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Nanostructure van der Waals interaction between a quantum well and a quantum dot atom

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Abstract

We examine the van der Waals interaction between mobile plasma electrons in a narrow quantum well nanostructure and a quantum dot atom. This formulation of the van der Waals interaction exhibits it to second order as the correlation energy (self-energy) of the dot-atom electrons mediated by the image potential arising from the dynamic, nonlocal and spatially inhomogeneous polarization of the quantum well plasma electrons. This image potential of the quantum-well plasma is, in turn, determined by the dynamic, nonlocal, inhomogeneous screening function of the quantum well, which involves the space–time matrix inversion of its spatially inhomogeneous, nonlocal and time-dependent dielectric function. The latter matrix inversion is carried out exactly, in closed form, and the van der Waals energy is evaluated in the electrostatic limit to dipole–dipole terms.

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1. Introduction: atom–surface van der Waals interaction and the plasma image

The van der Waals interaction between an atom and surface is based on the Coulomb interaction between the atomic electrons and the mobile electrons within the surface, and it *excludes* the possibility of sharing or exchanging electrons by penetration of the atomic electron wavefunctions into the surface, or vice versa. Moreover, the theory of van der Waals attraction assumes that the atom and its electrons are far enough from the mobile electrons within the surface so that exchange effects are negligibly small. These qualitative statements apply to all van der Waals (vdW) interactions, including atom–atom, as well as atom–surface.

While all electrons are indistinguishable in principle, the atomic electrons may be thought of as a group distinct from the mobile surface electrons if their separation is large enough so that exchange effects and wavefunction penetration (tunnelling, sharing) are small. On this basis, we write ψ_a^+ , ψ_a to represent creation/annihilation operators for bound electrons of the

atom, and ψ_m^+ , ψ_m to represent the corresponding operators for mobile electrons of the surface, with

$$\psi = \psi_a + \psi_m; \quad \psi^+ = \psi_a^+ + \psi_m^+.$$

Considering them to be mutually independent, we take ψ_a^+ , ψ_a to anticommute with ψ_m^+ , ψ_m individually. Our nonrelativistic treatment for the Coulomb interaction, \mathcal{V} , is based on the usual two-body part of the Hamiltonian:

$$H^{(2)} = \frac{1}{2!} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' (\psi_a^+(\mathbf{x}', t) + \psi_m^+(\mathbf{x}', t)) (\psi_a^+(\mathbf{x}'', t) + \psi_m^+(\mathbf{x}'', t)) \\ \times \mathcal{V}(\mathbf{x}' - \mathbf{x}'') (\psi_a(\mathbf{x}'', t) + \psi_m(\mathbf{x}'', t)) (\psi_a(\mathbf{x}', t) + \psi_m(\mathbf{x}', t)). \quad (1)$$

Of the 16 possible products in the integrand of equation (1), one represents the Coulomb interactions (and internal correlations) within the subsystem of atomic (a) electrons, H_{aa} , and, separately, there is a similar one, H_{mm} , for the Coulomb interactions (and internal correlations) within the subsystem of mobile (m) electrons of the surface. Correspondingly,

$$H_{\{aa\}}^{(2)} = \frac{1}{2!} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \psi_{\{a\}}^+(\mathbf{x}', t) \psi_{\{a\}}^+(\mathbf{x}'', t) \mathcal{V}(\mathbf{x}' - \mathbf{x}'') \psi_{\{a\}}(\mathbf{x}'', t) \psi_{\{a\}}(\mathbf{x}', t). \quad (2)$$

Of the remaining 14 possible products, eight involve products of three operators of one subsystem and just one of the other (for example, $\psi_m^+ \psi_a^+ \mathcal{V} \psi_a \psi_m$, etc). We take these to be negligible since such a Hamiltonian term would transfer electrons singly from the atom to the surface or vice versa, which is excluded from our considerations in accordance with the above remarks. The remaining six products involve two operators of the a -electrons and two of the m -electrons. Of these, two are of the type $\psi_a^+ \psi_a^+ \mathcal{V} \psi_m \psi_m$ or $\psi_m^+ \psi_m^+ \mathcal{V} \psi_a \psi_a$, which would transfer electrons in pairs from the atom to the surface or vice versa, which is similarly excluded. Of the remaining four products two are described by

$$\psi_{\{a\}}^+(\mathbf{x}', t) \psi_{\{m\}}^+(\mathbf{x}'', t) \mathcal{V}(\mathbf{x}' - \mathbf{x}'') \psi_{\{a\}}(\mathbf{x}'', t) \psi_{\{m\}}(\mathbf{x}', t), \quad (3)$$

which would annihilate a surface electron at \mathbf{x}' while creating an atomic electron at \mathbf{x}'' in its place and simultaneously annihilate an atomic electron at \mathbf{x}'' while a mobile surface electron is created in its place at \mathbf{x}' , etc. Again, these two terms exchange atomic and surface electrons, processes which are excluded from our present considerations. The final two terms involve just the product of the density operator ρ_a for a -electrons with that of m -electrons, ρ_m , and vice versa, and the two are actually the same since the anticommutation of $\psi_a(\mathbf{x}', t)$ through $\rho_m(\mathbf{x}'', t)$ invokes *two* minus signs, hence they commute, as do $\rho_a(\mathbf{x}', t)$ and $\rho_m(\mathbf{x}'', t)$, etc. Thus the $\rho_a \rho_m$ term doubles, cancelling the prefactor $\frac{1}{2!}$ in this part of $H^{(2)}$. In summary, vdW interaction involves the following Hamiltonian:

$$H^{(2)} = H_{aa}^{(2)} + H_{mm}^{(2)} + H_{am}^{(2)}, \quad (4)$$

where

$$H_{am}^{(2)} = \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \rho_a(\mathbf{x}', t) \mathcal{V}(\mathbf{x}' - \mathbf{x}'') \rho_m(\mathbf{x}'', t). \quad (5)$$

We will only treat those aspects of atom–surface van der Waals interaction here which illustrate the far reaching utility of the dynamic nonlocal dielectric screening concept. Consider first the Hamiltonian for the instantaneous Coulomb interaction of the atomic electrons written in the form:

$$H_{aa}^{(2)} = \frac{1}{2} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \int dt'' \psi_a^+(\mathbf{x}', t') \psi_a(\mathbf{x}', t') \mathcal{V}(\mathbf{x}' - \mathbf{x}'') \delta(t' - t'') \psi_a^+(\mathbf{x}'', t'') \psi_a(\mathbf{x}'', t''). \quad (6)$$

In a first approximation, the associated energy (with correlations of the atomic electrons in the presence of the nuclear potential which binds the electrons) may be written as the expectation value of $H_{aa}^{(2)}$ in the ground state of the atom. To develop an approximation directed at incorporating the role of $H_{am}^{(2)}$ (equation (5)) without undertaking a formal perturbation theory [1] (which leads to the same result), we replace $\mathcal{V}(\mathbf{x} - \mathbf{x}')\delta(t - t')$ in equation (6) by the effective potential between atomic electrons, $\mathcal{V}_{\text{eff}}(\mathbf{x}', \mathbf{x}'', t' - t'')$, part of which is generated by Coulomb interaction between atomic electrons and the surface electrons, i.e. the nonlocal dynamic *image* potential, $\mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}'', t' - t'')$, felt by the electrons of the atom. Thus, we write their corresponding part of equation (6) as a ‘van der Waals’ term, H_{vdW} , given by

$$H_{\text{vdW}}^{(2)} = \frac{1}{2} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \int dt'' \psi_a^+(\mathbf{x}', t') \psi_a(\mathbf{x}', t') \times \mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}'', t' - t'') \psi_a^+(\mathbf{x}'', t'') \psi_a(\mathbf{x}'', t''). \quad (7)$$

Estimating the van der Waals interaction energy contribution from this term as the ground state expectation value $\langle H_{\text{vdW}}^{(2)} \rangle$, we have

$$E_{\text{vdW}} \cong \langle H_{\text{vdW}}^{(2)} \rangle = -\frac{1}{2} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \int dt'' \mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}'', t' - t'') \times G_2^a(\mathbf{x}''t'', \mathbf{x}'t'; \mathbf{x}''t''^+, \mathbf{x}'t'^+). \quad (8)$$

Here, G_2^a is the two-particle Green’s function of the atomic electrons, including the full complement of intra-atom interactions, but with no effects from the surface electrons, averaged in the ground state of the atom $|\Phi_0^a\rangle$. The image potential, $\mathcal{V}_{\text{image}}$, due to the polarization of the surface electron plasma by the Coulomb field of a point charge outside may be written in terms of the G_2^m function of the plasma of surface electrons using the inverse dielectric (screening) function K^m of the surface plasma. Discarding G_1^m terms and δ -terms that are not pertinent to this discussion, we have

$$K^m(1, 2) \rightarrow i \int d^3\mathcal{V}(1 - 3)G_2^m(3, 2; 3^+, 2^+) = i \int d^{(3)}\mathbf{x}^{\text{iv}} \mathcal{V}(\mathbf{x}' - \mathbf{x}^{\text{iv}}) G_2^m(\mathbf{x}^{\text{iv}}t', \mathbf{x}''t''; \mathbf{x}^{\text{iv}}t'^+, \mathbf{x}''t''^+) \quad (9)$$

where G_2^m includes the effects of mobile electron–electron interactions within the surface, and \mathcal{V} is the unscreened Coulomb potential. The corresponding image potential, $\mathcal{V}_{\text{image}}$, is

$$\mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}'', t' - t'') = \int d^{(3)}\mathbf{x}''' [K^m(\mathbf{x}', \mathbf{x}'''; t' - t'') \mathcal{V}(\mathbf{x}''' - \mathbf{x}'')] - \mathcal{V}(\mathbf{x}' - \mathbf{x}'') = i \int d^{(3)}\mathbf{x}''' \int d^3\mathbf{x}^{\text{iv}} \mathcal{V}(\mathbf{x}' - \mathbf{x}^{\text{iv}}) G_2^m(\mathbf{x}^{\text{iv}}t', \mathbf{x}'''t''; \mathbf{x}^{\text{iv}}t'^+, \mathbf{x}'''t''^+) \mathcal{V}(\mathbf{x}''' - \mathbf{x}'') - \mathcal{V}(\mathbf{x}' - \mathbf{x}''), \quad (10)$$

which yields E_{vdW} in an alternative form as

$$E_{\text{vdW}} = -\frac{i}{2} \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \int d^{(3)}\mathbf{x}''' \int d^{(3)}\mathbf{x}^{\text{iv}} \int dt'' \mathcal{V}(\mathbf{x}' - \mathbf{x}^{\text{iv}}) \times G_2^m(\mathbf{x}^{\text{iv}}t', \mathbf{x}'''t''; \mathbf{x}^{\text{iv}}t'^+, \mathbf{x}'''t''^+) \mathcal{V}(\mathbf{x}''' - \mathbf{x}'') G_2^a(\mathbf{x}''t'', \mathbf{x}'t'; \mathbf{x}''t''^+, \mathbf{x}'t'^+) - \text{direct non-image counterpart}. \quad (11)$$

Noting that equation (11) is symmetric under the atom \leftrightarrow surface interchange, it is readily seen that another contribution to vdW energy identical to equation (11) comes from an analogous treatment of $H_{mm}^{(2)}$ in place of $H_{aa}^{(2)}$, *eliminating the 1/2 prefactor*. This result can also be obtained [1] using straightforward perturbation theory to second order in $H_{am}^{(2)}$ (equation (5)).

As in perturbation theory, G_2^m and G_2^a (alternatively, K^m and G_2^a) are to be determined in the absence of atom–surface coupling. It is convenient to write the result in the form of equation (8) (but without the eliminated 1/2 prefactor), as

$$E_{\text{vdW}} = - \int d^{(3)}\mathbf{x}' \int d^{(3)}\mathbf{x}'' \int dt'' \mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}'', t' - t'') G_2^a(\mathbf{x}'' t'', \mathbf{x}' t'; \mathbf{x}'' t''^+, \mathbf{x}' t'^+), \quad (12)$$

which suggests interpreting E_{vdW} in terms of a self-energy of the atomic electrons due to screening of their Coulomb interaction by the surface electrons. Here, we can fruitfully employ the determination of $\mathcal{V}_{\text{eff}} - \mathcal{V} = \mathcal{V}_{\text{image}}$ in the presence of dynamic, nonlocal screening by the mobile surface electrons as discussed below.

2. Effective potential and the 3D screening function of the 2D electron plasma of the quantum well

The effective potential $\mathcal{V}_{\text{eff}}(1)$ at a space–time point $1 = (\mathbf{r}_1, t_1)$ generated by the Coulomb potential $\mathcal{V}(2)$ impressed at $2 = (\mathbf{r}_2, t_2)$ by an atomic electron is associated with polarization of the 2D mobile electrons of the quantum well,

$$\mathcal{V}_{\text{eff}}(1) = \int d^{(4)}2 K^m(1, 2) \mathcal{V}(2), \quad (13)$$

where $K^m(1, 2)$ is the 3D screening function of the 2D plasma inverse to its direct dielectric function $\epsilon(3, 2)$ in a 3D space–time matrix sense

$$\int d^4 3 K^m(1, 3) \epsilon(3, 2) = \delta^4(1, 2). \quad (14)$$

Here, $\epsilon(3, 2)$ is the direct dielectric function of the 2D plasma in 3D real space–time representation. One must also recognize that there is a density perturbation involved in the response dynamics, such that

$$\begin{aligned} \rho(1) &= \int d^4 3 R(1, 3) \mathcal{V}_{\text{eff}}(3) \\ &= \int d^4 3 \int d^4 4 R(1, 3) K^m(3, 4) \mathcal{V}(4) \end{aligned} \quad (15)$$

with $R(1, 3) = \delta\rho(1)/\delta\mathcal{V}_{\text{eff}}(3)$ as the density-perturbation response function. Writing $\epsilon(3, 2)$ in terms of the polarizability $\alpha(3, 2)$, equation (14) becomes an RPA-type integral equation

$$K^m(1, 2) = \delta^4(1 - 2) - \int d^4 3 \alpha(1, 3) K^m(3, 2). \quad (16)$$

The polarizability $\alpha(1, 3)$ can be expressed in a form which describes both the free-electron response and an additive static background contribution (\mathcal{V} is the interelectron Coulomb interaction of the plasma, and $\alpha_0 = \epsilon_0 - 1$ is the additive background polarizability):

$$\alpha(1, 3) = - \int d^4 4 \mathcal{V}(1 - 4) R(4, 3) + \alpha_0 \delta^4(1 - 3). \quad (17)$$

This yields

$$K^m(1, 2) = \frac{1}{\epsilon_0} \delta^4(1 - 2) + \frac{1}{\epsilon_0} \int d^4 3 \int d^4 4 \mathcal{V}(1 - 4) R(4, 3) K^m(3, 2). \quad (18)$$

In the RPA, $R(4, 3)$ is the lowest ring diagram and the integral equation (18) is just the sum of ring diagrams. Considering translational invariance in the $\bar{r} = (x, y)$ plane of the quantum well walls and in time (but not for z), we Fourier transform

$$K^m(1, 2) = K^m(\bar{r}_1 - \bar{r}_2, z_1, z_2; t_1 - t_2) \rightarrow K^m(\bar{p}, z_1, z_2; \omega), \quad (19)$$

with respect to space $\bar{r}_1 - \bar{r}_2 \rightarrow \bar{p}$ and time $t_1 - t_2 \rightarrow \omega$.

To determine the 3D screening function $K^m(\bar{p}, z_1, z_2; \omega)$ that is the inverse of the 2D plasma dielectric function $\epsilon(\bar{p}, z_1, z_2; \omega)$ in 3D space, we employ the inversion condition of equation (14) in the form

$$\int dz_2 K(\bar{p}, z_1, z_2; \omega) \epsilon(\bar{p}, z_2, z_3; \omega) = \delta(z_1 - z_3), \quad (20)$$

which may be applied writing $\epsilon(\bar{p}, z_1, z_2; \omega)$ as

$$\epsilon(\bar{p}, z_1, z_2; \omega) = \delta(z_1 - z_2) + \alpha(\bar{p}, z_1, z_2; \omega) \quad (21)$$

in terms of the quantum well polarizability, $\alpha(\bar{p}, z_1, z_2; \omega)$. For electron motion confined to a single 2D plane sheet, the density-perturbation response function has its z arguments localized to the sheet by positional δ -functions of the form

$$R(\bar{p}, z_1, z_2; \omega) = \delta(z_1)\delta(z_2)R^{2D}(\bar{p}, \omega). \quad (22)$$

Here, $R^{2D}(\bar{p}, \omega)$ describes the electron density perturbation response properties on the 2D sheet, such that the 2D electron polarizability on the sheet is given by $\alpha^{2D}(\bar{p}, \omega) = -R^{2D}(\bar{p}, \omega)/p$ (where we introduced the 2D Fourier transform in the Coulomb potential in equation (17)). With this in view, we have

$$\epsilon(\bar{p}, z_1, z_2; \omega) = \epsilon_0 \delta(z_1 - z_2) + \delta(z_2) \alpha^{2D}(\bar{p}, \omega) e^{-p|z_1|}, \quad (23)$$

where $p = |\bar{p}|$ and $\epsilon_0 = 1 + \alpha_0$ for the background. We attempt inversion in the form

$$K^m(\bar{p}, z_1, z_2; \omega) = \frac{1}{\epsilon_0} \delta(z_1 - z_2) + \frac{1}{\epsilon_0} \delta(z_2) e^{-p|z_1|} [\tilde{K}^{2D}(\bar{p}, \omega) - 1]. \quad (24)$$

The determination of $\tilde{K}^{2D}(\bar{p}, \omega)$ is carried out by requiring satisfaction of the inversion condition in the form of equation (20). Equating coefficients of like positional delta functions, we obtain

$$\tilde{K}^{2D}(\bar{p}, \omega) = \left(1 + \frac{\alpha^{2D}(\bar{p}, \omega)}{\epsilon_0}\right)^{-1} \equiv [\tilde{\epsilon}^{2D}(\bar{p}, \omega)]^{-1}. \quad (25)$$

$\alpha^{2D}(\bar{p}, \omega)$ was determined by Stern [2] for null magnetic field and division by ϵ_0 corresponds to putting $\mathcal{V} \rightarrow \tilde{\mathcal{V}} = \mathcal{V}/\epsilon_0$ or $e^2 \rightarrow \tilde{e}^2 = e^2/\epsilon_0$. A simple example of the utility of equation (24) is provided in the determination of the statically screened Coulomb potential sited at $(0, 0, z_0)$ in 3D space, with the electron sheet on the 2D plane $z = 0$. Taking $\epsilon_0 \rightarrow 1$, we have the shielded potential as

$$\begin{aligned} \mathcal{V}(\mathbf{r}, t \rightarrow \infty) &= \int \frac{d^2 p}{(2\pi)^2} e^{i\bar{p}\cdot\bar{r}} \int dz' K^m(\bar{p}, z, z'; \omega \rightarrow 0) e^{-p|z'-z_0|}/p \\ &\times \int \frac{d^2 p}{(2\pi)^2} \frac{e^{i\bar{p}\cdot\bar{r}}}{p} \left(e^{-p|z-z_0|} - e^{-p(|z|+|z_0|)} \frac{\alpha^{2D}(\bar{p}, \omega \rightarrow 0)}{1 + \alpha^{2D}(\bar{p}, \omega \rightarrow 0)} \right). \end{aligned} \quad (26)$$

For a perfect metal sheet $\alpha^{2D} \rightarrow -\infty$, this yields a perfect image field of relative strength -1 on the same side of the sheet as the Coulomb site (same sign for z, z_0); and it also yields a completely shielded null result at points on the other side of the sheet (different signs for z, z_0 , as one should expect).

3. Nonlocal dipolar van der Waals interaction of an atom and a 2D quantum well: magnetic field effects

The atomic electron G_2^a function involved in E_{vdw} has the form

$$G_2^a \rightarrow \langle \Phi_0^a | \rho_a(\mathbf{x}'', t'') \rho_a(\mathbf{x}', t') | \Phi_0^a \rangle. \quad (27)$$

Recognizing that the atom has a fixed number of electrons and is electrically neutral (in the absence of ionization), we denote the energy eigenstates of the atomic electrons by $|\Phi_n^a\rangle$, with ground state $|\Phi_0^a\rangle$. These states of the atomic electrons bear the full complement of correlations due to electron–electron interactions of the electrons of the atom. Their completeness is expressed by

$$1 = \sum_n |\Phi_n^a\rangle\langle\Phi_n^a|, \quad (28)$$

so that

$$G_2^a(\mathbf{x}''t'', \mathbf{x}'t'; \mathbf{x}''t''+, \mathbf{x}'t'+) = \sum_n \langle\Phi_0^a| \rho_a(\mathbf{x}'', t'') |\Phi_n^a\rangle\langle\Phi_n^a| \rho_a(\mathbf{x}', t') |\Phi_0^a\rangle. \quad (29)$$

Employing an atomic electron time translation operator $e^{iH_a(t'-t'')}$ to bring the times of the two density operators into coincidence, we have

$$G_2^a(\mathbf{x}''t'', \mathbf{x}'t'; \mathbf{x}''t''+, \mathbf{x}'t'+) = \sum_n \langle\Phi_0^a| \rho_a(\mathbf{x}'', t'') |\Phi_n^a\rangle\langle\Phi_n^a| e^{iH_a(t'-t'')} \times \rho_a(\mathbf{x}', t') e^{-iH_a(t'-t'')} |\Phi_0^a\rangle, \quad (30)$$

and since

$$H_a |\Phi_n^a\rangle = E_n^a |\Phi_n^a\rangle, \quad (31)$$

we have

$$G_2^a(\mathbf{x}''t''; \mathbf{x}'t'; \mathbf{x}''t''+; \mathbf{x}'t'+) = \sum_n \langle\Phi_0^a| \rho_a(\mathbf{x}'', t'') |\Phi_n^a\rangle\langle\Phi_n^a| \rho_a(\mathbf{x}', t') |\Phi_0^a\rangle e^{i(E_n^a - E_0^a)(t'-t'')}. \quad (32)$$

Understanding that both density operators and the energy eigenstates are evaluated at the same time so that the matrix elements are independent of time, we write

$$\langle\Phi_0^a| \rho_a(\mathbf{x}'', t'') |\Phi_n^a\rangle = \langle\rho_a(\mathbf{x}'')\rangle_{0n}$$

and

$$\omega_{no}^a = E_n^a - E_0^a,$$

whence,

$$G_2^a(\mathbf{x}''t''; \mathbf{x}'t'; \mathbf{x}''t''+; \mathbf{x}'t'+) = \sum_n' \langle\rho_a(\mathbf{x}'')\rangle_{0n} \langle\rho_a(\mathbf{x}')\rangle_{n0} e^{i\omega_{no}^a(t'-t'')}. \quad (33)$$

(The prime on $\Sigma \rightarrow \Sigma'$ indicates that the $n = 0$ term is excluded since it has no time dependence and yields a constant, static contribution, which is irrelevant to the van der Waals interaction.) Substitution of this into equation (12) yields E_{vdW} in terms of the Fourier time transform of $\mathcal{V}_{\text{image}}(t' - t'') \rightarrow \mathcal{V}_{\text{image}}(\omega)$ as

$$E_{\text{vdW}} = \int d^3\mathbf{x}' \int d^3\mathbf{x}'' \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \mathcal{V}_{\text{image}}(\mathbf{x}', \mathbf{x}''; \omega) \sum_n' \left(\frac{\langle\rho_a(\mathbf{x}'')\rangle_{0n} \langle\rho_a(\mathbf{x}')\rangle_{n0}}{\omega - \omega_{no}^a} \right), \quad (34)$$

where we have taken account of nonlocality in time in performing the time integration. Considering spatial translational invariance in the lateral plane $\bar{\mathbf{x}} = (x, y) \rightarrow \bar{\mathbf{p}}$ and using $\mathcal{V}_{\text{image}}(z', z''; \bar{\mathbf{p}}, \omega)$ obtained from equations (24) and (25), we obtain the result for E_{vdW} using a multipole expansion mandated by the spatially confined distribution of the atomic electrons. To dipole–dipole terms, it is given by (\mathbf{D}_{on} is the matrix element of the dipole moment operator)

$$E_{\text{vdW}} = -\frac{4}{3\hbar\epsilon_0} \sum_n' \int_0^{\infty} \frac{d\omega}{2\pi i} \frac{\omega_{no}}{\omega^2 - \omega_{no}^2} \frac{|\mathbf{D}_{on}|^2}{\omega} \int_0^{\infty} dp p^2 e^{-2p|Z|} \frac{\alpha^{2D}(p, \omega)/\epsilon_0}{1 + \alpha^{2D}(p, \omega)/\epsilon_0}, \quad (35)$$

where $|Z|$ is the distance of the atom from the 2D planar quantum well.

Equation (35) is a useful point of departure to determine both local and nonlocal structure of the van der Waals interaction in a magnetic field normal to the quantum well. Expanding equation (35) in inverse powers of $|Z|$ under conditions of low density (such that $\omega_p < \omega_c, \omega_{no}$), and using the magnetic field dependent 2D polarizability [3, 4] we obtain (ω_c is the cyclotron frequency, which can exceed the 2D plasma frequency in semiconductors)

$$E_{\text{vdW}}^{(2)} = \frac{\pi e^2 n_{2D}}{4\hbar m \epsilon_0^2} \sum_n' |\mathbf{D}_{on}|^2 \omega_{no} \left\{ \frac{1}{|Z|^4} \frac{1}{\omega_c \omega_{no} (\omega_c + \omega_{no})} - \frac{1}{|Z|^6} \frac{5\sigma}{mn_{2D}\omega_c^2} \left(\frac{1}{\omega_c \omega_{no} (\omega_c + \omega_{no})} - \frac{1}{2\omega_c \omega_{no} (2\omega_c + \omega_{no})} \right) \right\}, \quad (36)$$

where n_{2D} is the 2D equilibrium density, which may be expressed in terms of the Fermi function $f_0(\omega)$ as

$$n_{2D} = 2 \int_0^\infty \frac{d\omega}{\hbar^2} f_0(\omega) \int_{-i\infty+\delta}^{i\infty+\delta} \frac{ds}{2\pi i} e^{\omega s} \frac{m\hbar\omega_c}{4\pi \tanh(\hbar\omega_c s/2)}. \quad (37)$$

and σ is defined as

$$\sigma = \int_0^\infty \frac{d\omega}{\hbar^2} f_0(\omega) \int_{-i\infty+\delta}^{i\infty+\delta} \frac{ds}{2\pi i} e^{\omega s} \frac{m(\hbar\omega_c)^2}{4\pi (\tanh \hbar\omega_c s/2)^2}. \quad (38)$$

It should be noted that the low-density approximation involved in obtaining equation (36), namely $\omega_p < \omega_c, \omega_{no}$, precludes taking the limit $\omega_c \rightarrow 0$ which would falsely indicate divergencies. Equations (36)–(38) will be discussed more fully elsewhere. They contain the full complement of both classical and quantum magnetic field effects due to Landau quantization of orbitals. The first term on the right of equation (36) is due to local 2D magneto-plasma response, and is proportional to $|Z|^{-4}$. It is important to bear in mind that the remaining terms ($O(|Z|^{-6})$) occur within the dipole–dipole approximation, devoid of higher multipole moments. They arise in consequence of the nonlocal plasma character of the 2D dielectric response. The formulation of van der Waals' interactions employed here is readily extended to Casimir forces, a subject of strong current interest [1, 5, 6].

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