Analytical asymptotic structure of the Kohn-Sham exchange potential at a metal surface

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In a recent paper we presented the analytical asymptotic structure of the Kohn-Sham exchange potential in the classically forbidden region at a metal-vacuum interface. This result is valid for self-consistently determined orbitals of the semi-infinite jellium and structureless-pseudopotential models of a metal surface. In this paper we provide the details of our derivation. The correctness of the analytical derivation is further substantiated through numerical work. [S0163-1829(97)09231-X]

In a recent paper,[1] we presented the *analytical* asymptotic structure of the exchange potential $\nu_x(\mathbf{r})$ component of the Kohn-Sham[2] (KS) density-functional theory[3] exchange-correlation potential $\nu_{\rm xc}(\mathbf{r})$ in the classically forbidden region of a metal-vacuum interface. The potentials $\nu_{\rm xc}(\mathbf{r})$ and $\nu_x(\mathbf{r})$ are defined as the functional derivatives $\delta E_{\rm xc}^{\rm KS}[\rho]/\delta\rho(\mathbf{r})$ and $\delta E_x^{\rm KS}[\rho]/\delta\rho(\mathbf{r})$ of the KS theory exchange-correlation $E_{\rm xc}^{\rm KS}[\rho]$ and exchange $E_x^{\rm KS}[\rho]$ energy functionals of the density $\rho(\mathbf{r})$, respectively. The asymptotic structure of $\nu_x(\mathbf{r})$, valid for the *self-consistent* orbitals of both the *semi-infinite* jellium[4,5] and structureless-pseudopotential[4,6] (stabilized-jellium) models, is image-potential-like of the form $-\alpha_{{\rm KS},x}(\beta)/x$, where x is the distance from the surface. The coefficient $\alpha_{{\rm KS},x}(\beta)$ depends upon the metal properties through the parameter $\beta=(W/\epsilon_F)^{1/2}$, where W is the surface-barrier height and ϵ_F the Fermi energy. For metallic densities corresponding to a Wigner-Seitz radius of $r_s=2-6$, the coefficient $\alpha_{{\rm KS},x}(\beta)$ varies from 0.195–0.274. For $\beta=2^{1/2}$, the coefficient $\alpha_{{\rm KS},x}(\beta)$ is exactly $\frac{1}{4}$, thereby leading to the classical image-potential structure for $\nu_x(\mathbf{r})$. The contrast of this result with the work of others[7–10] is discussed elsewhere.[1,11] We present in this paper only our derivation of the asymptotic structure of the potential $\nu_x(\mathbf{r})$.

The relationship between density-functional theory and many-body perturbation theory as established by Sham[3,7] is via the integral equation relating $\nu_{\rm xc}(\mathbf{r})$ to the nonlocal exchange-correlation component $\Sigma_{\rm xc}(\mathbf{r},\mathbf{r}';\omega)$ of the self-energy $\Sigma(\mathbf{r},\mathbf{r}';\omega)$. This equation is

$$\int d\mathbf{r}'\,\nu_{\rm xc}(\mathbf{r}')\int d\epsilon\; G_s(\mathbf{r},\mathbf{r}';\epsilon)G(\mathbf{r}',\mathbf{r};\epsilon) = \int\int d\mathbf{r}'\,d\mathbf{r}''\int d\epsilon\; G_s(\mathbf{r},\mathbf{r}';\epsilon)\Sigma_{\rm xc}(\mathbf{r}',\mathbf{r}'';\epsilon)G(\mathbf{r}'',\mathbf{r},\epsilon), \tag{1}$$

where $G(\mathbf{r},\mathbf{r}';\epsilon)$ is the one-particle Green function and $G_s(\mathbf{r},\mathbf{r}';\epsilon)$ the KS Green function. From this equation Sham[7] derived the asymptotic structure of $\nu_{\rm xc}(\mathbf{r})$ to be

$$\nu_{\rm xc}(\mathbf{r})=\frac{1}{2\Psi_{\mathbf{k}}(\mathbf{r})}\int d\mathbf{r}'\Sigma_{\rm xc}(\mathbf{r},\mathbf{r}';\epsilon_F)\Psi_{\mathbf{k}}(\mathbf{r}') + \frac{1}{2\Psi_{\mathbf{k}}^*(\mathbf{r})}\int d\mathbf{r}'\Psi_{\mathbf{k}}^*(\mathbf{r}')\Sigma_{\rm xc}(\mathbf{r}',\mathbf{r};\epsilon_F), \tag{2}$$

where the electron is at the Fermi level ϵ_F. The asymptotic structure of the exchange component $\nu_x(\mathbf{r})$ is obtained by substituting the self-energy $\Sigma_x(\mathbf{r},\mathbf{r}')=-\gamma_s(\mathbf{r},\mathbf{r}')/2|\mathbf{r}-\mathbf{r}'|$ into the above equation. Here $\gamma_S(\mathbf{r},\mathbf{r}')=2\Sigma_{\mathbf{k}}\Psi_{\mathbf{k}}^*(\mathbf{r})\Psi_{\mathbf{k}}(\mathbf{r}')$ is the idempotent density matrix constructed with the KS orbitals $\Psi_{\mathbf{k}}(\mathbf{r})$. The resulting expression is recognized to be the orbital-dependent potential[12] $\nu_{x,\mathbf{k}}(\mathbf{r})$ defined as

$$\nu_{x,k}(\mathbf{r})=\int\frac{\rho_{x,\mathbf{k}}(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}', \tag{3}$$

due to the orbital-dependent Fermi hole $\rho_{x,\mathbf{k}}(\mathbf{r},\mathbf{r}')$ of Hartree-Fock theory which in turn is defined as

$$\rho_{x,\mathbf{k}}(\mathbf{r},\mathbf{r}')=\sum_{\mathbf{k}'}\Psi_{\mathbf{k}'}^*(\mathbf{r})\Psi_{\mathbf{k}'}(\mathbf{r}')\Psi_{\mathbf{k}}(\mathbf{r}')/\Psi_{\mathbf{k}}(\mathbf{r}). \tag{4}$$

For both jellium and structureless-pseudopotential models of a metal surface, there is translational symmetry in the plane parallel to the surface, and since the effective potential in which the electrons move is local, the KS orbitals are of the form

$$\Psi_{\mathbf{k}}(\mathbf{r})=\left(\frac{2}{V}\right)^{1/2}e^{i\mathbf{k}_\parallel\cdot\mathbf{x}_\parallel}\phi_k(x), \tag{5}$$

where $(\mathbf{k}_\parallel,\mathbf{x}_\parallel)$ are the momentum and position vectors parallel to the surface, and (k,x) the components perpendicular to it. The structure of the component $\phi_k(x)$ of the orbitals for the two models is the same in the asymptotic vacuum and metal bulk regions. It is only in the surface region that the orbitals $\phi_k(x)$ differ.

Employing the KS orbitals of Eq. (5), Harbola and Sahni[9] derived the expression for the orbital-dependent-potential $\nu_{x,1}(z)$ corresponding to the Fermi-level electron with momentum perpendicular to the surface (in dimensionless variables),

$$\frac{\nu_{x,1}(z)}{(3k_F/2\pi)} = -\frac{4}{3\phi_1(z)}\int_{-\infty}^{\infty}\frac{dz'}{|z-z'|}\,\phi_1(z') \times \int_0^1 dk\;\phi_k^*(z')\phi_k(z)(1-e^{-\lambda|z-z'|}), \quad (6)$$

where $\lambda=(1-k^2)^{1/2}$ and $z=k_F x$. Noting that

$$\frac{1-e^{-\lambda|z-z'|}}{|z-z'|} = \int_0^\lambda dq\; e^{-q|z-z'|}, \quad (7)$$

the expression for $\nu_{x,1}(z)$ can be written in the following form:

$$\frac{\nu_{x,1}(z)}{(3k_F/2\pi)} = -\frac{2}{3\phi_1(z)}\int_0^1 dk\;\phi_k(z)\int_0^\lambda dq\; J(q,z), \quad (8)$$

where

$$J(q,z)=2\int_{-\infty}^{\infty}dz' e^{-q|z-z'|}\phi_k^*(z')\phi_1(z'). \quad (9)$$

In order to make the derivation of the asymptotic structure of $\nu_x(\mathbf{r})$ accessible, we first derive the structure for the orbitals of the effective finite-linear-potential model.[13] We then prove that the result is equally valid for the KS orbitals of the fully self-consistently determined effective potential. The orbitals corresponding to the finite-linear-potential model are

$$\phi_k(z)=\sin[kz+\delta(k)]\theta(-z)+[B_k\ \mathrm{Ai}(\zeta_k)+C_k\ \mathrm{Bi}(\zeta_k)] \times[\theta(z)-\theta(z-z_b)]+D_k\ \exp(-\kappa_k z)\,\theta(z-z_b), \quad (10)$$

where $k=\sqrt{2E}$, $\kappa_k=\sqrt{2(W-E)}$, $\zeta_k=zz_F^{-1/3}-\zeta_0$, $\zeta_0=k^2z_F^{2/3}$, $F=(k_F^2/2)/z_F$, $z_F=(k_F^2/2)z_b/W$, E is the energy, W the barrier height, and $\mathrm{Ai}(\zeta_k)$ and $\mathrm{Bi}(\zeta_k)$ the Airy functions. The phase factor $\delta(k)$ and the coefficients B_k, C_k, and D_k are determined by the requirement of continuity of the wave function and its logarithmic derivative at $z=0$ and $z=z_b$.

We first determine $J(q,z)$ of Eq. (9) for $z>0$ for these orbitals to obtain

$$J(q,z)=e^{-qz}\left[\frac{q\ \cos\ \delta_- + k_-\ \sin\ \delta_-}{q^2+k_-^2} - \frac{q\ \cos\ \delta_+ + k_+\ \sin\ \delta_+}{q^2+k_+^2} + 2\int_0^{z_b}dz' e^{qz'}\{B_k\ \mathrm{Ai}(\zeta_k')+C_k\ \mathrm{Bi}(\zeta_k')\} \times\{B_1\ \mathrm{Ai}(\zeta_1')+C_1\ \mathrm{Bi}(\zeta_1')\} + \frac{2D_kD_1}{\kappa_k+\kappa_1-q}\,e^{-(\kappa_k+\kappa_1-q)z_b}\right] - \frac{4qD_kD_1}{(\kappa_k+\kappa_1)^2-q^2}\,e^{-(\kappa_k+\kappa_1)z}, \quad (11)$$

where $k_\mp=1\mp k$ and $\delta_\mp=\delta(1)\mp\delta(k)$. In the asymptotic large z region, the effective value of $q\sim 1/z$ due to the e^{-qz} factor in $J(q,z)$. Furthermore, since $k\sim 1$ for large z, the effective value of $k_-\sim 1/z$ due to the $e^{-\kappa_k z}$ factor. Expanding $J(q,z)$ of Eq. (11) in q we obtain for the asymptotic region,

$$\underset{z\to\infty}{J(q,z)}\sim e^{-qz}\left[\frac{q}{q^2+k_-^2}\cos\ \delta_- + \frac{k_-}{q^2+k_-^2}\sin\ \delta_-\right] + e^{-qz}\left[-\frac{\sin\ \delta_+}{k_+} - \frac{q\ \cos\ \delta_+}{k_+^2} + \frac{2D_kD_1}{\kappa_k+\kappa_1} \times e^{-(\kappa_k+\kappa_1)z_b} + 2\int_0^{z_b}dz'\{B_k\ \mathrm{Ai}(\zeta_k')+C_k\ \mathrm{Bi}(\zeta_k')\} \times\{B_1\ \mathrm{Ai}(\zeta_1')+C_1\ \mathrm{Bi}(\zeta_1')\}\right] - \frac{4qD_kD_1}{(\kappa_k+\kappa_1)^2}\,e^{-(\kappa_k+\kappa_1)z}. \quad (12)$$

Next consider the contribution of $J(q,z)$ of Eq. (12) to the integral over q in Eq. (8). The last term of Eq. (12) is exponentially small in the vacuum region and does not contribute. The contribution of the second set of terms is

$$\frac{1-e^{-\lambda z}}{z}\left[-\frac{\sin\ \delta_+}{k_+}+\frac{2D_kD_1}{\kappa_k+\kappa_1}\,e^{-(\kappa_k+\kappa_1)z_b} + 2\int_0^{z_b}dz'\{\ \}\{\ \}\right]+\left[\frac{\lambda e^{-\lambda z}}{z}+0\left(\frac{1}{z^2}\right)\right]\frac{\cos\ \delta_+}{k_+^2}. \quad (13)$$

Now $\lambda z\sim k_-^{1/2}z=(k_-z)^{1/2}z^{1/2}\gg 1$ for large z since $k_-\sim 1/z$. Thus, the contribution of Eq. (13) is $0(1/z)$. The contribution of the first term of Eq. (12) to the integral over q in Eq. (8), with $qz=u$ and $a=k_-z$, is

$$\cos\ \delta_-\int_0^\infty du\,\frac{ue^{-u}}{u^2+a^2}+a\ \sin\ \delta_-\int_0^\infty du\,\frac{e^{-u}}{u^2+a^2}+0\left(\frac{1}{z}\right). \quad (14)$$

We next consider the integral over k in Eq. (8) and rewrite it as $(1/z)\int_0^\infty da$. Since for large z, $k\sim 1$, we have $\kappa_k z=\kappa_1 z+ca$ where $c=1/\kappa_1$, so that $\phi_k(z)\sim\phi_1(z)\exp(-ca)$. Substituting this $\phi_k(z)$ into Eq. (8) and using the fact that $\cos\ \delta_-\sim 1$ and $\sin\ \delta_-\sim 0$ for $k\sim 1$, we derive the expression for $\nu_{x,1}(z)$ to be

$$\nu_{x,1}(z)\sim -\frac{3k_F}{2\pi}\,\frac{2}{3\phi_1(z)}\,\phi_1(z)\,\frac{1}{z}\int_0^\infty da\int_0^\infty du\,\frac{ue^{-ba-u}}{u^2+a^2}, \quad (15)$$

or equivalently

$$\nu_x(x)=-\frac{\alpha_{\mathrm{KS},x}(\beta)}{x};$$

$$\alpha_{\mathrm{KS},x}(\beta)=\frac{\beta^2-1}{2\beta^2}\left[1-\frac{\ln(\beta^2-1)}{\pi(\beta^2-1)^{1/2}}\right]. \quad (16)$$

The above derivation also shows that, for the extended metal surface system for which the energy spectrum is continuous, to the leading order, the orbital-dependent potentials

$\nu_{x,\mathbf{k}}(\mathbf{r})$ for electrons within a shell of thickness $(1/z)$ about the Fermi level are the same. Thus, their average taken over this shell, which is the exchange potential, is equivalent in leading order to the orbital-dependent potential for electrons at the Fermi level. In the case of discrete systems such as atoms, it is of course more readily apparent that the asymptotic structure is due to the highest occupied orbital electrons.

To prove that the asymptotic structure of the Kohn-Sham exchange potential Eq. (16) is valid for the self-consistently determined effective potential, we divide the z axis into three parts: $z\leqslant -d$, $-d\leqslant z\leqslant d$, $z\geqslant d$, where d is an effective width of the surface region. In the first region, which corresponds to the metal bulk, the potential $\nu_{\mathrm{xc}}(z)$ is constant. Consequently, the orbitals are of the form $\phi_k(z)=\sin[kx+\delta(k)]$, where the $\delta(k)$ are the self-consistent phase shifts. The contribution to $J(q,z)$ of Eq. (9) from this region is then

$$J(q,z)=2e^{-qz}\int_{-\infty}^{d}dz'\,e^{qz'}\,\sin[kz'+\delta(k)]\sin[z'+\delta(1)]$$
$$=e^{-qz}e^{-qd}\left[\frac{q\,\cos(k_-d-\delta_-)-k_-\,\sin(k_-d-\delta_-)}{q^2+k_-^2}\right.$$
$$\left.-\frac{q\,\cos(k_+d-\delta_+)-k_+\,\sin(k_+d+\delta_+)}{q^2+k_+^2}\right]. \qquad (17)$$

Note that this contribution is the same as the corresponding terms of Eq. (11) except that they are modified by the factor d. Now, due to screening, the surface region is small in comparison to the asymptotic electron position: $d\ll z$ for $z\to\infty$. Furthermore, again the effective value of $q\sim 1/z$, so that on expansion in q this contribution of $J(q,z)$ is

$$J(q,z)=e^{-qz}\,\frac{q}{q^2+k_-^2}\cos\,\delta_-\,, \qquad (18)$$

which is the same result as derived previously [see Eq. (12)]. Recall, that it is this term which leads to the coefficient $\alpha_{\mathrm{KS},x}(\beta)$.

In the region $-d\leqslant z\leqslant d$, the self-consistent orbitals will, of course, differ from those of the model effective potential considered. However, the contribution from this region to $J(q,z)$, which is

$$J(q,z)=2\int_{-d}^{d}dz'\,e^{-q|z-z'|}\phi_k(z')\,\phi_1(z'), \qquad (19)$$

will be similar to the second set of terms of Eq. (12). Consequently, its contribution to $\nu_x(z)$ is $0(1/z^2)$.

In the region $z\geqslant d$, the orbitals of the model potential assumed previously were exponential [see Eq. (10)]. If, however, we assume that the asymptotic structure of the effective potential which is that of $\nu_{\mathrm{xc}}\sim -1/4x$, then the orbitals in this region are of the form[8] $\phi_k(z)\sim z^{\nu_k}e^{-\kappa_k z}$. [For an electron at the Fermi level $\nu_{k_F}=1/(4k_F\sqrt{\beta^2-1})$.] The expression for $J(q,z)$ in this region is

$$J(q,z)$$
$$=\int_d^\infty dz'\,e^{-q|z-z'|}\phi_k(z')\,\phi_1(z') \qquad (20)$$
$$\sim e^{-qz}\int_d^z dz'\,e^{qz'}(z')^{\nu_k+\nu_1}e^{-(\kappa_k+\kappa_1)z'}$$
$$+e^{qz}\int_z^\infty dz'\,e^{-qz'}(z')^{\nu_k+\nu_1}e^{-(\kappa_k+\kappa_1)z'}$$
$$=\frac{e^{-qz}\{\Gamma(\nu_k+\nu_1+1)-\Gamma[\nu_k+\nu_1+1,(\kappa_k+\kappa_1-q)z]\}}{(\kappa_k+\kappa_1-q)^{\nu_k+\nu_1+1}}$$
$$-\frac{e^{-qz}\gamma[\nu_k+\nu_1+1,(\kappa_k+\kappa_1-q)d]}{(\kappa_k+\kappa_1-q)^{\nu_k+\nu_1+1}}$$
$$+\frac{e^{qz}\Gamma[\nu_k+\nu_1+1,(\kappa_k+\kappa_1+q)z]}{(\kappa_k+\kappa_1+q)^{\nu_k+\nu_1+1}}, \qquad (21)$$

where

$$\gamma(\alpha,x)=\int_0^x e^{-t}t^{\alpha-1}dt,\quad \Gamma(\alpha,x)=\int_x^\infty e^{-t}t^{\alpha-1}dt, \qquad (22)$$

are the incomplete γ functions. Now[14] $\Gamma(\alpha,x)\sim x^{\alpha-1}e^{-x}$ as $x\to\infty$, so that

$$\underset{z\to\infty}{J(q,z)}=\frac{e^{-qz}\Gamma(\nu_k+\nu_1+1)}{(\kappa_k+\kappa_1-q)^{\nu_k+\nu_1+1}}-\frac{2qz^{\nu_k+\nu_1}}{(\kappa_k+\kappa_1)^2-q^2}\,e^{-(\kappa_k+\kappa_1)z}$$
$$-\frac{e^{-qz}\gamma[\nu_k+\nu_1+1,(\kappa_k+\kappa_1-q)d]}{(\kappa_k+\kappa_1-q)^{\nu_k+\nu_1+1}}. \qquad (23)$$

[See Eq. (11) for a comparison with the corresponding terms of the finite-linear-potential model.] The first and third terms of Eq. (23) give a $1/z^2$ contribution to $\nu_x(z)$. The second term has the functional dependence on z as $z^{\nu_k+\nu_1}e^{-(\kappa_k+\kappa_1)z}$ instead of $e^{-(\kappa_k+\kappa_1)z}$ of the model potential. The contribution of this term asymptotically to $\nu_x(z)$ vanishes.

Therefore, the asymptotic structure of the KS exchange potential for the self-consistently determined effective potential is the same as Eq. (16) derived previously. We emphasize again that this asymptotic structure of the potential in the vacuum region is governed and arises from the orbitals deep in the metal interior whose structure is $\phi_k(x)=\sin[kx+\delta(k)]$ irrespective of whether the effective potential at the surface is modeled or determined self-consistently.

To demonstrate the correctness of our derivation, we note that the KS exchange energy $E_x^{\mathrm{KS}}[\rho]$ and potential $\nu_x(\mathbf{r})$ may be expressed in terms of the Slater potential $V_x^S(\mathbf{r})$ as

$$E_x^{\mathrm{KS}}[\rho]=\frac{1}{2}\int d\mathbf{r}\;\rho(\mathbf{r})V_x^S(\mathbf{r}), \qquad (24)$$

and

$$\nu_x(\mathbf{r})=\frac{1}{2}\,V_x^S(\mathbf{r})+\frac{1}{2}\int d\mathbf{r}'\rho(\mathbf{r}')\,\frac{\delta V_x^S(\mathbf{r}')}{\delta\rho(\mathbf{r})}, \qquad (25)$$

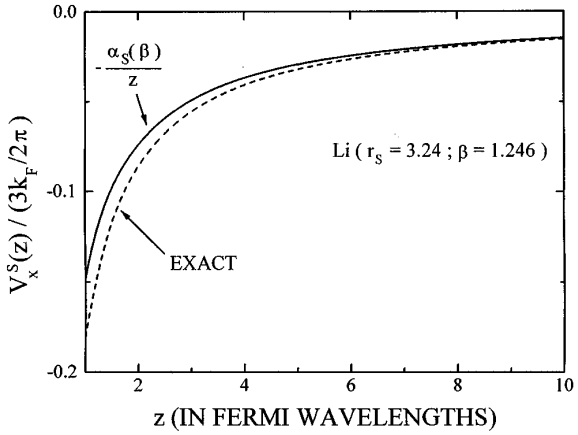

FIG. 1. Comparison of the *exact* Slater potential $V_x^S(\mathbf{r})$ as determined by its definition Eq. (26) with the analytical expression $-\alpha_S(\beta)/z$ for asymptotic positions of the electron in the vacuum.

respectively, where $V_x^S(\mathbf{r})$ is defined in terms of the Fermi hole $\rho_x(\mathbf{r},\mathbf{r}')=-|\gamma_s(\mathbf{r},\mathbf{r}')|^2/2\rho(\mathbf{r})$ as

$$V_x^S(\mathbf{r})=\int \frac{\rho_x(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}'. \tag{26}$$

Now, in our previous work,[1] we derived in a similar manner the asymptotic structure of $V_x^S(\mathbf{r})$ in the vacuum region to be $-\alpha_s(\beta)/x$, where the Slater coefficient $\alpha_S(\beta)=2\alpha_{\mathrm{KS},x}(\beta)$. Thus, the contribution of the second term of Eq. (25) in the vacuum region is zero in the leading order of $1/z$, so that in this asymptotic region

$$\nu_x(z)\approx\tfrac{1}{2}V_x^S(z). \tag{27}$$

The correctness of the derivation can therefore be shown by comparison of the asymptotic structure of $V_x^S(\mathbf{r})$ in the vacuum as determined by its definition of Eq. (26) with the function $-\alpha_S(\beta)/x$. An expression for $V_x^S(\mathbf{r})$ in terms of momentum space integrals has been derived[11] and given in Eqs. (2)–(5) of Ref. 1. This enables the easy determination of $V_x^S(\mathbf{r})$ throughout space since the integrals are then over the finite region from 0 to 1 in units normalized to the Fermi momentum. In Fig. 1 we plot for Li metal ($r_s=3.24$) the Slater potential $V_x^S(\mathbf{r})$ outside the metal as determined by this *exact* expression as well as the function $-\alpha_s(\beta)/z$. The calculations for the *exact* results are performed for the orbitals of the finite-linear-potential model for which the relationship between r_s and β is determined via energy minimization in the local-density approximation (see Appendix of Ref. 15). The same value of β is employed in the analytical expression for $\alpha_s(\beta)$. It is evident that the two curves merge by about ten Fermi wavelengths from the surface, thereby confirming the analytical results derived. It is interesting to note that in contrast the KS asymptotic function $-\alpha_{\mathrm{KS},x}(\beta)/z$ merges with an accurate approximate representation[16] of $\nu_x(\mathbf{r})$ by about one Fermi wavelength from the surface.

A similar analysis can be performed[17] for the asymptotic structure of the Pauli and correlation-kinetic components of the Kohn-Sham exchange potential $\nu_x(\mathbf{r})$. The Pauli component can be shown to decay asymptotically as $-\alpha_W(\beta)/x$ with the coefficient $\alpha_W(\beta)$ being derived as

$$\alpha_W(\beta)=\frac{\beta^2-1}{\beta^2}\left[\frac{2}{\pi\sqrt{\beta^2-1}}\left(1-\frac{(\beta^2-1)\ln(\beta^2-1)}{\beta^2}\right)+\frac{\beta^2-2}{\beta^2}\right]. \tag{28}$$

From this expression it is evident that the decay coefficients of the Kohn-Sham exchange potential $\nu_x(\mathbf{r})$ and its Pauli component differ. Furthermore, it can be seen that the correlation-kinetic component then also decays asymptotically as x^{-1}, and becomes more significant for low-density metals. This is in sharp contrast to the case of finite systems, such as atoms and molecules, where the asymptotic structure of the entire exchange-correlation potential is due to the Pauli component.

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