Calculation of the Average Potential of a Wigner Solid

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Abstract: The paper corrects a few errors occurring in the calculations of CALLAWAY J on the average potential of a Wigner solid. With respect to the monoatomic bcc and fcc metals, a theory of calculating the average potentials of them is established, and the theoretical results demonstrate that the average potential is directly proportional to the reciprocal of the lattice constant of the crystal. Moreover, the paper performs a great deal of calculations of the average potentials of various bcc and fcc metals, and obtains a lot of numerical results which are valuable for applications.

Keywords: Wigner Solid, Poisson's Equation, Average Potential, Lattice Constant

1. Introduction

The average potential of a crystal is an indispensible part of calculating the energy band, electrostatic energy or electrostatic binding energy of the crystal. It can be regarded as an approximation of zero order disturbance of the Hamilton of the electron in crystals. With respect to the calculation of electrostatic potential energy without the consideration of the average potential or regard it as zero, it will result in 20% even more corrections to the result.[1] Therefore, calculations of the average potential of crystals is one of the important and valuable subjects in the research field of the solid theory. The calculation about crystals is very complex, people hope explore and establish new theories to simplify the calculations. Wigner solid is a theoretical model, and similar to the plasma state. Because Wigner solid can be applied to many physical phenomena, such as inversion layers near the surface of semiconductors; an electron crystal slightly above a free surface of liquid helium subjected to a perpendicular electric field; white dwarf stars; and crusts of pulsars. It therefore attracts interesting and a lot of studies.[1-6] Wigner solid model is favorably applied to metals, because electrons in metals are free moving, so possibly toward to the uniform distribution of negative charges. CALLAWAY J calculated out the potential of an electron at Γ point of the BZ (Brillouin zone) for monoatomic bcc metals by use of this model, actually, it is identical with the average potential of the crystals,[7-8] but there are errors in his calculation theory; in Ref. [2, 5], CALLAWAY J et al. misinterpreted the potential function

$V(\vec{r})$ in Poisson equation as the function of potential energy. Besides, CALLAWAY J misused the calculation result of Ref. [1] to $\frac{1}{\Omega}\iiint r^2 d^3 r$, because the integral zone chosen by Ref. [1] is the proximity cell whose volume is $2a^3$, but the integral zone chosen by CALLAWAY J is the general cell whose volume is $\frac{1}{2}a^3$. The both zones are different from each other, so it is necessary to recalculate the integral. In consideration with most of metals are bcc or fcc lattice, the discussions of this paper will restrict to the average potentials of bcc and fcc metal crystals.

2. Wigner Solid

For the convenience of calculations, the present discussions merely consider monoatomic bcc and fcc metals. The so-called Wigner solid for the crystal of ionic lattice is composed of the point charge with positive charge $Z|e|$(e is the charge of an electron) resting at the lattices of the crystal and the background with uniform distribution of the negative charges [1-2], the quantity of negative charges in a cell is $-Z|e|$, the whole crystal is neutral. Z =atomic number－numbers of electrons inside the atomic core. The potential function of an electron in the crystal is determined by the Poisson's equation: [9]

$$\Delta V(\vec{r}) = -\frac{1}{\varepsilon_r \varepsilon_0} \rho(\vec{r}), \qquad (1)$$

where $\rho(\vec{r})$ represents the charge density in the crystal, ε_0 and ε_r respectively represent the dielectric constant in vacuum and the relative dielectric constant of the metal, for general metals, $\varepsilon_r < 10$. Either of $V(\vec{r})$ and $\rho(\vec{r})$ is the periodic function, using the Fouier transformation, they are expanded as:

$$V(\vec{r}) = \sum_s V(\vec{K}_s) \exp(i\vec{K}_s \cdot \vec{r}) \,; \rho(\vec{r}) = \sum_s \rho(\vec{K}_s) \exp(i\vec{K}_s \cdot \vec{r}). \quad (2)$$

The Fouier coefficients of $V(\vec{r})$ and $\rho(\vec{r})$ are respectively

$$V(\vec{K}_s) = \frac{1}{\Omega} \int \exp(-i\vec{K}_s \cdot \vec{r}) V_c(\vec{r}) d^3 r, \qquad (3)$$

and

$$\rho(\vec{K}_s) = \frac{1}{\Omega} \int \exp(-i\vec{K}_s \cdot \vec{r}) \rho_c(\vec{r}) d^3 r. \qquad (4)$$

Choosing the cell as the elementary unit, where $\vec{K}_s$ notes any reciprocal vector, $\rho_c(\vec{r})$ notes the charge density in a cell, Ω notes the volume of a cell. $V_c(\vec{r})$ is the potential term around every cell as the center. $V(\vec{r})$ can be written as:

$$V(\vec{r}) = \sum_\mu V_c(\vec{r} - \vec{R}_\mu). \qquad (5)$$

Similarly, $\rho(\vec{r})$ can be written as the sum of every cell term:

$$\rho(\vec{r}) = \sum_\mu \rho_c(\vec{r} - \vec{R}_\mu). \qquad (6)$$

Substituting eq.(2) into eq. (1), it obtains

$$V(\vec{K}_s) = -\frac{1}{\varepsilon_r \varepsilon_0} \cdot \vec{K}_s^{-2} \cdot \rho(\vec{K}_s). \qquad (7)$$

The theoretical calculations are very similar for various special points in BZ (Brillouin zone), the present calculations merely consider $\Gamma(\vec{K}_s = 0)$ point in BZ, it can be found that when $\vec{K}_s = 0$, eq.(3) represents the average potential of the crystal. [2, 7-8] This is necessary to be calculated if we want to calculate the energy band or electrostatic potential of the crystal by use of the theory of disturbance. Regarding $\vec{K}_s$ of

eq. (7) is the continuous variable, we define that $V(0)$ is the value of eq.(7)while $\vec{K}_s \to 0$. Leaving off the lower note of $\vec{K}_s$, in terms of eq. (7),

$$V(0) = -\frac{1}{\varepsilon_r \varepsilon_0} \lim_{\vec{K} \to 0} \frac{\rho(\vec{K})}{\vec{K}^2}. \qquad (8)$$

From eq. (4), expanding $\exp(-i\vec{K}_s \cdot \vec{r})$ and leaving off the lower note s, it arrives:

$$\rho(\vec{K}) = \frac{1}{\Omega} [\iiint \rho_c(\vec{r}) d^3 r - i \iiint \rho_c(\vec{r})(\vec{K} \cdot \vec{r}) d^3 r -$$
$$\frac{\vec{K}^2}{2} \iiint r^2 \rho_c(\vec{r}) \cos^2 \theta d^3 r + \cdots]. \qquad (9)$$

Where θ represents the angle between $\vec{K}$ and $\vec{r}$, Because the charge distribution in a cell of the crystal is neutral, the first integral is equal to zero. Besides, there is the symmetry of space inversion in a cell, thus the second integral is also zero; actually, $V(0)$ should be a real number, the second term of eq.(9) cannot be considered. Substituting eq. (9) into eq. (8), while $\vec{K} \to 0$, we get

$$V(0) = \frac{1}{2\varepsilon_r \varepsilon_0 \Omega} \iiint r^2 \rho_c(\vec{r}) \cos^2 \theta d^3 r, \qquad (10)$$

Where $\cos^2 \theta = \frac{1}{3} + \frac{2}{3} P_2(\cos\theta)$, $P_2(\cos\theta)$ is the second Legendre polynomials. Eq.(10)can be written as:

$$V(0) = \frac{1}{6\varepsilon_r \varepsilon_0 \Omega} \iiint [1 + 2P_2(\cos\theta)] r^2 \rho_c(\vec{r}) d^3 r. \qquad (11)$$

3. Calculating Bcc Metals

The charge distribution is uniform in the cell of crystals, it has the spherical symmetry, all the cell is neutral charge. Therefore, for the bcc metal crystals, the charge density in a cell can be written as [5, 7]

$$\rho_c(\vec{r}) = Z|e| [\delta(r) - \frac{1}{\Omega}]. \qquad (12)$$

$\rho_c(\vec{r})$ is cubic symmetry, substituting it into eq.(11) for calculations, the integral containing $P_2(\cos\theta)$ will be equal to zero, thus

$$V(0) = -\frac{Z|e|}{6\varepsilon_r \varepsilon_0 \Omega^2} \iiint r^2 d^3 r. \qquad (13)$$

With respect to the integral $\frac{1}{\Omega}\iiint r^2 d^3 r$, $\Omega = \frac{a^3}{2}$, we use the spherical approximation for the calculations [1-2]. The present calculations obtain the spherical radius $r_s \approx 0.4923846a$. It therefore calculated out the integral

$$\frac{1}{\Omega}\iiint r^2 d^3 r \approx 0.1454762a^2 , \qquad (14)$$

This result is consistent with the data provided by Ref.[2]. Eventually, it can be obtained from eq. (13) that the average potential of bcc metal crystals is:

$$V_b(0) = -8.77446 \times 10^{-10} \cdot \frac{Z}{\varepsilon_r} \cdot \frac{1}{a}. \qquad (15)$$

Eq. (15) shows that the average potential of bcc metals is proportional to $\frac{1}{a}$ (a is the lattice constant of the crystal), this is also consistent with the conclusion of other relative reference [5]. The paper performed numerical calculations for some bcc metals (superconductor elements), the results as shown as TABLE 1.

Table 1. *The numerical calculation results about the average potentials of various bcc metals.*

Metals	a	Z [b]	ionic polarizability	ε_r [d]	$V_b(0)$
	(experiment, nm)[a]		(10^{-3} nm^3)[c]		(V)
Li(78K)	0.349(78K)	1	0.029	1.0172	−2.4717
Na(5K)	0.423(5K)	1	0.179	1.0606	−1.9558
K (5K)	0.523(5K)	1	0.839	1.1550	−1.4526
Fe(α)	0.287	8	0.336(3+)	1.4055	−17.4019
Rb(5K)	0.559(5K)	1	1.40	1.2159	−1.2910
Nb	0.330	5	0.261(5+)	1.1944	−11.1308
W	0.316	6	0.280(6+)	1.2409	−13.4260
Cs	0.605	1	2.42	1.3023	−1.1137
Ba	0.502	2	1.55(2+)	1.3432	−6.6026
Ta	0.331	5	0.358(5+)	1.2705	−10.4325
Mo	0.315	6	0.19(6+)	1.1610	−14.3956
V	0.302	5	0.126(5+)	1.1196	−12.9754

a. See Ref.[10], the notes 78K and 5K on the right of lattice constants mean the temperature of the measurements, and others are measured in the room temperature.

b. Z =atomic number−the numbers of electrons in the atomic core.

c. See Ref.[11].

d. ε_r in TABLE 1 are theoretical results calculated by use of the Clausius –Mossotti formula in Ref.[10] and the ionic polarizabilities of metals.

4. Calculating Fcc Metals

With respect to fcc metals, $\Omega = \frac{a^3}{4}$, using spherical approximation to calculate the integral of eq. (13) $\frac{1}{\Omega}\iiint r^2 d^3 r$, from calculations we get the spherical radius $r_s \approx 0.3906694a$, thus

$$\frac{1}{\Omega}\iiint r^2 d^3 r \approx 0.0914843a^2 . \qquad (16)$$

From eq. (13) it eventually obtains

$$V_f(0) = -11.035847 \times 10^{-10} \cdot \frac{Z}{\varepsilon_r} \cdot \frac{1}{a}. \qquad (17)$$

The paper performed numerical calculations for some fcc metals, their results are shown in TABLE2.

Table 2. *The numerical calculation results about the average potentials of some fcc metals.*

Metals	a	Z [b]	ionic polarizabilities	ε_r [d]	$V_f(0)$
	(experiment, nm)[a]		(10^{-3}nm^3)[c]		(V)
Cu	0.361	1	0.428	1.5395	−1.9857
Ni	0.352	8	0.386(2+)	1.5223	−16.4760
Al	0.405	3	0.054(3+)	1.0414	−7.8497
Ca	0.558	2	0.472(2+)	1.1431	−3.4603
Rh	0.380	8	0.667(3+)	1.7673	−13.1462
Pb	0.495	4	0.618(4+)	1.2800	−6.9671
Ce	0.516	4	1.03(3+)	1.4310	−5.9783
Ag	0.409	1	1.72(1+)	3.1833	−0.8476

a. See Ref. [10].

b. Z =atomic number−numbers of electrons in atomic core.

c. See Ref. [11].

d. ε_r in TABLE 2 are the theoretical results calculated by Clausius – Mossotti formula in Ref.[10] and the electropolarizabilities.

5. Conclusion

As a supposing model Wigner solid has been extensively applied in research fields of solid state theory. With respect to monoatomic bcc and fcc metals, the paper calculated and derived the formulas of the average potentials eq. (15) and eq. (17), which can be respectively and directly applied to bcc and fcc metals. Moreover, it performed the numerical calculations of average potentials for some bcc and fcc metals, and the results are shown in TABLE 1 and TABLE 2. Although it has not found the experimental data and other theoretical results to compare with, it can be found from eq. (15) and eq. (17) that the average potentials of metals are proportional to the reciprocal of their lattice constants, this result is consistent with the conclusion of Ref. [5]. The theory established by this paper can similarly applied to the metals with other lattice.

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