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ANALYTIC FORMULA FOR THE ELECTRON DENSITY OF METAL SURFACES

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1. Recently increasing attention has been paid to the electron density at metal surfaces. The self-consistent calculations for the electron density are numerically cumbersome, therefore it is a great advantage if an analytic expression can be found that closely approximates the results of the self-consistent calculation [1]. In addition, the availability of analytic density may be very useful for studying other fundamental problems depending on the properties of an inhomogeneous electron gas. This paper presents an analytic expression for density, which closely approximates the self-consistent results of LANG [2]. The final formula is very simple, which makes it possible to calculate very easily the density for all metals, while the electron density of metal surfaces was computed originally by LANG only for parameters $r_s = 2,3,4,5,6$ a.u.

The value of r_s can be computed from the density, according to the following expression:

$$\frac{4r_s^3\pi}{3} = \frac{1}{N \cdot b},$$

$$r_s = 0.2879 \cdot \frac{1}{N'b}\,[\mathrm{nm}].$$

where $N = N' \cdot 10^{22}$ atom/cm^3 is the atomic density, b is the number of the free electrons per atom.

The parameter r_s of several atoms can be found in Table I.

2. A numerical approximation was worked out to LANG's results yielding the following expression for the electron density [4]:

$$n(x) = -0.5 \cdot \mathrm{th}[p(x+\varphi)] + k\left\{-\frac{\sin q(x+\varphi)}{[q(x+\varphi)]^2} + \frac{\cos q(x+\varphi)}{q(x+\varphi)}\right\} + 0.5\,,$$

if $$x < -\varphi\,;$$

Table I

The value of density and the parameter r_s of several atoms

Metal	N' [10^{22} atom/cm^3]*	r_s [nm]	b
Li	4.629	0.173	1
Na	2.532	0.211	1
Ka	1.31	0.263	1
Cu	8.467	0.112	2
Rb	1.075	0.281	1
Ag	5.864	0.160	1
Cs	0.8855	0.300	1
Au	5.896	0.159	1
Be	12.35	0.099	2
Mg	4.30	0.141	2
Ca	2.3	0.173	2
Zn	6.62	0.122	2
Sr	1.775	0.189	2
Cd	4.63	0.137	2
Ba	1.576	0.196	2
Hg	4.35	0.140	2
Al	6.023	0.110	3
Ga	5.103	0.116	3
In	3.824	0.128	3
Tl	3.519	0.131	3
Si	4.994	0.106	4
Ti	5.500	0.113	3
Ge	4.417	0.111	4
Zr	4.189	0.119	4
Sn	2.928	0.127	4
Sn	3.696	0.117	4
Pb	3.297	0.122	4
V	7.119	0.119	2
Sb	3.31	0.112	5
Ta	5.535	0.113	2
Bi	2.827	0.141	3
Cr	8.333	0·113	3
Mo	6.417	0.107	3
Se	2.94	0.127	4
W	6.308	0.124	2
Mn	7.935	0.115	2
Fe	8.496	0.112	2
Co	8.471	0.110	2
Ni	9.14	0.109	2
Pd	6.795	0.121	2
Pt	6.625	0.122	2

* Thanks are due Mr. Zs. BALASSA for computing the atomic density N.

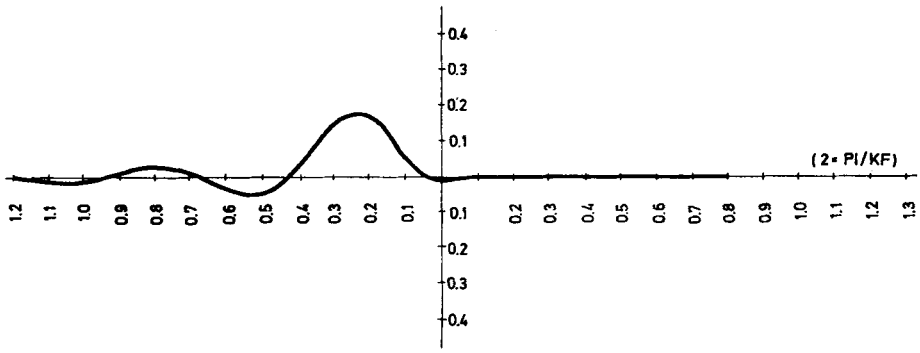

Fig. 1

$$n(x) = -0.5 \cdot \mathrm{th}[p(x + \varphi)] + 0.5 ,$$

if $$x > -\varphi ,$$

where

$$\varphi = 0.01 \cdot (r_s)^{0,54} ,$$

$$p = 3.34 \cdot (r_s)^{0,48} ,$$

$$q = 8.73 \cdot (r_s)^{0,05^8} ,$$

$$k = 0.08 \cdot (r_s)^{0,9} .$$

Here $n(x)$ is in units of $\bar{n}$ (the bulk density) and x is in units of the inverse Fermi wavelength $(2\pi/K_F)$. The inverse Fermi wavelength can be computed from the following expression:

$$E_F = \frac{\hbar^2 K_F^2}{2m} .$$

The term th$x$ is very accurate. The "difference function" (the term th$x$ subtracted from LANG's results) can be seen in Fig. 1 (for $r_s = 5$). It is easy to observe that if $x > -\varphi$ the difference is very small. (under 0.008) and if $x < -\varphi$ the Friedel oscillation appears clearly. The presence of the Bessel function term ensures the oscillation. Subtracting the corresponding values from LANG's results we obtain the error of our approximation. For $r_s = 2$ it can be seen in Table II.

The analytic expression gives a fairly good approximation for every computed integer r_s value. In addition we can compute $n(x)$ also for not integer

Table II

The distance X from the surface of the positive background is given in units of $2\pi/k_F$.

The error is in units of $\bar{n}$ (the bulk density)

X	Error	X	Error
−1.200	0.001	−0.100	0.017
−1.200	0.001	−0.075	0.018
−1.100	0.015	−0.050	0.017
−1.050	0.021	−0.025	0.014
−1.000	0.021	0.000	0.014
−0.950	0.016	0.025	0.017
−0.900	0.007	0.050	0.017
−0.850	0.006	0.075	0.015
−0.800	0.019	0.100	0.012
−0.750	0.028	0.125	0.009
−0.700	0.031	0.150	0.005
−0.650	0.027	0.200	0.000
−0.600	0.017	0.250	0.004
−0.550	0.004	0.300	0.005
−0.500	0.007	0.350	0.005
−0.450	0.014	0.400	0.005
−0.400	0.015	0.450	0.004
−0.375	0.013	0.500	0.003
−0.350	0.011	0.550	0.002
−0.325	0.008	0.600	0.002
−0.300	0.005	0.650	0.001
−0.275	0.003	0.700	0.001
−0.250	0.002	0.750	0.001
−0.225	0.003	0.800	0.001
−0.200	0.004	0.850	0.000
−0.175	0.007	0.900	0.000
−0.150	0.011	0.950	0.000
−0.125	0.014	1.000	0.000

r_s values. This is the most important advantage of the analytic formula. The error of the approximation has a minimum at $r_s = 2$. Since the r_s value of most metals is near to 2, it is a fairly good approximation.

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REFERENCES

1. J. E. HIMBERGEN and R. SILBEY, Phys. Rev. B, **18**, 2674, 1978.
2. N. D. LANG, Solid State Commun., **7**, 1047, 1969.
3. N. D. LANG and W. KOHN, Phys. Rev. B, **1**, 4555, 1970.
4. Z. SZEIFERT, Thesis (unpublished).