering only linear terms with respect to $r$, Eq. (3) can be written as

$$\begin{aligned} V_{\rm cd}(\mathbf{R}) = &-\frac{\pi ke^2}{2\kappa\rho_0}\left[H_0\left(\frac{R}{\rho_0}\right) - Y_0\left(\frac{R}{\rho_0}\right)\right] \\ &+ \frac{\pi ke^2}{2\kappa\rho_0}\left[H_0\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}\right]\right)\right. \\ &\left.-Y_0\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}\right]\right)\right]. \end{aligned} \tag{5}$$

Expand the Struve $H_0(\frac{R}{\rho_0}[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}])$ and Bessel $Y_0(\frac{R}{\rho_0}[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}])$ functions in terms of power of $\frac{r}{R}$ when $R \gg r$ and consider linear terms with respect to $r$,

$$\begin{aligned} H_0\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}\right]\right) &\simeq H_0\left(\frac{R}{\rho_0}\right) + H_0'(x)|_{x=R/\rho_0}\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}}{R^2} \\ &= H_0\left(\frac{R}{\rho_0}\right) + H_{-1}\left(\frac{R}{\rho_0}\right)\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}}{R^2}, \end{aligned} \tag{6}$$

$$\begin{aligned} Y_0\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}}{R^2}\right]\right) &\simeq Y_0\left(\frac{R}{\rho_0}\right) + Y_0'(x)|_{x=\frac{R}{\rho_0}}\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}}{R^2} \\ &= Y_0\left(\frac{R}{\rho_0}\right) + Y_{-1}\left(\frac{R}{\rho_0}\right)\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}}{R^2}. \end{aligned} \tag{7}$$

Here we use that $H_0'(x) = H_{-1}(x)$ and $Y_0'(x) = -Y_1(x) = Y_{-1}(x)$ [11–13]. Using (6) and (7) Eq. (5) can be written as

$$V_{\rm cd}(\mathbf{R}) = \frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{r}}{R}, \tag{8}$$

or

$$V_{\rm cd}(\mathbf{R}) = \frac{\pi ke}{2\kappa\rho_0}\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{d}}{\rho_0 R}. \tag{9}$$

Consider the asymptotic of $V_{\rm cd}(\mathbf{R})$ interaction when $R \to \infty$. For the difference of $H_{-1}(x) - Y_{-1}(x)$ when $x \to \infty$ we have [11,12,14]

$$H_\nu(x) - Y_\nu(x) \xrightarrow[x\to\infty]{} \frac{\left(\frac{x}{2}\right)^{\nu-1}}{\sqrt{\pi}\,\Gamma(\nu+1/2)}. \tag{10}$$

For $\nu = -1$ $H_{-1}(\frac{R}{\rho_0}) - Y_{-1}(\frac{R}{\rho_0}) = \frac{4\rho_0^2}{R^2}\frac{1}{\sqrt{\pi}\Gamma(-1/2)}$. Therefore,

$$V_{\rm cd}(\mathbf{R}) \xrightarrow[R\to\infty]{} -\frac{ke}{\kappa}\frac{\mathbf{R}\cdot\mathbf{d}}{R^3}, \tag{11}$$

where we use $\Gamma(-1/2) = -2\sqrt{\pi}$. Thus, one can conclude that in 2D configuration space the charge-dipole interaction has the form (9) that has the asymptotic (11).

Evidently, the charge-dipole potential goes like $\frac{1}{R^2}$ at large $R$ and it falls off more rapidly than potential (1). For the charge-dipole interaction in 3D configuration space we have well known expression,

$$V^{C}_{\mathrm{cd}}(\mathbf{R}) = -\frac{ke}{\kappa}\frac{\mathbf{R}\cdot\mathbf{d}}{R^3}. \tag{12}$$

Here $\kappa = \varepsilon$ is the dielectric constant of the bulk material. We can conclude that $V_{\mathrm{cd}}(\mathbf{R})$ in 2D and $V^{C}_{\mathrm{cd}}(\mathbf{R})$ in 3D configuration spaces, respectively, vary as $\frac{1}{R^2}$ at large separation of the charge and the dipole.

## III. DIPOLE-DIPOLE INTERACTION IN 2D CONFIGURATION SPACE

Consider two dipole $\mathbf{d}_1 = e\mathbf{r}_1$ and $\mathbf{d}_2 = e\mathbf{r}_2$ interaction in 2D configuration space. One can consider a dipole-dipole interaction as the interactions of positive and negative charges of one dipole with the second dipole. Following notations in Fig. 1 for a dipole-dipole interaction in 2D space we have

$$V_{\mathrm{dd}}(\mathbf{R}) = V_{\mathrm{hd}}\left(\frac{R}{\rho_0}\right) + V_{\mathrm{ed}}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right). \tag{13}$$

Using (9) for the charge-dipole interaction in Eq. (13), we have

$$V_{\mathrm{dd}}(\mathbf{R}) = \frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{r}_1}{R} - \frac{\pi ke}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right) - Y_{-1}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right)\right]\frac{(\mathbf{R}+\mathbf{r}_2)\cdot\mathbf{r}_1}{|\mathbf{R}+\mathbf{r}_2|}. \tag{14}$$

We focus on the second term in Eq. (14), which represents the second term in Eq. (13). For $R \gg r_2$ considering the terms linear with respect to $r_2$, we have $|\mathbf{R}+\mathbf{r}_2| = R(1 + \frac{2\mathbf{R}\cdot\mathbf{r}_2}{R^2} + \frac{r_2^2}{R^2})^{1/2} \simeq R(1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2})$ and $\frac{1}{|\mathbf{R}+\mathbf{r}_2|} = \frac{1}{R}(1 + \frac{2\mathbf{R}\cdot\mathbf{r}_2}{R^2} + \frac{r_2^2}{R^2})^{-1/2} \simeq \frac{1}{R}(1 - \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2})$ and the second term in (14) becomes

$$\begin{aligned} V_{\mathrm{ed}}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right) &= -\frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right) - Y_{-1}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right)\right]\frac{(\mathbf{R}+\mathbf{r}_2)\cdot\mathbf{r}_1}{|\mathbf{R}+\mathbf{r}_2|} \\ &= -\frac{\pi ke^2}{2\kappa\rho_0^2}\left\{H_{-1}\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}\right]\right) - Y_{-1}\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}\right]\right)\right\}\left(\frac{(\mathbf{R}+\mathbf{r}_2)\cdot\mathbf{r}_1}{R} - \frac{\mathbf{R}\cdot\mathbf{r}_1\mathbf{R}\cdot\mathbf{r}_2}{R^3}\right). \end{aligned} \tag{15}$$

Expand the Struve $H_{-1}(\frac{R}{\rho_0}[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}])$ and Bessel $Y_{-1}(\frac{R}{\rho_0}[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}])$ functions in terms of the power of $\frac{r_2}{R}$ when $R \gg r_2$ and consider linear terms with respect to $r_2$,

$$H_{-1}\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}\right]\right) \simeq H_{-1}\left(\frac{R}{\rho_0}\right) + H'_{-1}(x)|_{x=R/\rho_0}\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}, \tag{16}$$

$$Y_{-1}\left(\frac{R}{\rho_0}\left[1 + \frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}\right]\right) \simeq Y_{-1}\left(\frac{R}{\rho_0}\right) + Y'_{-1}(x)|_{x=R/\rho_0}\frac{R}{\rho_0}\frac{\mathbf{R}\cdot\mathbf{r}_2}{R^2}. \tag{17}$$

When $R \gg r_1$ and $R \gg r_2$ by considering only terms linear with respect to $r_1$ and $r_2$ and using (16) and (17) finally, Eq. (15) can be written as

$$\begin{aligned} V_{\mathrm{ed}}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right) = &-\frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\left(\frac{\mathbf{R}\cdot\mathbf{r}_1}{R} + \frac{\mathbf{r}_1\cdot\mathbf{r}_2}{R} - \frac{\mathbf{R}\cdot\mathbf{r}_1\mathbf{R}\cdot\mathbf{r}_2}{R^3}\right) \\ &-\frac{\pi ke^2}{2\kappa\rho_0^2}\left[H'_{-1}\left(\frac{R}{\rho_0}\right) - Y'_{-1}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{r}_1\mathbf{R}\cdot\mathbf{r}_2}{\rho_0 R^2}. \end{aligned} \tag{18}$$

Let us find $H'_{-1}(\frac{R}{\rho_0}) - Y'_{-1}(\frac{R}{\rho_0})$ which presents in (18). The recurrence relations for the Struve functions $H_{\nu-1}(x) + H_{\nu+1}(x) = \frac{2\nu}{x}H_\nu(x) + (\frac{x}{2})^\nu\frac{1}{\sqrt{\pi}\Gamma(\nu+3/2)}$ and $H_{\nu-1}(x) - H_{\nu+1}(x) = 2H'_\nu(x) - (\frac{x}{2})^\nu\frac{1}{\sqrt{\pi}\Gamma(\nu+3/2)}$ [11,12] lead to $H'_\nu(x) = H_{\nu-1}(x) + \frac{1}{x}H_{-1}(x)$. On the other hand, for the second kind Bessel function $Y'_\nu(x) = Y_{\nu-1}(x) - \frac{\nu}{x}Y_\nu(x)$ [11]. Therefore, for $\nu = -1$ we obtain: $H'_{-1}(\frac{R}{\rho_0}) - Y'_{-1}(\frac{R}{\rho_0}) = H_{-2}(\frac{R}{\rho_0}) - Y_{-2}(\frac{R}{\rho_0}) + \frac{\rho_0}{R}[H_{-1}(\frac{R}{\rho_0}) - Y_{-1}(\frac{R}{\rho_0})]$. The latter expression allows to rewrite Eq. (18) as

$$V_{\mathrm{ed}}\left(\frac{|\mathbf{R}+\mathbf{r}_2|}{\rho_0}\right) = -\frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\left(\frac{\mathbf{R}\cdot\mathbf{r}_1}{R} + \frac{\mathbf{r}_1\cdot\mathbf{r}_2}{R}\right) - \frac{\pi ke^2}{2\kappa\rho_0^2}\left[H_{-2}\left(\frac{R}{\rho_0}\right) - Y_{-2}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{r}_1\mathbf{R}\cdot\mathbf{r}_2}{\rho_0 R^2}. \tag{19}$$

Replacing the second term in Eq. (14) by expression (19) we obtain the dipole-dipole interaction in 2D configuration space,

$$V_{\mathrm{dd}}(R) = -\frac{\pi k}{2\kappa\rho_0}\left\{\left[H_{-1}\left(\frac{R}{\rho_0}\right) - Y_{-1}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{d}_1\cdot\mathbf{d}_2}{\rho_0 R} + \left[H_{-2}\left(\frac{R}{\rho_0}\right) - Y_{-2}\left(\frac{R}{\rho_0}\right)\right]\frac{\mathbf{R}\cdot\mathbf{d}_1\mathbf{R}\cdot\mathbf{d}_2}{\rho_0^2 R^2}\right\}. \tag{20}$$

Using Eq. (10) for $\nu = -1$ and $\nu = -2$ for the first and second terms in Eq. (20), respectively, one can find the asymptotic of the $V_{\mathrm{dd}}(\mathbf{R})$ interaction when $R \to \infty$. The first term in Eq. (20) has the following asymptotic behavior $(\frac{R}{2\rho_0})^{-2}\frac{1}{\sqrt{\pi}\Gamma(-1/2)}\frac{\mathbf{d}_1\cdot\mathbf{d}_2}{\rho_0 R} = -\frac{2\rho_0}{\pi}\frac{\mathbf{d}_1\cdot\mathbf{d}_2}{R^3}$. Whereas the asymptotic of the second term is $(\frac{R}{2\rho_0})^{-3}\frac{1}{\sqrt{\pi}\Gamma(-3/2)}\frac{\mathbf{R}\cdot\mathbf{d}_1\mathbf{R}\cdot\mathbf{d}_2}{\rho_0^2 R^2} = \frac{6\rho_0}{\pi}\frac{\mathbf{R}\cdot\mathbf{d}_1\mathbf{R}\cdot\mathbf{d}_2}{R^5}$.

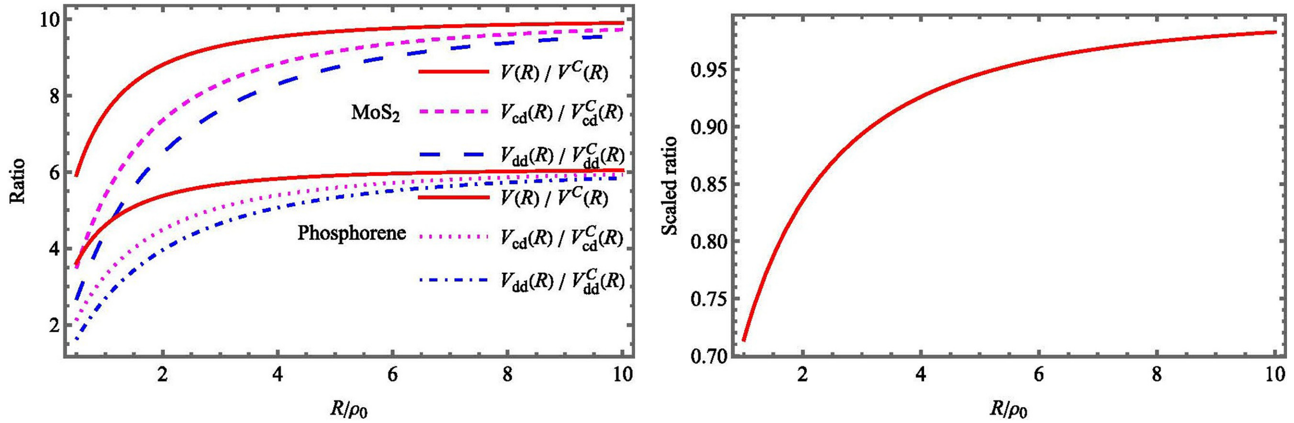

FIG. 2. Left panel: The ratios of effective 2D (1) and Coulomb potentials, charge-dipole interaction $V_{\rm cd}$ in 2D configuration space, and $V^C_{\rm cd}$ for bulk materials and the second factors of the dipole-dipole interaction in a monolayer and bulk material. Calculations are performed for the phosphorene and MoS$_2$. Right panel: The universal dependence of the ratio of $V_{\rm cd}/V^C_{\rm cd}$ and $V(R)/V^C(R)$ on $R/\rho_0$ for any 2D material.

Combining the latter expressions we obtain

$$V_{\rm dd}(\mathbf{R}) \xrightarrow[R\to\infty]{} \frac{k}{\kappa}\frac{1}{R^3}\left[\mathbf{d}_1\cdot\mathbf{d}_2 - 3\frac{(\mathbf{R}\cdot\mathbf{d}_1)(\mathbf{R}\cdot\mathbf{d}_2)}{R^2}\right]. \qquad (21)$$

For comparison the dipole-dipole interaction in 3D configuration space has the following form:

$$V^C_{\rm dd}(\mathbf{R}) = \frac{k}{\kappa}\frac{1}{R^3}\left[\mathbf{d}_1\cdot\mathbf{d}_2 - 3\frac{(\mathbf{R}\cdot\mathbf{d}_1)(\mathbf{R}\cdot\mathbf{d}_2)}{R^2}\right], \qquad (22)$$

where $\kappa = \epsilon$ is the dielectric constant of the bulk material. Thus, $V_{\rm dd}(\mathbf{R})$ asymptotic coincides with the dipole-dipole interaction in 3D configuration space where charges interact via the Coulomb potential. In numerical calculations, we focus only on freestanding phosphorene and monolayer MoS$_2$. We use for MoS$_2$ polarizability $\chi_{2D} = 6.6$ Å [9] obtained within density functional theory and subsequent random-phase approximation calculations for TMDC monolayers. For the phosphorene polarizabilty the value of $\chi_{2D} = 4.1$ Å [15] is used. The right panel in Fig. 2 presents the ratio of charge-dipole interaction potentials $V_{\rm cd}(\mathbf{R})$ in phosphorene and MoS$_2$ and $V^C_{\rm cd}(\mathbf{R})$ in the same bulk materials. The values of the negative order Struve $H_{-1}(\frac{R}{\rho_0})$ and Bessel $Y_{-1}(\frac{R}{\rho_0})$ functions were evaluated with the in-built codes in *Mathematica*. There are five distinguished features: (i) The value of $V_{\rm cd}(\mathbf{R})$ is bigger than the value of $V^C_{\rm cd}(\mathbf{R})$; (ii) at short distances $V_{\rm cd}(\mathbf{R})$ falls more slowly than the Coulomb potential induced charge-dipole interaction in the same bulk material; (iii) at short distances the slope of the ratio fall demonstrate the sensitivity of $V_{\rm cd}(\mathbf{R})$ to the 2D polarizability and dependence on the ratio of dielectric constant of the bulk material and the polarizability of monolayer; (v) the asymptotic of the ratio is the value of the dielectric constant of the bulk material. This means that when $R \to \infty$ the charge-dipole interaction in a monolayer is the same as in vacuum.

Both dipole-dipole interactions (20) and (22) have two terms: One is proportional to $\mathbf{d}_1\cdot\mathbf{d}_2$, and the other one is proportional to $(\mathbf{R}\cdot\mathbf{d}_1)(\mathbf{R}\cdot\mathbf{d}_2)$. The comparison of factors in front of $\mathbf{d}_1\cdot\mathbf{d}_2$ shows that their ratio has the same dependence as the ratio $V_{\rm cd}/V^C_{\rm cd}$. The ratios of factors in front of $(\mathbf{R}\cdot\mathbf{d}_1)(\mathbf{R}\cdot\mathbf{d}_2)$ for phosphorene and MoS$_2$ are shown in Fig. 2. These ratios are smaller than $V_{\rm cd}/V^C_{\rm cd}$ and demonstrate the same features as that are listed above for $V_{\rm cd}/V^C_{\rm cd}$. However, the ratios fall more smoothly than $V_{\rm cd}/V^C_{\rm cd}$. As is seen from Fig. 2 $V/V^C > V_{\rm cd}/V^C_{\rm cd} > V_{\rm dd}/V^C_{\rm dd}$ and all ratios converging to the dielectric constant of bulk materials. At short distances $V/V^C$ increases more rapidly than $V_{\rm cd}/V^C_{\rm cd}$ and $V_{\rm cd}/V^C_{\rm cd}$ increases faster than the second term of $V_{\rm dd}/V^C_{\rm dd}$. Interestingly enough, the ratio,

$$[V_{\rm cd}/V^C_{\rm cd}]/[V/V^C] = x\frac{H_{-1}(x) - Y_{-1}(x)}{H_0(x) - Y_0(x)} \quad \text{where } x = \frac{R}{\rho_0} \qquad (23)$$

shows the universality in its dependence on $\frac{R}{\rho_0}$ that is the same for any monolayer material. This ratio we named as a scaled ratio that is the ratio of $V_{\rm cd}(R)$ scaled to the corresponding $V^C_{\rm cd}(R)$ and $V(R)$ scaled to the Coulomb potential. The dependence of this ratio on $R/\rho_0$ is shown in the right panel in Fig. 2.

*Concluding remarks.* In this Letter we study the influence of the reduction of dimensionality on the charge-dipole and dipole-dipole interactions in 2D configuration space. We demonstrate that the screened nature of Coulomb interaction imposes peculiarities in the 2D charge-dipole and dipole-dipole interactions behavior. The analytical expression for the charge-dipole and dipole-dipole interactions in 2D configuration space is derived. These charge-dipole and dipole-dipole interactions will find wide application in studies of 2D materials and contribute to the advancement of research on novel two-dimensional materials. Recently, a new potential form for the electron-hole interaction, which takes into account the three atomic sheets that compose a monolayer of transition-metal dichalcogenides was derived [16]. Without losing any generality our approach can be extended for this form of the potential.

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