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Exchange and correlation in positronium-molecule scattering

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Abstract

Exchange and correlations play a particularly important role in positronium (Ps) collisions with atoms and molecules, since the static potential for Ps interaction with a neutral system is zero. Theoretical description of both effects is a very challenging task. In the present work we use the free-electron-gas model to describe exchange and correlations in Ps collisions with molecules similar to the approach widely used in the theory of electron-molecule collisions. The results for exchange and correlation energies are presented as functions of the Fermi momentum of the electron gas and the Ps incident energy. Using the Thomas-Fermi model, these functions can be converted into exchange and correlation potentials for Ps interaction with molecules as functions of the distance between the projectile and the target.

PACS numbers:

I. INTRODUCTION

Since the discovery [1–3] of similarity between electron and positronium (Ps) scattering by atoms and molecules, a lot of theoretical effort [4–9] has been directed at explaining this intriguing phenomenon. The similarity of cross sections for equivelocity electrons and Ps can be justified by the impulse approximation [4]. However, the impulse approximation breaks down at low energies, particularly below the threshold for Ps ionization (break-up), therefore a more sophisticated analysis is required in the low-energy region. Generally at the Ps velocities above about 0.2 a.u. (energies above 1 eV) the Ps interaction with atoms is mostly controlled by electrons. Because of the symmetry of the Ps wavefunction with respect to interchange of the electron and positron coordinates, the direct static potential (without exchange) between Ps and the atomic or molecular target is zero [10], therefore the exchange interaction and short-range correlations play an especially important role in Ps scattering. At low collision energies the long-range van der Waals force between Ps and the target also becomes important.

In our previous treatment of Ps collisions with rare-gas atoms [5, 8] and molecular hydrogen [7] we constructed pseudopotentials for the Ps-target interaction based on electron and positron scattering phase shifts. These pseudopotentials contain repulsive cores which mock orthogonality between the wavefunction of the scattered electron and the occupied molecular orbitals. However, for the complete inclusion of exchange in electron-molecule collisions the orthogonality constraint is not sufficient. For example in e -N₂ collisions the Π_g resonance is mainly due to the exchange interaction [11, 12]. This important effect cannot be incorporated by the orthogonality constraint used, for example, in Ref. [13] since there is no occupied π_g orbital in N₂. Combination of a model attractive exchange potential with the orthogonality constraint usually gives the best results in terms of agreement with calculations which incorporate exchange exactly. Because of complexity of the exact exchange potential this method has been widely used in electron-molecule scattering calculations [11].

Exact inclusion of electron exchange in Ps collisions with atoms and molecules is an even more challenging task [10] and has been accomplished only for simple targets such as the hydrogen atom [14, 15] and rare-gas atoms [16–19].

Studies of electron-molecule collisions [11] show that the electron scattering phase shifts can be obtained with good accuracy by using, in addition to the static potential, a local

exchange potential obtained from calculation of the exchange energy of interaction of a free electron with a free electron gas (FEG). Originally this potential for electron-molecule collisions was proposed by Hara [20], and is therefore called the Hara free electron gas exchange (HFEGE) potential. It was successfully used for treatment of electron scattering by N_2 [12], CO_2 [21], and other targets [22, 23]. Systematic studies of the HFEGE approximation [12, 24] have shown that it strongly improves the results obtained in the static approximation without exchange, although at low electron energies the scattering cross sections might still differ from those incorporating exchange exactly by 50%. However, with the growth of energy the HFEGE results are improving fast. Further improvement can be achieved by enforcing the orthogonality of continuum orbitals to the occupied molecular orbitals [24].

Similarly, the treatment of the short-range correlations in electron or positron scattering by atoms and molecules can be based on the free electron gas model [25, 26]. The full correlation potential is then obtained by joining the short-range form with the long-range polarization potential which behaves as $-\alpha/(2r^4)$ at large projectile-target distances, where α is the dipole polarizability of the target. Alternatively, correlations can be included by using the potential

$$V_{\text{pol}}(r) = -\frac{\alpha}{2r^4} \left[1 - \exp(-(r/r_c)^6) \right] \quad (1)$$

where r_c is a parameter which can be adjusted by comparing calculated cross section with experimental or completely *ab initio* results. (For simplicity we write here the potential for electron-atom scattering which contains only the isotropic term). Similarly, for Ps-atom collisions we can use an empirical potential of the form

$$V_{\text{corr}}(R) = -\frac{C_W}{R^6} \left[1 - \exp(-(R/R_c)^8) \right] \quad (2)$$

where R is the distance between the center of mass of Ps and the center of mass of the target atom, and C_W is the van der Waals constant.

The problem with potentials (1) and (2) is that they can underestimate the short-range correlations due to uncertainty in the cut-off parameter. The ultimate choice of the cut-off parameter is often dictated by experiments, but this makes the whole calculation empirical and diminishes its physical significance, especially in the case of Ps scattering as compared to electron scattering, since the short-range electron-target interaction is typically dominated by the static potential, and for Ps scattering the static potential is zero. In addition, the effective cut-off parameter might be energy dependent. Some indication of this deficiency

can be observed in pseudopotential calculations [7] of Ps-H₂ scattering which employed the van der Waals potential in the form of Eq. (2). Whereas, with a physically reasonable choice of R_c , agreement with experiment is good at low Ps velocities below 1.5 a.u., the theoretical cross section decreases significantly for $v > 1.5$ a.u., whereas the experimental cross section remains basically flat. The same tendency was observed in preliminary results for Ps-N₂ scattering [9] which were obtained with the van der Waals potential (2). This might indicate that short-range correlations are not included properly.

In the present paper we generalize exchange and correlation potentials, developed for electron scattering, to Ps-molecule scattering and apply them in the next paper of this series to Ps-N₂ scattering [27]. Based on the results of the previous studies of the accuracy of the FEG approximation for electron scattering [12, 24], we assume that the same level of accuracy can be achieved in employing the FEG model for Ps scattering. Atomic units are used throughout unless stated otherwise.

II. EXCHANGE POTENTIAL FOR POSITRONIUM-MOLECULE SCATTERING

A. First-order perturbation theory

The Hara exchange potential [20] was derived for a free incident electron. We want to extend it to the electron bound in the Ps atom. Consider first the wavefunction describing Ps in the presence of a free electron in a Fermi sea. The unperturbed wavefunction has the form

$$\Psi(q_1, q_2, \mathbf{r}_p) = \frac{1}{\sqrt{2}} \left[\Psi^{(0)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_p) \chi_{m_1 m_2}(1, 2) - \Psi^{(0)}(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_p) \chi_{m_1 m_2}(2, 1) \right] \quad (3)$$

where q_1, q_2 are all electron coordinates including spin coordinates, $\mathbf{r}_1, \mathbf{r}_2$ are spatial electron coordinates, \mathbf{r}_p spatial positron coordinates, $\chi_{m_1 m_2}(1, 2)$ the electron part of the spin function (the inessential positron part is omitted), and

$$\Psi^{(0)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_p) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}_1} \Psi_{\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p) \quad (4)$$

where \mathbf{k} is the momentum of the electron in the Fermi sea, V is the normalization volume, and $\Psi_{\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p)$ is the wavefunction of Ps moving with the momentum \mathbf{p} ,

$$\Psi_{\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p) = \frac{1}{\sqrt{V}} e^{i\mathbf{p} \cdot \mathbf{R}_2} \psi_{100}(\boldsymbol{\rho}_2) \quad (5)$$

where $\psi_{100}(\boldsymbol{\rho}_1)$ is the Ps ground state,

$$\psi_{100}(\boldsymbol{\rho}) = \frac{e^{-\rho/2}}{(8\pi)^{1/2}}. \quad (6)$$

The coordinates \mathbf{R}_i , $\boldsymbol{\rho}_i$, $i = 1, 2$, are related to \mathbf{r}_i , \mathbf{r}_p by the transformation

$$\mathbf{R}_i = \frac{1}{2}(\mathbf{r}_i + \mathbf{r}_p), \quad \boldsymbol{\rho}_i = \mathbf{r}_i - \mathbf{r}_p.$$

The total Hamiltonian of the system can be written in two alternative forms

$$H = H_0(1) + H_{\text{Ps}}(2) - \frac{1}{r_{1p}} + \frac{1}{r_{12}}$$

or

$$H = H_0(2) + H_{\text{Ps}}(1) - \frac{1}{r_{2p}} + \frac{1}{r_{12}}$$

where H_0 is the Hamiltonian of a free electron, and H_{Ps} is the Hamiltonian of the Ps. Note that the function $\Psi^{(0)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_p) \equiv \Psi_1^{(0)}$ is the eigenstate of the Hamiltonian $H_0(1) + H_{\text{Ps}}(2)$, and the function $\Psi^{(0)}(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_p) \equiv \Psi_2^{(0)}$ is the eigenstate of the Hamiltonian $H_0(2) + H_{\text{Ps}}(1)$ with the eigenvalue

$$E^{(0)} = \frac{k^2}{2} + \frac{p^2}{4} + \epsilon_1$$

where $\epsilon_1 = -0.25$ a.u. is the energy of the ground-state Ps. Therefore the expectation value of the Hamiltonian over the unperturbed state is

$$\langle \Psi | H | \Psi \rangle = E^{(0)} + \frac{1}{\sqrt{2}} \langle \Psi | -\frac{1}{r_{1p}} + \frac{1}{r_{12}} | \Psi_1^{(0)} \chi_{m_1 m_2}(1, 2) \rangle - \frac{1}{\sqrt{2}} \langle \Psi | -\frac{1}{r_{2p}} + \frac{1}{r_{12}} | \Psi_2^{(0)} \chi_{m_1 m_2}(2, 1) \rangle.$$

Both contributions to the energy correction in the right-hand side are identical, therefore the correction can be written as

$$E^{(1)} = \langle \Psi_1^{(0)} | -\frac{1}{r_{1p}} + \frac{1}{r_{12}} | \Psi_1^{(0)} \rangle - \langle \Psi_2^{(0)} \chi_{m_1 m_2}(2, 1) | -\frac{1}{r_{1p}} + \frac{1}{r_{12}} | \Psi_1^{(0)} \chi_{m_1 m_2}(1, 2) \rangle.$$

The first (direct) contribution gives zero result because the integrand is odd under interchange of \mathbf{r}_2 and \mathbf{r}_p . This is a particular case of a general result: interaction of any system of charges with Ps averaged over the Ps density distribution is zero. In particular, the static Ps-atom interaction is zero. The second (exchange) contribution is reduced to the integral

$$E^{(1)} = -\frac{\delta_{m_1 m_2}}{V} \int e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \Psi_{\mathbf{p}}^*(\mathbf{r}_1, \mathbf{r}_p) \Psi_{\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p) \left(\frac{1}{r_{12}} - \frac{1}{r_{1p}} \right) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_p.$$

As expected, it is nonzero only for $m_1 = m_2$.

We add now summation over all electrons below the Fermi level which have the same spin direction as the electron in Ps. This leads to the following expression for the exchange energy E_{ex} in the first order of the perturbation theory

$$E_{\text{ex}} = -\frac{1}{V^2} \sum_{\mathbf{k}} \int e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} e^{i\mathbf{p}\cdot(\mathbf{R}_2-\mathbf{R}_1)} \psi_{100}(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_2) \left(\frac{1}{r_{12}} - \frac{1}{r_{1p}} \right) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_p$$

Using the transformation

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1, \quad \boldsymbol{\rho}_1 = \mathbf{r}_1 - \mathbf{r}_p, \quad \mathbf{r}'_p = \mathbf{r}_p$$

whose Jacobian equals 1, and integrating over \mathbf{r}'_p , we obtain

$$E_{\text{ex}} = -\frac{1}{V} \sum_{\mathbf{k}} \int e^{-i\mathbf{k}\cdot\mathbf{r} + i\mathbf{p}\cdot\mathbf{r}/2} \psi_{100}(\rho_1) \psi_{100}(|\boldsymbol{\rho}_1 + \mathbf{r}|) \left(\frac{1}{r} - \frac{1}{\rho_1} \right) d\mathbf{r} d\boldsymbol{\rho}_1$$

Perform now summation over \mathbf{k} :

$$\frac{1}{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{(2\pi)^3} \int d\hat{\mathbf{k}} \int_0^{k_F} e^{i\mathbf{k}\cdot\mathbf{r}} k^2 dk = \frac{k_F^2}{2\pi^2 r} j_1(k_F r)$$

where k_F is the Fermi momentum. and j_1 is the spherical Bessel function. Therefore

$$E_{\text{ex}} = - \int \frac{k_F^2}{2\pi^2 r} j_1(k_F r) e^{i\mathbf{p}\cdot\mathbf{r}/2} \psi(\rho_1) \psi(|\boldsymbol{\rho}_1 + \mathbf{r}|) \left(\frac{1}{r} - \frac{1}{\rho_1} \right) d\mathbf{r} d\boldsymbol{\rho}_1. \quad (7)$$

This result does not depend on the Ps position due to uniformity of the electron gas. For collisions with atomic and molecular targets k_F can be made coordinate-dependent by the use of the Thomas-Fermi model, and this is what makes the exchange energy dependent on the projectile coordinate (Hara prescription [20]). According to this approach, k_F in expression (7) should be taken at the coordinate $\mathbf{R}_1 + \boldsymbol{\rho}_1/2$ for the electron part of the interaction and at the coordinate $\mathbf{R}_1 - \boldsymbol{\rho}_1/2$ for the Ps part of interaction where the coordinate dependence of k_F is given by

$$k_F(\mathbf{r}) = [3\pi^2 n(\mathbf{r})]^{1/3}$$

where $n(\mathbf{r})$ is the electron number density in the target. However, such a substitution in the integrand of Eq. (7) would be inconsistent since until now we assumed that \mathbf{k} is a position-independent wavevector in the plane wave. Indeed such a substitution would lead to a complex exchange energy which is physically unjustified. Instead we will assume that k_F is a slowly varying function of coordinates and take it at the center of the Ps atom corresponding to the average position of electron and positron in Ps. This ansatz is justified

due to the weak dependence of k_F on the number density n . Near the nuclei n varies with \mathbf{r} rather rapidly, and $k_F(\mathbf{r})$ dependence might become significant. However, at low projectile energies which we are mostly interested in, the short-range part of the interaction does not affect partial cross sections except possibly the s -wave contribution. This could create some error in the Σ_g contribution to the scattering cross section.

For calculation of the integral we use the explicit form of the ground-state Ps wavefunction, Eq. (6), and perform the expansions

$$e^{-|\mathbf{r}+\boldsymbol{\rho}_1|/2} = \sum_l (2l+1) F_l(r, \rho_1) P_l(\cos \theta_{r-\rho_1}) \quad (8)$$

$$e^{i\mathbf{p}\cdot\mathbf{r}/2} = \sum_l i^l (2l+1) j_l(pr/2) P_l(\cos \theta_{pr}) \quad (9)$$

where θ_{pr} is the angle between vectors \mathbf{r} and \mathbf{p} , $\theta_{r-\rho_1}$ is the angle between vectors \mathbf{r} and $-\boldsymbol{\rho}_1$, P_l is Legendre polynomial, and F_l is the function introduced in Ref. [5]:

$$F_l(r_1, r_2) = (-1)^{l+1} \frac{d}{d\kappa} \left[\kappa \hat{h}_l(\kappa r_>) \hat{j}_l(\kappa r_<) \right] \Big|_{\kappa=1/2}.$$

Here $r_<$, $r_>$ are less and greater of r_1 , r_2 , and \hat{h}_l , \hat{j}_l are real functions which can be expressed in terms of spherical Bessel functions as

$$\hat{h}_l(x) = -i^l h_l^{(1)}(ix), \quad \hat{j}_l(x) = i^l j_l(ix).$$

Integration over angles is performed using

$$\int P_l(\cos \theta_{pr}) P_{l'}(\cos \theta_{r-\rho_1}) d\hat{\mathbf{r}} d\hat{\boldsymbol{\rho}}_1 = (4\pi)^2 \delta_{l0} \delta_{l'0}.$$

Finally we obtain

$$E_{\text{ex}} = -\frac{k_F^2}{\pi} \int e^{-\rho/2} j_1(k_F r) j_0(pr/2) F_0(r, \rho) (\rho - r) \rho dr d\rho. \quad (10)$$

B. Choice of Ps momentum

When the projectile interacts with the target, its momentum is not equal to the incident momentum at infinity p . Hara, when deriving the free-electron-gas exchange potential, assumed that the potential acting on the incident electron is the same as the potential acting on the electron in the Fermi gas. This resulted in the following effective momentum p^* [20]

$$p^* = \sqrt{2E^*}, \quad E^* = E + E_F + I \quad (11)$$

where E is the energy of the incident electron, $E_F = k_F^2/2$ is the Fermi energy, and I is the ionization potential. The dependence of p^* on the distance R between the projectile and the target is due to dependence of the Fermi momentum on the electron density. Riley and Truhlar [22] argued that this expression becomes inconsistent at the infinite projectile-target separation where, according to Eqs. (11), $E^* = E + I$ whereas the correct relation should be $E^* = E$. Therefore they suggested using instead what they called the “asymptotically-adjusted” relation between E^* and E ,

$$E^* = E + E_F.$$

Neither expression would work for Ps as a projectile since the potential experienced by Ps is different from that experienced by an electron. It would be more consistent to assume

$$E^* = E - E_{\text{ex}}, \quad p^* = \sqrt{4E^*} \quad (12)$$

where $E = p^2/4$ is the kinetic energy of the incident Ps. However, calculation of $E_{\text{ex}}(R)$ requires the effective momentum as an input. Therefore an iterative procedure has been developed. We start with $p^* = p$, calculate E_{ex} from Eq. (10) and E^* from Eq. (12), and repeat the same calculation until the change in E_{ex} between two iterations is small enough. This method works quite well for sufficiently large E_{ex} . If it is too small, the integration error is becoming too large at higher iteration steps. This typically occurs at small k_F , corresponding to large distances R , where E_{ex} calculated with $p^* = p$ seems to be sufficient. At $k_F > 1$ the difference between E_{ex} calculated with different values of p^* starts to increase, but even at $k_F = 2.8$ it is only about 10%.

C. Exchange energies

In Fig. 1 we present the exchange energy as a function of the Fermi momentum k_F for several Ps momenta p which were chosen to be nonmodified. It is interesting to discuss the sign of the exchange energy. It is well known that, due to the Pauli exclusion principle, electron interaction with the electron gas results in the “Fermi hole” [28, 29] which creates an effective attraction between the individual electron and electron gas, therefore the exchange energy is negative. The same hole creates an effective repulsion between the positron in Ps and the gas. However, the electron and positron motion in Ps are correlated in such a way

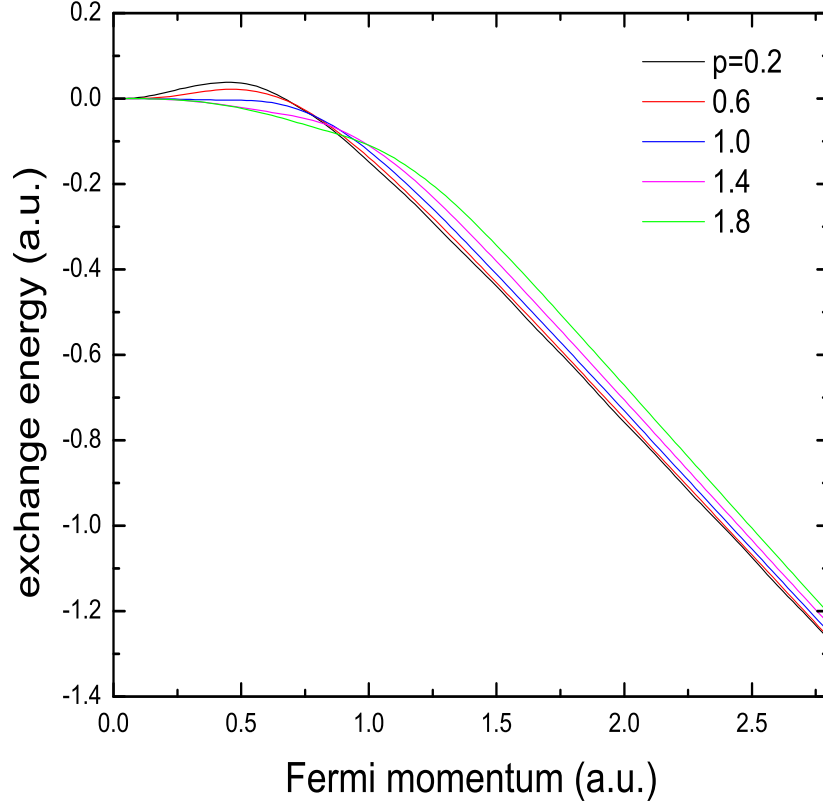


FIG. 1: (Color online) FEG exchange energy as a function of the Fermi momentum k_F for several Ps momenta p

that the net energy is in most cases negative, although with some exceptions. As can be observed from the figure, at $p < 1$ a.u. and $k_F < 0.6$ a.u. the net exchange energy becomes positive. This means that at low incident momenta and large distances there is an effective repulsion between Ps and the target. However, typically this repulsion is small compared to the van der Waals interaction, therefore the net Ps-target interaction is still attractive.

To show the role of $e - e$ interaction in the exchange energy, in Fig. 2 we compare the total exchange energy with the $e - e$ contribution. It confirms that the $e - e$ interaction is dominant.

It is also apparent from Fig. 1 that the dependence of the E_{ex} on the Ps momentum p is weak, therefore the exchange potential should not be very sensitive to the exact choice of p .

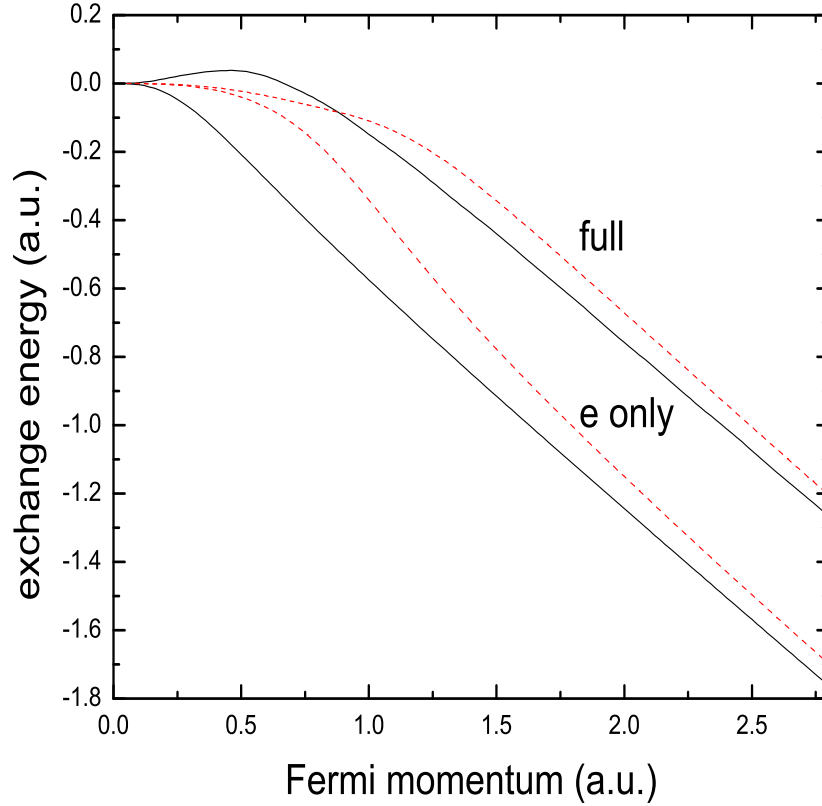


FIG. 2: (Color online) Full FEG exchange energy (upper curves) compared with the $e - e$ contribution (lower curves). Solid curves: $p = 0.2$ a.u., dashed curves: $p = 1.8$ a.u.

In Fig. 3 we present comparison of exchange energy, calculated with the original Ps momentum p , with the energy calculated with the adjusted momentum given by Eq. (12). As in the case of Hara potential, the adjustment decreases the absolute value of the exchange energy. However, in the present case this change is significantly smaller than in the case of electron scattering because of the relative weakness of the Ps-molecule interaction.

III. FEG CORRELATION ENERGY

Inclusion of short-range correlations in lepton-atom scattering is a very challenging task. One way to do this is to calculate the second-order correction to the projectile energy in

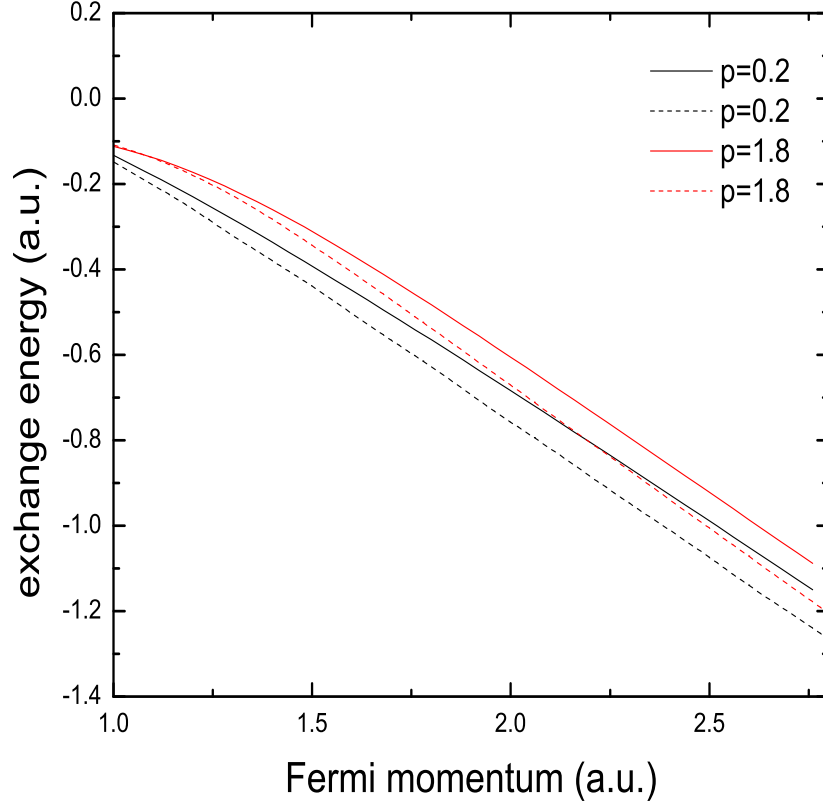


FIG. 3: (Color online) FEG exchange energy as a function of the Fermi momentum k_F calculated with the modified Ps momenta for several Ps momenta p^* , Eq. (12) (solid lines) and nonmodified momenta (dashed lines) for $p = 0.2$ and $p = 1.8$.

a free electron gas. It is well known (see, e.g., Ref. [30]) that in the case of the projectile electron this correction is diverging due to the singularity of the Coulomb potential at low momentum transfer, and it is necessary to go to higher-order perturbation theory. In particular in the high-density approximation it is possible to sum all ring diagrams [31] and obtain the correction equivalent to the random-phase approximation of Bohm and Pines [32]. In what follows below we will show that for Ps the second-order correction is not diverging, and will obtain formulas for its evaluation.

A. Second-order correction

We start again with the unperturbed wavefunction describing Ps and a free electron in a Fermi sea, Eq. (3).

We will include now the virtual excitations of Ps, therefore we replace Eqs. (4), (5) by

$$\Psi^{(0)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_p) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}_1} \Psi_{nlm\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p)$$

and

$$\Psi_{nlm\mathbf{p}}(\mathbf{r}_2, \mathbf{r}_p) = \frac{1}{\sqrt{V}} e^{i\mathbf{p} \cdot \mathbf{R}_2} \psi_{nlm}(\boldsymbol{\rho}_2)$$

where $\psi_{nlm}(\boldsymbol{\rho}_1)$ is the Ps wavefunction in the state with the principal quantum number n , orbital angular momentum l and its projection m . The eigenvalues of the unperturbed Hamiltonian are

$$E_{n\mathbf{p}\mathbf{k}} = \frac{k^2}{2} + \frac{p^2}{4} + \epsilon_n$$

where ϵ_n is the energy of the Ps in the state $\{nlm\}$.

The second-order correction to the ground-state Ps energy interacting with an electron in the Fermi sea is

$$E_{1\mathbf{p}\mathbf{k}}^{(2)} = \sum_{nlm\mathbf{p}'\mathbf{k}'m'_1m'_2} \frac{|\langle nlm\mathbf{p}'\mathbf{k}' | H' | 100\mathbf{p}\mathbf{k} \rangle|^2}{E_{1\mathbf{p}\mathbf{k}} - E_{n\mathbf{p}'\mathbf{k}'} + i\eta} \quad (13)$$

where H' is the perturbation

$$H' = \frac{1}{r_{12}} - \frac{1}{r_{2p}},$$

summation is restricted to electron energies above the Fermi level, $k' > k_F$, and the infinitesimal $i\eta$ in the denominator provides outgoing-wave boundary condition in the inelastic channels. The total Ps correlation energy is

$$E_{1\mathbf{p}}^{\text{corr}} = \sum_{\mathbf{k}} E_{1\mathbf{p}\mathbf{k}}^{(2)}$$

where the summation is over the occupied states below the Fermi level, $k < k_F$.

Due to the antisymmetry of the wavefunction with respect to interchange of q_1 and q_2 , the matrix element of the perturbation H' is reduced to two terms, the direct and exchange terms. The direct term has the form

$$M_{\text{dir}} = \frac{\delta_{m_1 m'_1} \delta_{m_2 m'_2}}{V^2} \int e^{i\mathbf{R}_1 \cdot \mathbf{Q}} e^{i\mathbf{r}_2 \cdot \mathbf{q}} \psi_{nlm}^*(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_1) \left(\frac{1}{r_{12}} - \frac{1}{r_{2p}} \right) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_p \quad (14)$$

where $\mathbf{Q} = \mathbf{p} - \mathbf{p}'$, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. Due to the symmetry properties of the Ps wavefunction under the inversion

$$\psi_{nlm}^*(-\boldsymbol{\rho})\psi_{100}(-\boldsymbol{\rho}) = (-1)^l \psi_{nlm}^*(\boldsymbol{\rho})\psi_{100}(\boldsymbol{\rho})$$

the integrand is odd under interchange of \mathbf{r}_1 and \mathbf{r}_p , if l is even, therefore the integral is nonzero only for odd l .

Perform now integration over \mathbf{r}_2 :

$$\begin{aligned} \int \frac{e^{i\mathbf{r}_2 \cdot \mathbf{q}}}{r_{12}} d\mathbf{r}_2 &= e^{i\mathbf{r}_1 \cdot \mathbf{q}} \frac{4\pi}{q^2} \\ \int \frac{e^{i\mathbf{r}_2 \cdot \mathbf{q}}}{r_{2p}} d\mathbf{r}_2 &= e^{i\mathbf{r}_p \cdot \mathbf{q}} \frac{4\pi}{q^2} \end{aligned}$$

Then

$$M_{dir} = \frac{4\pi\delta_{m_1m'_1}\delta_{m_2m'_2}}{V^2q^2} \int e^{i\mathbf{Q} \cdot \mathbf{R}_1} \psi_{nlm}^*(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_1) (e^{i\mathbf{q} \cdot \mathbf{r}_1} - e^{i\mathbf{q} \cdot \mathbf{r}_p}) d\mathbf{R}_1 d\mathbf{r}_p.$$

Changing now integration variables to $\boldsymbol{\rho}_1$ and \mathbf{R}_1 , we obtain

$$M_{dir} = \frac{4\pi\delta_{m_1m'_1}\delta_{m_2m'_2}}{V^2q^2} \int \psi_{nlm}^*(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_1) (e^{i\mathbf{q} \cdot (\mathbf{R}_1 + \boldsymbol{\rho}_1/2)} - e^{i\mathbf{q} \cdot (\mathbf{R}_1 - \boldsymbol{\rho}_1/2)}) e^{i\mathbf{Q} \cdot \mathbf{R}_1} d\mathbf{R}_1 d\boldsymbol{\rho}_1.$$

Integration over \mathbf{R}_1 leads to the conservation of momentum, $\mathbf{Q} + \mathbf{q} = 0$, and we obtain

$$M_{dir} = \frac{8\pi i \delta_{m_1m'_1} \delta_{m_2m'_2} \delta_{\mathbf{P}\mathbf{P}'}}{Vq^2} \int \sin(\mathbf{q} \cdot \boldsymbol{\rho}_1/2) \psi_{nlm}^*(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_1) d\boldsymbol{\rho}_1 \quad (15)$$

where $\mathbf{P} = \mathbf{p} + \mathbf{k}$. The square modulus of this matrix element can be expressed through the atomic form factor

$$F_n(q) = \sum_{lm} \left| \int \sin(\mathbf{q} \cdot \boldsymbol{\rho}_1/2) \psi_{nlm}^*(\boldsymbol{\rho}_1) \psi_{100}(\boldsymbol{\rho}_1) d\boldsymbol{\rho}_1 \right|^2 \quad (16)$$

which appears in the expression of many collision cross sections in terms of momentum transfer [33], for example in the Born approximation. Methods of its evaluation were reviewed by Beigman and Lebedev [33]. However, for our purposes it is more convenient to use the method developed in Appendix A.

Summation over \mathbf{k} and \mathbf{k}' can be replaced by summation over \mathbf{k} and \mathbf{q} . Then in the denominator of Eq. (13)

$$\frac{k^2 - (k')^2}{2} + \frac{p^2 - (p')^2}{4} = -\frac{3}{4}q^2 + \mathbf{q} \cdot (\mathbf{k} - \frac{1}{2}\mathbf{p})$$

and

$$E_{1\mathbf{p}}^{\text{corr}} = \frac{2(8\pi)^2}{V^2} \sum_{k < k_F} \sum_{|\mathbf{k}-\mathbf{q}| > k_F} \sum_n \frac{F_n(q)}{q^4 \left(-\frac{3}{4}q^2 + \mathbf{q} \cdot (\mathbf{k} - \frac{1}{2}\mathbf{p}) + \epsilon_1 - \epsilon_n + i\eta \right)},$$

where we have summed over m'_1, m'_2 and included an extra factor 2 due to sum over spin states below the Fermi level.

Using the standard switching from summation over wavevectors to integration, we obtain

$$E_{1\mathbf{p}}^{\text{corr}} = \frac{2}{\pi^4} \sum_n \int d^3k \int d^3q \frac{F_n(q) \theta(|\mathbf{k} - \mathbf{q}| - k_F) \theta(k_F - k)}{q^4 \left(-\frac{3}{4}q^2 + \mathbf{q} \cdot (\mathbf{k} - \frac{1}{2}\mathbf{p}) + \epsilon_1 - \epsilon_n + i\eta \right)}. \quad (17)$$

where we have introduced step (Heaviside) functions to account for the constraints on the integration region. Since $F_n(q)$ behaves as q^2 near the origin, the integral is convergent in q (in contrast to what happens with the free electron correlation energy). The nontrivial integration variables here are q , k , $\cos \zeta$, and $\cos \theta$, where ζ is the angle between \mathbf{k} and \mathbf{q} , and θ is the angle between \mathbf{p} and \mathbf{q} . Angular integration and integration in k can be performed analytically, as shown in Appendix B, and calculation of $E_{1\mathbf{p}}^{\text{corr}}$ is reduced to numerical integration in q and summation over n .

Eq. (17) includes only the direct term. Calculation of the exchange-correlation term is a much more formidable task, and we have neglected it in the present work. A justification for this approximation can be found in the recent paper of Green *et al.* [19] who used the diagram technique to calculate the correlation energy in Ps-atom interaction. In particular they showed that the main contribution to the correlation energy is given by the direct electron-hole loop diagram, and it provides the required van der Waals asymptotic form for the correlation potential. On the other hand, the two leading contributions to the exchange-correlation correction partly cancel each other, therefore the total exchange-correlation contribution can be neglected.

In accordance with the Thomas-Fermi model, the correlation energy can be used for description of Ps-target correlation potential if k_F is considered as a function of the projectile position \mathbf{R} , similar to the method used in electron-atom and electron-molecule scattering. Outside the target where $n(\mathbf{R})$ and $k_F(\mathbf{R})$ become small, the energy is matched with the van der Waals interaction $-C_W/R^6$. This approach is similar to that used in electron-molecule collisions [25, 26] where the correlation potential is matched to its long-range part $-\alpha/(2r^4)$ outside the target.

B. Results for FEG correlation energy

In specific calculations we kept a finite sum in n in Eq. (17) and neglected completely the integral over the Ps continuum. Calculations show that sum in n is convergent reasonably well, although sometimes n up to 20 should be included. Physically it is also clear that highly-excited Rydberg states of Ps should not contribute because of the screening effects which are not accounted for in the second-order perturbation theory. Some discussion of the screening effects is given in Sec. IV. At large Ps-target distances the screening effects become negligible, and the complete sum in all Ps eigenstates, including integration over the Ps continuum, should be included. However, outside the target we match the correlation energy with the van der Waals interaction with the proper van der Waals constant. In this way we incorporate the effect of the Ps continuum implicitly.

In Fig. 4 we present the real part of the correlation energy as a function of the Fermi momentum. As in the case of the exchange energy, the dependence on Ps momentum p is weak.

Calculations also show that the imaginary part of the correlation energy is negligible in the domain $p < 2$ a.u., $k_F < 3$ a.u. Mathematically this means that the denominator in Eq. (17) turns to zero for such values of q where the numerator, $F_n(q)$, is small. Physically this corresponds to insignificance of the inelastic channels, electron-hole excitations and excitations of Ps. For higher momenta $\text{Im}E^{\text{corr}}$ starts to grow. The most important inelastic channel in Ps-atom and Ps-molecule collisions is the Ps ionization which can be included explicitly by impulse [34] or binary-encounter [7, 8] approximations. In the present application of the method to Ps-N₂ collisions [27] we neglect $\text{Im}E^{\text{corr}}$ and calculate the contribution of the Ps ionization channel explicitly.

IV. SCREENING EFFECTS

A. Review of the electron gas theory

Screening effects play an important role in the theory of the electron gas. The electron self-energy in the electron gas is divergent in the second-order perturbation theory [31], and only accounting for screening effects makes it finite [30]. We will summarize the results for electron gas first.

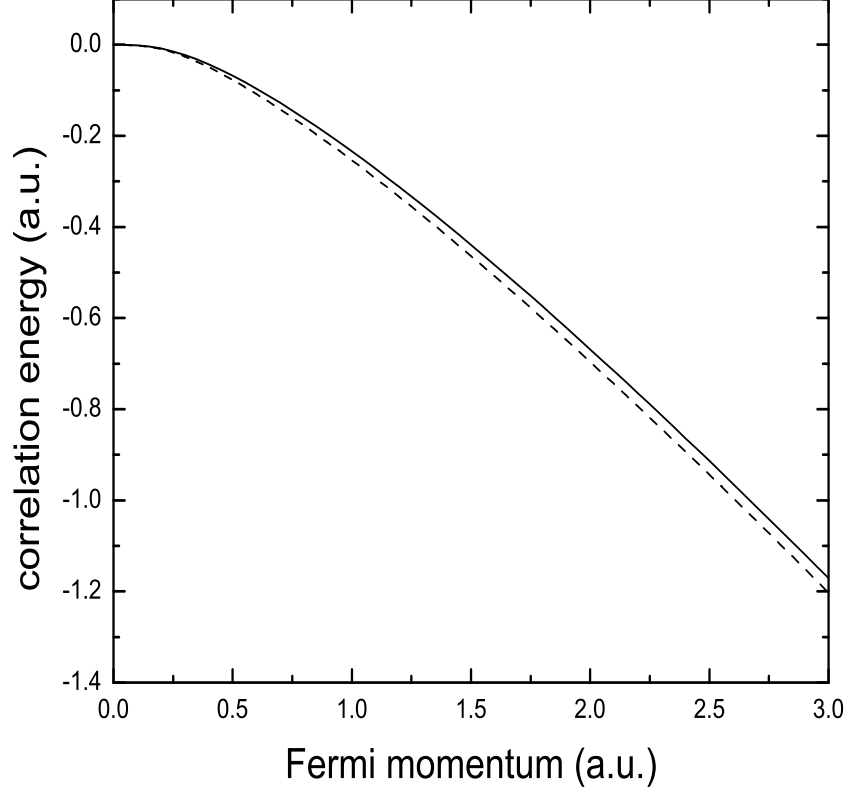


FIG. 4: Correlation energy for Ps in an electron gas as a function of the Fermi momentum k_F . Solid line, Ps momentum $p = 0.2$ a.u. Dashed line, $p = 1.0$ a.u.

The electron-electron Coulomb interaction in momentum space

$$V(\mathbf{q}) = \frac{4\pi}{q^2}, \quad \mathbf{q} = \mathbf{k} - \mathbf{k}' \quad (18)$$

with account of screening is modified as

$$V_s(\mathbf{q}) = \frac{4\pi}{q^2 + \xi^2}$$

where ξ is the screening constant. Generally, if the external perturbation is time-dependent, it depends on q and frequency ω , but in the static approximation

$$\xi^2(q) = \frac{2k_F}{\pi} \left[1 - \left(\frac{1}{q} - \frac{1}{4}q \right) \ln \left| \frac{1 - q/2}{1 + q/2} \right| \right].$$

In the limit $q \rightarrow 0$ we get the Thomas-Fermi screening constant [31, 32]

$$\xi_{\text{TF}}^2 = \frac{4k_F}{\pi}.$$

The Fourier transform of $V_s(q)$ with q -independent Thomas-Fermi screening constant produces the Yukawa potential. However, when q -dependence of ξ is taken into account, the dependence of $V_s(r)$ on r is more complicated: at large r it decays as $1/r^3$ with superimposed oscillations (Friedel oscillations [35]):

$$V_s(r) = \text{const} \cdot \frac{\cos(2k_F r)}{r^3}.$$

Calculations of the electron exchange energy E_{ex} accounting for screening show a significant reduction of E_{ex} , but the results obtained with the Thomas-Fermi screening constant and dynamical screening constant are very close to each other.

B. Electron exchange and correlations in Ps-atom scattering

Calculation of screening effects in Ps interaction with an electron gas is a much more challenging task than calculation of screening effects for a point charge. If the q -dependence of the screening constant is not important, we can assume that the electron or positron in Ps interacts with an electron in the Fermi gas by the potential

$$V_s(r) = -Z \frac{e^{-\xi r}}{r}$$

where $Z = -1$ for electron, and $Z = 1$ for positron. However, such an approach would be very approximate, if not wrong, since it treats polarization of the electron gas due to the electron and positron in Ps independently.

Regarding the Ps self-energy, the second-order correction gives a finite result, as was discussed above. A simple replacement of the Coulomb potential by the screened potential in Eq. (14) produces an unrealistically small correlation energy. It is clear, though, from the discussion above that such a substitution would be inconsistent: it accounts for screening in interaction of the Ps electron with the Fermi gas and Ps positron with the Fermi gas, but not for screening in interaction between Ps electron and positron. It is obvious that a consistent account of screening in Ps interaction with the electron gas requires a much more advanced theory. On the other hand, Green *et al* [19], using the diagram technique, found

that the lowest-order diagram describing creation of electron-hole pair, is sufficient for an adequate description of Ps-atom scattering. This lowest-order diagram corresponds to our correlation energy E^{corr} . Generally, it is reasonable to assume that since Ps is a neutral system, the screening effect in this case will not be as significant as for an electron, as is apparent from comparison of the Fourier transform of the Coulomb potential, Eq. (18) with the Fourier transform of the Ps-electron interaction, Eq. (15).

V. CONCLUSION

In conclusion we have constructed new FEG exchange and correlation energies allowing us to describe more completely these effects as compared to our previous treatment of exchange and correlations in Ps-atom and Ps-molecule scattering. The major difference in methods used in [5, 8] and the present is that in Refs. [5, 8] we constructed a pseudopotential for the projectile-target interaction using the electron and positron scattering phase shifts whereas in the present method is based on the FEG exchange and correlation potentials without adding a repulsive core mocking the orthogonality condition. Whereas the present method is more direct in the sense that it does not require electron and positron scattering data, it includes exchange and correlation effects approximately by modeling the target electrons as a free electron gas. In the next paper of this series [27] we apply the method developed in the present paper to the problem of Ps-N₂ scattering and show that the new method describes well the resonant Ps-N₂ scattering and high-energy behavior of the total cross section.

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Appendix A. Hydrogen-like formfactors

For calculation of Ps formfactors, Eq. (16), we start with the integral

$$I_{nl} = \int e^{i\mathbf{q}\cdot\boldsymbol{\rho}/2} \psi_{nlm}^*(\boldsymbol{\rho}) \psi_{100}(\boldsymbol{\rho}) d\boldsymbol{\rho}.$$

This has a nonzero value only for $m = 0$, if we direct the quantization axis along the momentum transfer \mathbf{q} .

Expanding the plane wave in spherical harmonics and using the standard expressions for the hydrogen-like wavefunctions:

$$\psi_{nlm}(\boldsymbol{\rho}) = \frac{u_{nl}(\rho)}{\rho} Y_{lm}(\hat{\rho})$$

$$u_{nl}(\rho) = N_{nl} x^{l+1} e^{-x/2} F(l+1-n, 2l+2, x), \quad x = \frac{2\rho}{na_0}$$

where F is the confluent hypergeometric function, a_0 is the Bohr radius for the hydrogenlike system (for Ps $a_0 = 2$ a.u.), and N_{nl} is the normalization constant

$$N_{nl} = \frac{1}{(2l+1)!} \left[\frac{(n+l)!}{2n(n-l-1)!} \right]^{1/2} \left(\frac{2}{na_0} \right)^{l+3/2}.$$

Then

$$I_{nl} = i^l (2l+1)^{1/2} \int j_l(q\rho/2) u_{nl}(\rho) u_{10}(\rho) d\rho$$

where j_l is the spherical Bessel function. Since only the imaginary part of I_{nl} contributes to the formfactor, Eq. (16), we are interested only in odd values of l .

Use now the polynomial representation of F

$$F(-n_r, 2l+2, x) = \sum_{k=0}^{n_r} \frac{(-n_r)_k}{k!(2l+2)_k} x^k, \quad n_r = n-l-1$$

and the integral [36]

$$\int_0^\infty \rho^{l+k+3/2} \exp\left[-\frac{\rho}{a_0} \left(1 + \frac{1}{n}\right)\right] J_{l+1/2}(q\rho/2) d\rho = a_0^{l+k+5/2} \frac{\Gamma(2l+k+3)(qa_0/4)^{l+1/2}}{y^{2l+k+3}\Gamma(l+3/2)} {}_2F_1\left(l + \frac{k+3}{2}, -\frac{k+1}{2}; l + \frac{3}{2}; z\right) \quad (19)$$

where

$$y^2 = \left(1 + \frac{1}{n}\right)^2 + \frac{1}{4}q^2 a_0^2, \quad z = \frac{q^2 a_0^2}{4y^2}$$

and ${}_2F_1$ is the Gauss's hypergeometric function.

Then we obtain

$$I_{nl} = \frac{i^l}{(2l+1)!\Gamma(l+3/2)} \left[\frac{\pi(2l+1)(n+l)!}{2nn_r!} \right]^{1/2} \left(\frac{qa_0}{4} \right)^l \sum_{k=0}^{n_r} \frac{(-n_r)_k}{k!(2l+2)_k} \left(\frac{2}{n} \right)^{k+l+3/2} \frac{\Gamma(2l+k+3)}{y^{2l+3+k}} {}_2F_1\left(l + \frac{k+3}{2}, -\frac{k+1}{2}; l + \frac{3}{2}; z\right). \quad (20)$$

The hypergeometric function can be reduced to a polynomial. If k is odd, $k = 2m + 1$, $m = 0, 1, \dots$, then the hypergeometric series is truncated as

$${}_2F_1(l + m + 2, -(m + 1); l + 3/2; z) = \sum_{s=0}^{m+1} \frac{(l + m + 2)_s (-m - 1)_s}{(l + 3/2)_s s!} z^s.$$

If k is even, $k = 2m$, we use [36]

$${}_2F_1(a, b; c; z) = (1 - z)^{-b} {}_2F_1\left(c - a, b; c; \frac{z}{z - 1}\right).$$

Then

$${}_2F_1\left(l + m + \frac{3}{2}, -m - \frac{1}{2}; l + \frac{3}{2}; z\right) = (1 - z)^{m+1/2} \sum_{s=0}^m \frac{(-1)^s (-m)_s (-m - 1/2)_s}{s! (l + 3/2)_s} \left(\frac{z}{1 - z}\right)^s.$$

Appendix B. Calculation of correlation energy

To calculate the correlation energy, we start first with Eq. (17) and perform integration over orientation of the vector \mathbf{k} in the coordinate system with the polar axis along vector \mathbf{q} . The integral is reduced to

$$I_1(\mathbf{q}, \mathbf{k}) = 2\pi \int_{-1}^{x_{\max}} \frac{dx}{qkx + t(\mathbf{q})}$$

where $t(\mathbf{q}) = -3q^2/4 - \mathbf{q} \cdot \mathbf{p}/2 + \epsilon_1 - \epsilon_n + i\eta$. The upper integration limit x_{\max} is determined from the constraint $|\mathbf{k} - \mathbf{q}| > k_F$ which leads to

$$x = \cos \zeta < \beta(q, k)$$

where

$$\beta(q, k) = \frac{k^2 + q^2 - k_F^2}{2kq}$$

Therefore

$$x_{\max} = \min[1, \beta(q, k)]. \quad (21)$$

To find the right-hand-side in Eq. (21), we look for a domain in the (q, k) plane where $\beta(q, k) < 1$. This occurs for

$$k - k_F < q < k + k_F.$$

Since $k < k_F$, this constraint is simply reduced to $q < k + k_F$. Look now for the domain where $\beta(q, k) < -1$. This occurs if $q < k_F - k$. In summary

$$I_1(\mathbf{q}, \mathbf{k}) = \frac{2\pi}{qk} \left[\theta(k + k_F - q) \ln \frac{\beta(q, k) + t(\mathbf{q})/qk}{-1 + t(\mathbf{q})/qk} + \theta(q - k - k_F) \ln \frac{1 + t(\mathbf{q})/qk}{-1 + t(\mathbf{q})/qk} \right] \text{ if } k > k_F - q$$

and

$$I_1(\mathbf{q}, \mathbf{k}) = 0 \quad \text{if } k < k_F - q.$$

Here and below \ln is defined as analytic function with the branch cut along the negative real axis and with the account of $\text{Im}t > 0$. Perform now integration over orientation of \mathbf{q} in the coordinate system with the polar vector along \mathbf{p} . Since

$$t(\mathbf{q}) = s(q) - qpy/2, \quad y = \cos \theta, \quad s(q) = -3q^2/4 + \epsilon_1 - \epsilon_n + i\eta,$$

the integration is reduced to

$$I_2(q, k) = \frac{(2\pi)^2}{qk} \int_{-1}^1 dy \left[\theta(k + k_F - q) \ln \frac{2k/p + v - y}{v - 2k/p - y} + \theta(q - k - k_F) \ln \frac{u(q) + k^2/pq - y}{v - 2k/p - y} \right]$$

where

$$u(q) = \frac{q^2 - k_F^2 + 2s(q)}{pq}, \quad v(q) = \frac{2s(q)}{pq}$$

Using the integral

$$\lambda(a) \equiv \int_{-1}^1 \ln(y - a) dy = (1 - a) \ln(1 - a) + (1 + a) \ln(-1 - a) - 2$$

we obtain

$$I_2(q, k) = \frac{(2\pi)^2}{qk} \left[\lambda \left(\frac{k^2}{pq} + u(q) \right) - \lambda \left(v - \frac{2k}{p} \right) \right] \quad \text{if } k > q - k_F, \quad (22)$$

$$I_2(q, k) = \frac{(2\pi)^2}{qk} \left[\lambda \left(v + \frac{2k}{p} \right) - \lambda \left(v - \frac{2k}{p} \right) \right] \quad \text{if } k < q - k_F. \quad (23)$$

Integration in the (q, k) plane can be organized now as

$$\begin{aligned} \int_0^\infty dq \int_0^{k_F} dk &= \int_0^{k_F} dq \int_{k_F - q}^{k_F} dk I_2'(q, k) + \int_{k_F}^{2k_F} dq \left(\int_0^{q - k_F} I_2''(q, k) + \int_{q - k_F}^{k_F} dk I'(q, k) \right) \\ &\quad + \int_{2k_F}^\infty dq \int_0^{k_F} dk I_2'' \end{aligned}$$

where for I_2' we use Eq. (22), and for I_2'' Eq. (23).

Integration in k can be performed using the following integrals

$$G_1(a, b, x) \equiv \int (ax^2 + bx) \ln(ax + b) dx = \left(\frac{1}{3}ax^3 + \frac{1}{2}bx^2 - \frac{b^3}{6a^2} \right) \ln(ax + b) - \frac{1}{9}ax^3 - \frac{1}{12}bx^2 + \frac{b^2}{6a}x$$

$$G_2(a, b, x) \equiv \int (ax^3 + bx) \ln(ax^2 + bx) dx = \left(\frac{1}{4}ax^4 + \frac{1}{2}bx^2 + \frac{b^2}{4a} \right) \ln(ax^2 + b) - \frac{1}{8}ax^4 - \frac{1}{4}bx^2$$

Finally

$$E_{100}^{\text{corr}} = \frac{8}{\pi^2} \sum_{n>1} \int_0^\infty \frac{dq}{q^3} F_n(q) G(q)$$

where

$$\begin{aligned} G(q) = & G_2(-(pq)^{-1}, 1 - u(q); k_F) - G_2(-(pq)^{-1}, 1 - u(q); k_F - q) \\ & - G_2(-(pq)^{-1}, -1 - u(q); k_F) + G_2(-(pq)^{-1}, -1 - u(q); k_F - q) \\ & - G_1(2p^{-1}, 1 - v(q); k_F) + G_1(2p^{-1}, 1 - v(q); k_F - q) \\ & + G_1(2p^{-1}, -1 - v(q); k_F) - G_1(2p^{-1}, -1 - v(q); k_F - q) \quad \text{if } 0 < q < k_F \end{aligned} \quad (24)$$

$$\begin{aligned} G(q) = & G_1(-2p^{-1}, 1 - v(q); q - k_F) - G_1(-2p^{-1}, -1 - v(q); q - k_F) \\ & - G_1(2p^{-1}, 1 - v(q); q - k_F) + G_1(2p^{-1}, -1 - v(q); q - k_F) \\ & + G_2(-(pq)^{-1}, 1 - u(q); k_F) - G_2(-(pq)^{-1}, 1 - u(q); q - k_F) \\ & - G_2(-(pq)^{-1}, -1 - u(q); k_F) + G_2(-(pq)^{-1}, -1 - u(q); q - k_F) \\ & - G_1(2p^{-1}, 1 - v(q); k_F) + G_1(2p^{-1}, 1 - v(q); q - k_F) \\ & + G_1(2p^{-1}, -1 - v(q); k_F) - G_1(2p^{-1}, -1 - v(q); q - k_F) \quad \text{if } k_F < q < 2k_F \end{aligned} \quad (25)$$

$$\begin{aligned} G(q) = & G_1(-2p^{-1}, 1 - v(q); k_F) - G_1(-2p^{-1}, -1 - v(q); k_F) \\ & - G_1(2p^{-1}, 1 - v(q); k_F) + G_1(2p^{-1}, -1 - v(q); k_F) \quad \text{if } q > 2k_F. \end{aligned} \quad (26)$$

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