Journal of Statistical Physics, Vol. 53, Nos. 1/2, 1988

On the Energy per Particle in Three- and Two-Dimensional Wigner Lattices

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Received February 4, 1988

We come back to the 1979 controversy about the value of the energy per particle Φ_i in an infinite Wigner lattice of electrons in a uniform compensating background. For simplicity we restrict ourselves to the simple cubic (and square) lattice. We present an accurate calculation of the energy Φ_{el} of one electron in the field of the other electrons plus background for the case that the system (system I) is considered as an infinite arrangement of neutral cubes (Wigner–Seitz cells). The value obtained is checked by computer calculations. We confirm the conclusion of de Wette that for this system the relation $\Phi_i = \frac{1}{2}\Phi_{el}$ (often accepted without discussion) does not hold and we calculate the difference $\Delta\Phi$, which represents the average potential in the system. On the other hand, if the system is considered as the limit of a set of spheres with increasing radii, such that the spheres are neutral (system II), we obtain a different value of Φ_{el} and in this case $\Phi_i = \frac{1}{2}\Phi_{el}$. We show explicitly that the Ewald method of summation, used by Fuchs and others, leads to the same analytical expression as the limit obtained for a set of neutral spheres (system II). We extend the calculations to the two-dimensional square lattice. Here the equality $\Phi_i = \frac{1}{2}\Phi_{el}$ holds also in the case of an infinite arrangement of neutral squares (system I).

KEY WORDS: Wigner lattice; energy per particle; Ewald method of summation.

1. INTRODUCTION

In the elementary electron theory of solids it is assumed that the valence electrons move independently in a periodic field. Attempts to take into account the interaction between the electrons in a more rigorous way

This paper is dedicated to our friend and colleague Nico van Kampen in honor of his lifelong dedication to science in general and to theoretical physics in particular.

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0022-4715/88/1000-0361$06.00/0

originated more than 50 years ago in the work of Wigner.[1] The problem is often simplified by neglecting the periodic structure of the system and considering an electron gas moving in a uniform, positively charged background, sometimes called a jelly, in order to make the system electrically neutral. The electron density ρ is usually expressed in terms of the dimensionless quantity r_s defined by

$$1/\rho = 4/3\pi r_s^3 a_0^3 \tag{1.1}$$

where $a_0 \equiv \hbar^2/me^2$ is the Bohr radius; i.e., r_s is the radius (expressed in atomic units) of a sphere with volume equal to the volume per electron. Small r_s means high density, large r_s means low density; for real metals r_s is of the order of 5.

In modern many-body theory refined perturbation methods have been successfully used in treating the interaction between electrons. They lead to an expansion for the energy of an electron gas for small values of r_s, i.e., it is essentially a high-densty expansion. In order to develop interpolation formulas for the case of realistic r_s values it is obviously useful to consider the low-density limit also, i.e., the case of a dilute electron gas (large r_s). Wigner, in the papers referred to above, argued that in the limit of large r_s values the kinetic energy of the electrons, which is proportional to r_s^{-2}, could be neglected in comparison with the potential energy (proportional to r_s^{-1}) and he suggested that in a dilute electron gas the electrons would arrange themselves in a configuration of minimum potential energy, "probably a body-centered cubic lattice." Fuchs[2] was the first to perform an accurate calculation of the potential energy of an electron lattice in a positive compensating background for the bcc and fcc lattices and he found that the bcc structure was indeed the more stable one, though the difference turned out to be very small.

In 1960 Coldwell-Horsfall and Maradudin[3] evaluated the potential energy per electron for the three primitive cubic electron lattices in much the same way. Like Fuchs, they used summation methods introduced by Ewald and in addition to the static energy they also calculated the correction (proportional to $r_s^{-3/2}$) to the energy due to the zero-point vibrations around the lattice positions. Their results for the static lattices were, in Rydberg units $e^2/2a_0$,

$$\begin{aligned} E_{\text{bcc}} &= -1.791860(1/r_s) \\ E_{\text{fcc}} &= -1.791753(1/r_s) \\ E_{\text{sc}} &= -1.760119(1/r_s) \end{aligned} \tag{1.2}$$

Several people confirmed, simplified, or generalized the calculation, among them Foldy[4] and Nijboer.[5] In the latter paper it was remarked that the

potential energy per electron of an electron gas in a neutralizing background can be expressed as

$$E = -\frac{e^2}{2a_0}\left(\frac{4\pi}{3}\right)^{-1/3}\frac{1}{r_s}\int [1-g(\mathbf{r})]\frac{d^3r}{r} \tag{1.3}$$

where $g(\mathbf{r})$ is the so-called pair-distribution function and the cubic root of the volume per particle is taken as the unit of length in the integral.

The integral can be calculated by the following Ewald-like mathematical transformation:

$$\int \frac{1-g(\mathbf{r})}{r}d^3r = \int \frac{1-g(\mathbf{r})}{r}\Phi(\sqrt{\pi}\cdot r)\,d^3r + \int \frac{1-g(\mathbf{r})}{r}[1-\Phi(\sqrt{\pi}\cdot r)]\,d^3r$$

where

$$\Phi(x) = \mathrm{Erfc}(x) = \frac{\Gamma(1/2, x^2)}{\Gamma(1/2)} = 2\pi^{-1/2}\int_x^\infty \exp(-t^2)\,dt$$

Because

$$\int [\exp(2\pi i\mathbf{h}\cdot\mathbf{r})]\frac{1-\Phi(\sqrt{\pi}\cdot r)}{r}d^3r = \frac{1}{\pi h^2}\exp(-\pi h^2)$$

we find, applying Parseval's theorem,

$$\begin{aligned}\int \frac{1-g(\mathbf{r})}{r}d^3r &= \int [1-g(\mathbf{r})]\frac{\Phi(\sqrt{\pi}\cdot r)}{r}d^3r + \int \frac{1-S(\mathbf{h})}{\pi h^2}\exp(-\pi h^2)\,d^3h \\ &= 3 - \int g(r)\frac{\Phi(\sqrt{\pi}\cdot r)}{r}d^3r - \int S(\mathbf{h})\frac{\exp(-\pi h^2)}{\pi h^2}d^3h \end{aligned} \tag{1.4}$$

Here $S(\mathbf{h})$ is the so-called structure function; $S(\mathbf{h})-1$ is the Fourier transform of $g(\mathbf{r})-1$. For a Bravais lattice $g(\mathbf{r})$ is a sum of δ-functions and $S(\mathbf{h})$ a sum of δ-functions in the reciprocal lattice. For lattices the integrals in (1.4) reduce to lattice sums and they converge very rapidly. This is because $g(0)=0$ and $S(0)$ is also very small, as it represents the relative compressibility of the system (relative with respect to that of an ideal gas).

For the simple cubic lattice, to which for simplicity we will restrict ourselves in the following, one finds[2]

$$\int \frac{1-g(\mathbf{r})}{r} d^3r = 2.837298 \tag{1.5}$$

This number leads with (1.3) to the value mentioned in (1.2) for the energy per electron in an sc lattice. We want to stress that (1.4) may be easily applied to other lattices and also holds for liquids.

In 1979 Hall, referring to unpublished work of Plaskett, published an extensive paper[7] in which he stated that the numbers quoted in (1.2) were incorrect and that a correction term should be applied, depending on the lattice considered and which for the sc lattice amounted to

$$+0.324815(1/r_s) \tag{1.6}$$

resulting in an energy per particle of

$$-1.435304(1/r_s) \quad \text{Ry} \tag{1.7}$$

Hall's paper created at the time quite a controversy. Several authors, among whom we mention in particular de Wette[8] and Ihm and Cohen,[9] argued that Fuchs' values for the energy per particle given in (1.2) were nevertheless correct. One should distinguish between Φ_{el}, which is the energy of one electron in the field due to the other electrons plus the positive background, and Φ_i, which is the energy per particle. This notation is the one used by de Wette. In some types of calculation $\Phi_i = \frac{1}{2}\Phi_{\text{el}}$, an equality which often is assumed to hold without further discussion, e.g., by Fuchs as well as by Hall. Also, in using the expression (1.3) for the energy per particle we have without further discussion identified Φ_i with $\frac{1}{2}\Phi_{\text{el}}$. In other types of calculation (e.g., that by Hall) the equality does not hold. The problem is that one deals with an infinite system and the sums (and integrals) occurring are only conditionally convergent. In the present paper we will present exact calculations of the energies Φ_{el} and Φ_i in a simple cubic lattice by various methods. All of them will turn out to lead to the value for Φ_i quoted in (1.2), thus confirming in more detail the points of view of the authors quoted in references 8

[2] This number had already been found by the same method for the integral $\int \{[1-g(\mathbf{r})]/\pi r^2\}\, d^3r$ for an sc lattice by Placzek *et al.*[6] in 1951, where it occurs in a paper on the scattering of neutrons in dense media. In general one can easily show that the latter integral for a certain Bravais lattice is equal to $\int \{[1-g(\mathbf{r})]/r\}\, d^3r$ for its reciprocal lattice; cf. also ref. 5. By the way, we have checked that if we replace the Coulomb interaction $1/r$ by $1/r^2$ the calculation of the quantity Φ_{el} yields for system I the same value as for system II.

and 9. We will also apply these methods to a two-dimensional simple square Wigner lattice. Here the equality $\Phi_i = \frac{1}{2}\Phi_{el}$ turns out to hold for all methods considered.

2. CALCULATION OF Φ_{el} FOR AN INFINITE SYSTEM OF NEUTRAL CUBES (OR SQUARES); SYSTEM I

2.1. Dimension 3

We consider a simple cubic lattice of electrons (charge $-e$). Each electron is surrounded by a little cube (Wigner–Seitz cell) with edge a, which carries a uniform positive charge density $\rho = e/a^3$. We want to calculate Φ_{el}, which is the energy required to bring an electron from infinity to an empty lattice site in the presence of electrons occupying the remaining sites and the neutralizing positive background. We first consider a finite system consisting of an integer number of these neutral little cubes and then let the dimensions of the system go to infinity in all directions: system I. We only count the contribution of the cells the centers of which fall inside a sphere with arbitrary radius R and then let R go to infinity. Alternatively, we may consider a large cube with edges Na, so that its boundary consists of faces of the little cubes. An infinite system is then obtained by letting N go to infinity. It will be clear that the result for Φ_{el} will be the same in both cases. This is because a multipole expansion of the potential of a neutral cube starts with $l = 4$ and the potential therefore decreases with r^{-5}, where r is the distance from the origin to the center of the little cube [cf. (2.15)].

We first calculate the potential energy $\varphi(\mathbf{r})$ of an electron in the field of one neutral little cube, where $\mathbf{r}$ is the vector between electron and the center of the cell:

$$\varphi(\mathbf{r}) = \frac{e^2}{r} - e\rho \int_* \frac{dr'}{|\mathbf{r} - \mathbf{r}'|} \tag{2.1}$$

where the asterisk indicates that the integration extends over a little cube with edge a. Introducing the dimensionless vectors $\mathbf{u} = \mathbf{r}/a$ and $\mathbf{u}' = \mathbf{r}'/a$, we write (2.1) in the form

$$\varphi(a\mathbf{u}) = (e^2/a)[1/u - I(\mathbf{u})] \tag{2.2}$$

where

$$I(\mathbf{u}) = \int_* \frac{d\mathbf{u}'}{|\mathbf{u} - \mathbf{u}'|} \tag{2.3}$$

is a three-dimensional integral over a cell with unit edges. This integral can be reduced in dimension by substituting

$$\frac{1}{|\mathbf{u}-\mathbf{u}'|}=\frac{2}{\sqrt{\pi}}\int_0^\infty \exp(-\mathbf{t}^2\,|\mathbf{u}-\mathbf{u}'|^2)\,dt \tag{2.4}$$

The integration over the components of $\mathbf{u}'$ may now be performed, leading to the error function

$$\Psi(t)=\frac{2}{\sqrt{\pi}}\int_0^t \exp(-x^2)\,dx$$

After partial integration and using

$$\frac{d\Psi^3}{dt}=\frac{6}{\sqrt{\pi}}\,\Psi^2(t)\,e^{-t^2} \tag{2.5}$$

the final expression for $I(\mathbf{u})$ becomes $(\mathbf{u}=x,\ y,\ z)$

$$I(x,\ y,\ z)=\frac{1}{8}\int_0^\infty \frac{dt}{t^2}\frac{\partial}{\partial t}\,[h(x,\ t)\,h(y,\ t)\,h(z,\ t)] \tag{2.6}$$

with

$$h(x,\ t)=\Psi\{(x+\tfrac{1}{2})\,t\}-\Psi\{(x-\tfrac{1}{2})\,t\} \tag{2.7}$$

For the special case $\mathbf{u}=0$ we find

$$I(0)=\int_* \frac{d\mathbf{r}}{r}=\frac{3}{2}\sqrt{\pi}\int_0^\infty \frac{dt}{t^2}\,\Psi^2(t)\,e^{-t^2} \tag{2.8}$$

This integral can be evaluated explicitly. After some partial integrations we obtain

$$I(0)=-\frac{\pi}{2}+6\int_0^\infty e^{-2t^2}\Psi(t)\,\frac{dt}{t}$$

$$-\frac{\pi}{2}+\frac{6}{\sqrt{2\pi}}\int_0^\infty \frac{e^{-x}}{\sqrt{x}}\,{}_1F_1(1/2;\,3/2;\,-1/2x)\,dx$$

where ${}_1F_1$ is the confluent hypergeometric function. Using the relation

$${}_1F_1(1/2;\,3/2;\,-1/2x)=\exp(-1/2x)\;{}_1F_1(1;\,3/2;\,1/2x)$$

one can perform the integration. The result is[3]

$$I(0) = -\frac{\pi}{2} + 3 \log \frac{\sqrt{3}+1}{\sqrt{3}-1} = 2.380077 \tag{2.9}$$

The integral in (2.6) converges rapidly to zero for $t \to \infty$ and may be calculated numerically, using, e.g., the representation of the error function given in ref. 10. The potential energy Φ_{el} can now be expressed as a sum of contributions from all cubic cells with the central cell treated separately. We find

$$\Phi_{el} = \frac{e^2}{a}\left[-I(0) + \sum_{k,l,m}{}' \{(k^2+l^2+m^2)^{-1/2} - I(k,l,m)\} \right] \tag{2.10}$$

the term $k = l = m = 0$ being omitted from the sum. This sum is absolutely convergent and can easily be calculated numerically. In Table I (first column) we list the values of the expression between braces in (2.10), when the sum is truncated at the value $n = k^2 + l^2 + m^2$.

It is seen that the series converges very rapidly to a limiting value, which in Rydberg units is given by

$$\Phi_{el} = -2.0 * 1.43531(1/r_s) \quad \text{Ry} \tag{2.11}$$

Notice that $I(0)$ taken alone deviates only about 3% from the final sum. The value (2.11) agrees with the computer result obtained by de Wette,[8] presumably by using the scaled result (2.9) for a large cube and

[3] We thank Dr. F. W. de Wette for reminding us of this result. It had actually been derived by one of us (B.N.) already in 1964 (unpublished), but forgotten in the mean time.

Table I

n	Term in $\{\cdot\}$ in (2.10)	Multipoles
0	−2.380077	-
1	−2.304807	−2.30637
2	−2.310437	−2.31469
3	−2.315897	−2.31494
4	−2.313237	−2.31449
5	−2.311887	−2.31447
6	−2.312907	−2.31447
8	−2.313127	−2.31443
100	−2.312967	—

adding the contributions from the lattice points inside that cube. The same value had been found by Hall[7] by applying a correction to Fuchs' value for Φ_i.

Another way to calculate the potential of a neutral cube (2.1) is by way of a multipole expansion. Using the convention for spherical harmonics as given by Jackson,[11] we can write

$$\varphi(\mathbf{r}) = -e \sum_{l,m} 4\pi(2l+1)^{-1} Q_{lm} r^{-l-1} Y_{lm}(\theta, \varphi), \qquad r > \tfrac{1}{2}a\sqrt{3} \tag{2.12}$$

with the multipole moment

$$Q_{l,m} = \frac{e}{a^3} \int_* r'^l Y^*_{lm}(\theta, \varphi)\, d\mathbf{r}', \qquad Q_{00} = 0 \tag{2.13}$$

However, an expansion in terms of harmonic functions which have cubic symmetry is perhaps more convenient. If $Y_l(x, y, z)$ is such a harmonic of degree l, then $\Delta(r^{-l-1}Y_l) = 0$ should hold. For each $l \leqslant 10$ these functions are uniquely defined, up to a normalizing factor. They are

$$\begin{aligned}
Y_4 &= 3r^4 - 5(x^4 + y^4 + z^4) \\
Y_6 &= 17(x^6 + y^6 + z^6) - 15r^2(x^4 + y^4 + z^4) + 180x^2y^2z^2 \\
Y_8 &= 5(x^8 + y^8 + z^8) + 28r^2(x^6 + y^6 + z^6) - 35(x^4 + y^4 + z^4)^2 \\
Y_{10} &= 5(x^{10} + y^{10} + z^{10}) - 45r^2(x^8 + y^8 + z^8) + 42(x^6 + y^6 + z^6)(x^4 + y^4 + z^4) \\
&\quad + 1638x^2y^2z^2(x^4 + y^4 + z^4) - 630x^2y^2z^2r^4
\end{aligned} \tag{2.14}$$

The normalization chosen was such that $Y_{2l}(1, 0, 0) = 2(-1)^{l+1}$. The expansion of $\varphi(\mathbf{r})$ may now be written as

$$\varphi(x, y, z) = e^2 \sum_{l=4}^{10} \frac{(-1)^{l/2} a^l}{2^{l+1}} M_l \frac{Y_l(x, y, z)}{r^{2l+1}} + \cdots \tag{2.15}$$

The moments M_l can be expressed in terms of the multipole moments Q_{lm}. In this way we find

$$M_l = \int_0^1 \int_0^1 \int_0^1 r^l P_l\left(\frac{z}{r}\right) dx\, dy\, dz \tag{2.16}$$

The calculation of these moments is tedious, but the results have been checked in an independent way:

$$M_4 = -7/30, \qquad M_6 = 2/21, \qquad M_8 = 11/40, \qquad M_{10} = -13/33 \tag{2.17}$$

With the potential $\varphi(x, y, z)$ of (2.15) we calculated Φ_{el} again by adding the contributions (up to $l=10$) of all neutral cubes the center of which lie inside a sphere with radius $\sqrt{n}$. For the central cube we took the value given in (2.9). The results obtained in this way are given in the second column of Table I, where they may be compared with the exact values.

2.2. Dimension 2

For the two-dimensional square lattice the integral (2.3) for $I(\mathbf{u})$ can be expressed in terms of elementary functions. With $\mathbf{u}=(x, y)$ we find the symmetric expression:

$$\begin{aligned} I(\mathbf{u}) = (x+\tfrac{1}{2})[f(y-\tfrac{1}{2}, x+\tfrac{1}{2}) - f(y+\tfrac{1}{2}, x+\tfrac{1}{2})] \\ + (x-\tfrac{1}{2})[f(y+\tfrac{1}{2}, x-\tfrac{1}{2}) - f(y-\tfrac{1}{2}, x-\tfrac{1}{2})] \\ + \text{same expression with } x \text{ and } y \text{ interchanged} \end{aligned} \tag{2.18}$$

in which

$$f(x, y) = \log[(x^2+y^2)^{1/2} - x] \tag{2.19}$$

Using again (2.10), but now summing over the two-dimensional square lattice, we obtain for the individual terms in the sum the numbers shown in Table II. There we also list the value of $\varphi_{as}(k, l) = -1/24(k^2+l^2)^{-3/2}$, giving the asymptotic behavior of $(k^2+l^2)^{-1/2} - I(k, l)$. The sum is again absolutely convergent, but the rate is less than in three dimensions. For the case of neutral squares with centers inside a circle of radius R we obtain $\Phi_{el} = -e^2/aI_R$, with

$$I_{50} = 3.895026, \qquad I_{100} = 3.897647 \tag{2.20}$$

Table II

k, l	Term in $[\cdot]$ in (2.10)	φ_{as}
0, 0	−3.525494	—
1, 0	−0.038050	−0.041667
1, 1	−0.017591	−0.014731
2, 0	−0.005092	−0.005208
2, 1	−0.003875	−0.003727
2, 2	−0.001932	−0.001841

Since the approach to the limiting value is slow, we should add the contribution of the squares outside the circle. For large R this may be approximated by

$$\frac{2\pi}{24}\int_R^\infty \frac{r\,dr}{r^3} = \frac{\pi}{12R} \tag{2.21}$$

Finally we obtain the value for the two-dimensional square lattice

$$I_\infty = 3.90026 \tag{2.22}$$

3. CALCULATION OF Φ_{el} FOR NEUTRAL SPHERES (OR CIRCLES) WITH INCREASING RADII; SYSTEM II

3.1. Dimension 3

We consider again a simple cubic lattice, the sites of which are occupied by electrons, and there is a neutralizing positive background with uniform charge density $\rho = e/a^3$. As in Section 2, we want to calculate the value of Φ_{el} for a set of spheres with increasing radii, but now the spheres do not contain an integer number of neutral little cubes, but the radii $a\sqrt{p_i}$ are chosen in such a way that the whole sphere is electrically neutral, that is,

$$\frac{4\pi}{3} p_i^{3/2} = \sum_{n=0}^{p_i} g(n) \tag{3.1}$$

Here $a^2 n = a^2(n_1^2 + n_2^2 + n_3^2)$ is the square of the distance of lattice point (n_1, n_2, n_3) to the origin, $g(n)$ is the number of lattice points which have a distance $a\sqrt{n}$ to the center of the sphere, and $\sum_{n=0}^{p_i}$ extends to the largest integer $[p_i] \leqslant p_i$. Notice that for most integer values of p the sum $\sum_{n=1}^{p} [g(n)/\sqrt{n}]$ jumps by an amount of order 2π (see Appendix A), but in $\sum_{n=1}^{p_i}$ we mean to include the value of $g(n)/\sqrt{n}$ at $n = [p_i]$. As the contribution of the positive charge inside the sphere to Φ_{el} is given by $(2\pi e^2/a)\, p_i$, we should calculate

$$\Phi_{el} = \lim_{i \to \infty} \frac{e^2}{a} \left\{ \sum_{n=1}^{p_i} \frac{g(n)}{\sqrt{n}} - 2\pi p_i \right\} \tag{3.2}$$

We replace this limit of a sequence for discrete values p_i by the limit of a continuous function of p, which for $p = p_i$ has according to (3.1) the above values:

$$\Phi_{el} = \lim_{p \to \infty} \frac{e^2}{a} \left\{ \sum_{n=1}^{p} \frac{g(n)}{\sqrt{n}} - \frac{2\pi}{3} p - \frac{1}{\sqrt{p}} \sum_{n=0}^{p} g(n) \right\} \equiv \lim_{p \to \infty} \frac{e^2}{a} f(p) \tag{3.3}$$

This limit is evaluated by introducing the (modified) Laplace transform

$$\bar{f}(s) \equiv \int_0^\infty e^{-sp} p^{1/2} f(p)\, dp \tag{3.4}$$

of the function $f(p)$ and then applying an appropriate form of Tauber's theorem[12] (see Appendix A).

When the result is written as $\Phi_{el} = -(e^2/a)\,\mathscr{I}$, the dimensionless quantity $\mathscr{I}$ is found to be given by

$$\mathscr{I} = 3 - \sum_{n=1}^{\infty} g(n) \frac{e^{-n\pi}}{n\pi} - \sum_{n=1}^{\infty} g(n) \frac{\Phi(\sqrt{\pi}\, n)}{\sqrt{n}} \tag{3.5}$$

This is exactly the same expression as is obtained by the Ewald-like transformation briefly explained in the Introduction. When the general result of this transformation (1.4) is applied to the simple cubic lattice, (3.5) is found. The two series in (3.5) converge very rapidly; only three or four terms are needed to lead to the values

$$\begin{aligned} \mathscr{I} &= 2.837298 \\ \Phi_{el} &= -2.0 * 1.760119(1/r_s) \quad \text{Ry} \end{aligned} \tag{3.7}$$

already mentioned in the Introduction.

This result for system II deviates considerably from the result (2.11) obtained in Section 2 by summing over a large number of neutral cells (system I) and this deviation actually led to the controversy mentioned in the Introduction. We want to stress that the boundaries of the finite series considered in the two systems are different.

By performing a computer calculation of the limit (3.2), we found that the value (3.7) was indeed obtained for a series of p_i corresponding to neutral spheres. In this calculation one starts with a sphere the radius of which is the square root of an integer N. For most N there are a number of lattice points $g(N)$ on that sphere. Usually the volume of this sphere is a little smaller than the number of lattice points $\sum_{n=0}^{N} g(n)$ on and within that sphere. Then one increases the radius a little so that $\sum_{n=0}^{p} g(n) = (4\pi/3)\, p^{3/2}$. One should be careful, however, that the p found in this way remains smaller than $N+1$.

We have come to the conclusion that the Ewald-like method of summation (integration) is equivalent to summation over large neutral spheres.

3.2. Dimension 2

We have performed an analogous calculation summing over a sequence of neutral circles with increasing radius. It is described in some

detail in Appendix A. Again in this case the analytical expression for Φ_{el} found by the Laplace-transform method is identical to that obtained by the Ewald transformation, also briefly described in that Appendix. We find [see (A.17)]

$$\Phi_{el} = -(e^2/a)\,\mathscr{I}, \qquad \text{with} \quad \mathscr{I} = 3.90025 \tag{3.8}$$

However, in two dimensions this value agrees closely with that found in (2.22) by summation over a large integer number of neutral squares. Hence, in two dimensions systems I and II give the same outcome.

For the two-dimensional case we did a computer calculation for large values of p of the function

$$f(p) \equiv \sum_{n=0}^{p} \frac{g(n)}{\sqrt{n}} - 2\pi\sqrt{p} \tag{3.9}$$

for two series of p values. The first series of p_i was chosen such that

$$\sum_{n=0}^{p_i} g(n) = \pi p_i \tag{3.10}$$

corresponding to neutral circles. In the second series of p values such a condition was not imposed. For the first series the value of $f(p_i)$ rapidly approached the value of $\mathscr{I}$ given in (3.8). For the second series the fluctuations in $f(p)$ were larger, but also in this case the limit $\mathscr{I}$ was approached eventually. The explanation for this behavior, which was different in three dimensions, lies in the fact that in two dimensions $g(n)$ is either 4 or 8 (or 0), so that the discontinuities in $f(p)$ go to zero for $p \to \infty$.

4. THE RELATION BETWEEN Φ_{el} AND Φ_i

Remember that Φ_{el} has been defined as the potential energy of an electron at a lattice point of an infinite Wigner lattice due to the other electrons and the uniform positive background (self-energy of this electron omitted); Φ_i is defined as the potential energy per electron in the same system. In Sections 2 and 3 we have shown by exact calculations that in the three-dimensional case Φ_{el} calculated for the limit of a large system built up of an integer number of neutral cells (system I) differs from Φ_{el} calculated for a set of neutral spheres with increasing radius (system II). As far as we know this conclusion was first drawn by de Wette in his paper[8] mentioned in the Introduction by applying the so-called spherical

approximation. In this paper and also by Ihm and Cohen[9] it has further been shown that the following relation holds:

$$\Phi_i = \tfrac{1}{2}(\Phi_{\mathrm{el}} + eV_{\mathrm{av}}) \tag{4.1}$$

where V_{av} is the average potential in the lattice: $V_{\mathrm{av}} = (1/v_{\mathrm{cell}}) \int_{\mathrm{cell}} V(\mathbf{r})\, d\mathbf{r}$. We observe that in Φ_{el} the self-energy of the electron is omitted, but that in the definition of V_{av} the singularity at the position of the electron is included. It has been mentioned before that in the past the equality of Φ_i and $\frac{1}{2}\Phi_{\mathrm{el}}$ had usually been accepted without discussion. De Wette[8] calculated V_{av} in spherical approximation for system I and from (4.1) also Φ_i. This Φ_i turned out to have the same value as that calculated directly in the same approximation, and it was shown to be close to the exact Fuchs value given in (1.2).

In this section we discuss these problems in somewhat greater detail. We calculate V_{av} for system I exactly and we give a simple direct proof that in the Ewald method V_{av} is zero.

For the total potential energy of system I we have

$$\Phi = \sum_i \Phi_i = \sum_i \left[\frac{e^2}{2} \sum_{j \neq i} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} - e\rho \int_V \frac{d\mathbf{r}}{|\mathbf{r} - \mathbf{R}_i|} + \frac{\rho^2}{2} \int_{(i)} \int_V \frac{d\mathbf{r}_i\, d\mathbf{r}'}{|\mathbf{r}_i - \mathbf{r}'|} \right] \tag{4.2}$$

i and j number the neutral cubic cells, V is the total volume containing an integer number of cells and going to infinity, $\mathbf{R}_i$ and $\mathbf{R}_j$ indicate the lattice points, and ρ is the positive charge density e/a^3. The summand may be written as

$$\Phi_i = \sum_{j \neq i} \left[\frac{e^2}{2} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} - e\rho \int_{(j)} \frac{d\mathbf{r}_j}{|\mathbf{r}_j - \mathbf{R}_i|} + \frac{\rho^2}{2} \int_{(i)} \int_{(j)} \frac{d\mathbf{r}_i\, d\mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|} \right]$$
$$- e\rho \int_{(i)} \frac{d\mathbf{r}_i}{|\mathbf{r}_i - \mathbf{R}_i|} + \frac{\rho^2}{2} \int_{(i)} \int_{(i)} \frac{d\mathbf{r}\, d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \tag{4.3}$$

The term between brackets indicates the interaction between neutral cells i and j. For large distance $|\mathbf{R}_i - \mathbf{R}_j|$ it becomes very small, so that $\sum_{j \neq i}$ is a rapidly converging series, which for V sufficiently large no longer depends on $\mathbf{R}_i$. The two remaining terms give the self-energy of a neutral cell (self-energy of the electron omitted). Hence Φ_i is independent of $\mathbf{R}_i$.

The potential energy of an electron at lattice point $\mathbf{R}_i$ is

$$\Phi_{\mathrm{el}}(i) = e^2 \sum_{j \neq i} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} - e\rho \int_V \frac{d\mathbf{r}}{|\mathbf{r} - \mathbf{R}_i|} \tag{4.4}$$

and may be written as

$$\Phi_{\rm el}(i)=\sum_{j\neq i}\left[\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}-e\rho\int_{(j)}\frac{d\mathbf{r}_j}{|\mathbf{r}_j-\mathbf{R}_i|}\right]-e\rho\int_{(i)}\frac{d\mathbf{r}_i}{|\mathbf{r}_i-\mathbf{R}_i|} \tag{4.5}$$

Here the term between brackets is the contribution to the potential energy of the electron at $\mathbf{R}_i$ from the neutral cell j. This series is again rapidly convergent, and hence for sufficiently large V, $\Phi_{\rm el}$ again does not depend on $\mathbf{R}_i$.

If we now write

$$\Phi_i=\tfrac{1}{2}\Phi_{\rm el}+\Delta\Phi \tag{4.6}$$

we find

$$\begin{aligned}\Delta\Phi&=\sum_{j\neq i}\left\{-\frac{1}{2}e\rho\int_{(j)}\frac{d\mathbf{r}_j}{|\mathbf{r}_j-\mathbf{R}_i|}+\frac{\rho^2}{2}\int_{(i)}\int_{(j)}\frac{d\mathbf{r}_i\,d\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}\right\}\\&\quad-\frac{1}{2}e\rho\int_{(i)}\frac{d\mathbf{r}_i}{|\mathbf{r}_i-\mathbf{R}_i|}+\frac{1}{2}\rho^2\int_{(i)}\int_{(i)}\frac{d\mathbf{r}_i\,d\mathbf{r}_i'}{|\mathbf{r}_i-\mathbf{r}_i'|}\\&=\sum_{\text{all }j}\left\{-\frac{1}{2}e\rho\int_{(j)}\frac{d\mathbf{r}_j}{|\mathbf{r}_j-\mathbf{R}_i|}+\frac{1}{2}\rho^2\int_{(i)}\int_{(j)}\frac{d\mathbf{r}_i\,d\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}\right\}\end{aligned} \tag{4.7}$$

A little reflection shows that we may alternatively write

$$\Delta\Phi=\sum_{\text{all }j}\left\{-\frac{1}{2}e\rho\int_{(i)}\frac{d\mathbf{r}_i}{|\mathbf{r}_i-\mathbf{R}_j|}+\frac{1}{2}\rho^2\int_{(i)}\int_{(j)}\frac{d\mathbf{r}_i\,d\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}\right\} \tag{4.8}$$

This is (except for a factor $\frac{1}{2}$) the expression B in Eq. (6) of the paper of Ihm and Cohen[9] and we see that it represents indeed one-half of the average potential $V_{\rm av}$. In (4.7) we take the lattice $\mathbf{R}_i$ as origin of coordinates; (i) is the central cubic cell with edge a. We write

$$\Delta\Phi=\frac{e^2}{2a^6}\int_{(i)}d\mathbf{r}_i\int d\mathbf{r}_j\left(\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\frac{1}{r_j}\right) \tag{4.9}$$

Now, for $r_j>r_i$,

$$\begin{aligned}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\frac{1}{r_j}&=\frac{1}{r_j}\sum_{l=0}^{\infty}P_l(\cos\theta_{ij})\left(\frac{r_i}{r_j}\right)^l-\frac{1}{r_j}\\&=\frac{1}{r_j}\sum_{l=1}^{\infty}P_l(\cos\theta_{ij})\left(\frac{r_i}{r_j}\right)^l\end{aligned} \tag{4.10}$$

With the addition theorem of spherical harmonics we can express $P_l(\cos\theta_{ij})$ in terms of the polar angles of $\mathbf{r}_i$ and $\mathbf{r}_j$ separately and we conclude that the integration over the polar angles of $\mathbf{r}_j$ gives zero.

On the other hand, for $r_j < r_i$,

$$\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{1}{r_j} = \frac{1}{r_i} \sum_{l=0}^{\infty} P_l(\cos\theta_{ij}) \left(\frac{r_j}{r_i}\right)^l - \frac{1}{r_j} \tag{4.11}$$

If now we integrate over the angles of $\mathbf{r}_j$, the terms with $l > 0$ vanish and we obtain

$$\begin{aligned} \Delta\phi &= \frac{e^2}{2a^6} \iint_{-1/2a}^{+1/2a} \int dx_i\, dy_i\, dz_i \int_0^{r_i} 4\pi \left(\frac{1}{r_i} - \frac{1}{r_j}\right) r_j^2\, dr_j \\ &= -\frac{e^2}{2a^6} \iint_{-1/2a}^{+1/2a} \int dx_i\, dy_i\, dz_i \frac{2\pi}{3} r_i^2 = -\frac{\pi e^2}{12a} \end{aligned} \tag{4.12}$$

This result corresponds with $-\frac{1}{2}A$, where A is Hall's correction term,[7] and with the term $\frac{1}{2}B$ of Ihm and Cohen.[9] With the relation (4.6) and the value of Φ_{el} obtained for system I in (2.11) we now find for the simple cubic lattice for the energy per particle Φ_i the value $-1.760119(1/r_s)$ Ry already mentioned in (1.2) of the Introduction, which had been found by several authors when calculating Φ_{el} by the Ewald method or (which is equivalent, as we have seen) for system II.

In view of the relation (4.1), this would mean that in the Ewald method the average potential V_{av} must be zero. This is indeed true; in this respect one often refers to a paper by Birman.[13] In Appendix B we give a simple direct proof for the particular case of a Wigner lattice. Because, as was shown in Section 3, the calculation for system II (spheres with increasing radius such that they are neutral) leads to the same analytical expression (3.5) for Φ_{el} as the Ewald method, we come to the conclusion that also for system II the average potential is zero. A direct proof of this statement seems to be difficult and has not been given.

In this paper we have investigated two kinds of infinite simple cubic Wigner lattices, which we called systems I and II, respectively. We found that, though Φ_{el} was different for these two types, Φ_i has the same value. One might of course also imagine infinite systems as the limit of other shapes, e.g., neutral ellipsoids or parallelopipeds. We think it highly probable that for these, Φ_{el} again may have a different value and that Φ_i is unique. But a proof has not been given.

In Sections 2 and 3 we have also briefly discussed the two-dimensional analogues of systems I and II for the simple square Wigner lattice. We found that Φ_{el} has the same value for both systems and that in both cases

$\Phi_i = \frac{1}{2}\Phi_{\rm el}$. We should expect, therefore, that the two-dimensional analogue of (4.9) for $\Delta\Phi$ would give zero, in contrast with the three-dimensional case. This turns out to be correct.

To calculate for two dimensions

$$\int_{(i)} d\mathbf{r}_i \int d\mathbf{r}_j \left(\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{1}{r_j} \right)$$

of (4.9), we first integrate the second integral over the angle φ between $\mathbf{r}_i$ and $\mathbf{r}_j$,[14]

$$\int_0^{2\pi} \frac{d\varphi}{(r_i^2 + r_j^2 - 2r_i r_j \cos\varphi)^{1/2}} = 4r_>^{-1} K\left(\frac{r_<}{r_>}\right) \tag{4.13}$$

Here $r_>$ is the largest, $r_<$ is the smallest, from r_i and r_j, and K is the complete elliptic integral of the first kind. Hence

$$\Delta\Phi = \frac{e^2}{2a^4} \int_{(i)} d\mathbf{r}_i \left\{ \int_0^{r_i} r_j\, dr_j \left[\frac{4}{r_i} K\left(\frac{r_j}{r_i}\right) - \frac{2\pi}{r_i} \right] + \int_{r_i}^{\infty} r_j\, dr_j \left[\frac{4}{r_j} K\left(\frac{r_i}{r_j}\right) - \frac{2\pi}{r_j} \right] \right\} \equiv \frac{e^2}{2a} \int_* r\, d\mathbf{r}\, J \tag{4.14}$$

with

$$J = \int_0^1 dx \left[4xK(x) - 2\pi + \frac{4}{x^2} K(x) - \frac{2\pi}{x^2} \right]$$

and $\int_*$ means integration over a square with unit side. With the help of formulas 6.146, 5.112.9, and 8.114.1 of ref. 14, one finds $J = 0$ and therefore $\Delta\Phi = 0$. We conclude that the average potential is $\Phi_{\rm av} = 0$ in two dimensions also for system I.

APPENDIX A. SUMMATION OVER NEUTRAL SPHERES (OR CIRCLES) WITH INCREASING RADIUS

A1. Dimension 3[4]

Consider a simple cubic lattice of electrons with lattice constant 1. The distance of a lattice point n_1, n_2, n_3 to the origin $n_i = 0$ is given by

[4] The following derivation had been completed in 1979 at the time of the controversy mentioned in the Introduction. A substantial contribution was then made by our student W. J. Ventevogel.

$n^{1/2} = (n_1^2 + n_2^2 + n_3^2)^{1/2}$. Let us call $g(n)$ the number of lattice points on the spherical surface with radius $n^{1/2}$. We want to investigate $\sum_{n=1}^{N} [g(n)/n^{1/2}]$ for large values of N. Except for a factor $-e$ (the electron charge), this sum gives the potential at the origin due to the electrons inside and on the surface of a sphere with radius $N^{1/2}$ (the self-energy of the electron at the origin excluded). Inside the sphere we have also a uniform compensating positive charge with density $+e$. The potential energy of an electron at the origin due to the other electrons and the uniform charge inside the sphere is then

$$\Phi_{\text{el}} = e^2 \left(\sum_{n=1}^{N} \frac{g(n)}{n^{1/2}} - 2\pi N \right) \tag{A.1}$$

Now, for almost all integers n, $g(n) \approx 4\pi/3[n^{3/2} - (n-1)^{3/2}] \approx 2\pi n^{1/2}$ for large n. Hence, the sum in the expression above jumps for almost all integer numbers N by an amount of about 2π and therefore has no proper limit. We now consider a sequence of neutral spheres with radius $p_i^{1/2}$ such that

$$\frac{4\pi}{3} p_i^{3/2} = \sum_{n=0}^{p_i} g(n) \tag{A.2}$$

Here $\sum_{n=0}^{p}$ is defined as $\sum_{n=0}^{[p]}$, where $[p]$ is the largest integer $\leqslant p$. If (A.2) is satisfied, the uniform charge exactly compensates the charge of the electrons inside (or on) the sphere. We now want to calculate

$$\lim_{i \to \infty} \left[\sum_{1}^{p_i} \frac{g(n)}{n^{1/2}} - 2\pi p_i \right] \tag{A.3}$$

or rather, if we replace this limit by the limit of a continuous function of p, which for $p = p_i$ has the above values

$$\lim_{p \to \infty} \left[\sum_{n=1}^{p} \frac{g(n)}{n^{1/2}} - \frac{2\pi}{3} p - \frac{1}{p^{1/2}} \sum_{n=0}^{p} g(n) \right] \tag{A.4}$$

Let us call the expression between brackets $f(p) = f_1(p) + f_2(p) + f_3(p)$. We now introduce the (modified) Laplace transform

$$\bar{f}(s) \equiv \int_0^{\infty} e^{-sp} p^{1/2} f(p)\, dp \tag{A.5}$$

and apply the well-known Tauber theorem,[12] which says

$$\lim_{p \to \infty} f(p) = \lim_{s \to 0} \frac{2}{\pi^{1/2}} s^{3/2} \bar{f}(s) \tag{A.6}$$

Now

$$\bar{f}_2(s) \equiv -\frac{2\pi}{3}\int_0^\infty e^{-sp}p^{3/2}\,dp = -\frac{1}{2}\pi^{3/2}s^{-5/2}$$

$$\bar{f}_3(s) = -\int_0^\infty e^{-sp}\sum_{n=0}^{p} g(n)\,dp = -s^{-1}\sum_{n=0}^{\infty} g(n)\,e^{-sn}$$

$$\bar{f}_1(s) = \int_0^\infty e^{-sp}p^{1/2}\sum_{n=1}^{p}\frac{g(n)}{n^{1/2}}\,dp = s^{-3/2}\int_s^\infty \sum_{n=1}^{\infty} ng(n)\,e^{-nt}t^{1/2}\,dt$$

$$= -s^{-3/2}\int_s^\infty t^{1/2}\frac{\partial}{\partial t}\sum_{n=1}^{\infty} g(n)\,e^{-nt}\,dt$$

$$= s^{-1}\sum_{n=1}^{\infty} g(n)\,e^{-sn} + \frac{1}{2}s^{-3/2}\int_s^\infty \sum_{n=1}^{\infty} g(n)\,e^{-nt}\frac{dt}{t^{1/2}}$$

Hence

$$2\pi^{-1/2}s^{3/2}\bar{f}(s) = -\pi s^{-1} - 2(s/\pi)^{1/2} + \pi^{-1/2}\int_s^\infty t^{-1/2}\sum_{n=1}^{\infty} g(n)\,e^{-nt}\,dt \qquad \text{(A.7)}$$

Notice that

$$\sum_{n=1}^{\infty} g(n)\,e^{-nt} \equiv \left(\sum_{m=-\infty}^{-\infty} e^{-m^2t}\right)^3 - 1$$

and according to a well-known relation of the theta function,

$$\sum_{m=-\infty}^{+\infty} \exp(-m^2t) = (\pi/t)^{1/2}\sum_{m=-\infty}^{+\infty} \exp(-m^2\pi^2t^{-1})$$

We want to study the expression (A.7) for small s and split the integral $\int_s^\infty = \int_s^\pi + \int_\pi^\infty$. Then

$$\pi^{-1/2}\int_s^\pi t^{-1/2}\sum_{n=1}^{\infty} g(n)\,e^{-nt}\,dt$$

$$= \pi^{-1/2}\int_s^\pi t^{-1/2}\left\{(\pi/t)^{3/2}\left[\sum_{m=-\infty}^{+\infty}\exp(-m^2\pi^2t^{-1})\right]^3 - 1\right\}dt$$

$$= \pi\int_s^\pi t^{-2}\left\{\left[\sum_{m=-\infty}^{+\infty}\exp(-\pi^2m^2t^{-1})\right]^3 - 1\right\}dt$$

$$+ \pi\int_s^\pi t^{-2}\,dt - \pi^{-1/2}\int_s^\pi t^{-1/2}\,dt$$

$$= \pi^{-1}\int_\pi^{\pi^2/s}\left\{\left[\sum_{-\infty}^{+\infty}\exp(-m^2u)\right]^3 - 1\right\}du + \pi/s - 1 - 2 + 2(s/\pi)^{1/2} \qquad \text{(A.8)}$$

Finally, from (A.6), (A.7) and (A.8),

$$\lim_{p\to\infty} f(p) = \pi^{-1}\int_{\pi}^{\infty}\left\{\left[\sum_{m=-\infty}^{+\infty}\exp(-m^2u)\right]^3 - 1\right\}du$$
$$+\pi^{-1/2}\int_{\pi}^{\infty} t^{-1/2}\left\{\left[\sum_{m=-\infty}^{+\infty}\exp(-m^2t)\right]^3 - 1\right\}dt - 3$$
$$= \sum_{n=1}^{\infty} g(n)\frac{e^{-\pi n}}{\pi n} + \sum_{n=1}^{\infty} g(n)\frac{\Phi(\sqrt{\pi}\,n)}{\sqrt{n}} - 3$$
$$= 0.086169 + 0.076533 - 3 = -2.837297 \qquad \text{(A.9)}$$

This is the result (1.4) from the Introduction when applied to a simple cubic lattice. For the potential energy of an electron in the field of the other electrons plus background we then find

$$\Phi_{\text{el}} = -2 * 1.760119(1/r_s) \quad \text{Ry} \qquad \text{(A.10)}$$

i.e., twice the value of the energy per electron given in the Introduction.

A2. Dimension 2 (Summation over Neutral Circles with Increasing Radius)

Consider a simple square lattice with lattice constant 1. Again $g(n)$ is the number of lattice points on a circle with radius $n^{1/2} = (n_1^2 + n_2^2)^{1/2}$. Now $g(n)$ is roughly of order π for large n, so that the jumps in $\sum_{n=1}^{N}[g(n)/n^{1/2}]$ for large N go to zero. We now consider circles with radius $p_i^{1/2}$, such that

$$\pi p_i = \sum_{n=0}^{p_i} g(n) \qquad \text{(A.11)}$$

The uniform charge inside such a neutral circle contributes a potential $2\pi e p_i^{1/2}$ at the origin. Hence, we should calculate

$$\lim_{p_i\to\infty}\left[\sum_{n=1}^{p_i}\frac{g(n)}{n^{1/2}} - 2\pi p_i^{1/2}\right] = \lim_{p\to\infty}\left[\sum_{n=1}^{p}\frac{g(n)}{n^{1/2}} - 2\pi p^{1/2}\right] \qquad \text{(A.12)}$$

We now use the ordinary Laplace transform $\tilde{f}(s) \equiv \int_0^\infty e^{-sp} f(p)\,dp$ and apply Tauber's theorem,[12] which says

$$\lim_{p\to\infty} f(p) = \lim_{s\to 0} s\tilde{f}(s) \qquad \text{(A.13)}$$

If we write

$$\sum_{n=1}^{p}\frac{g(n)}{n^{1/2}} \equiv f_1(p), \qquad -2\pi p^{1/2} \equiv f_2(p)$$

we then have

$$s\bar{f}_1(s) = \sum_{n=1}^{\infty} \frac{g(n)\, e^{-ns}}{n^{1/2}} = \pi^{-1/2} \int_0^{\infty} \left\{ \left[\Theta\left(\frac{x+s}{\pi}\right) \right]^2 - 1 \right\} x^{-1/2}\, dx \tag{A.14}$$

where the theta function $\Theta(x) \equiv \sum_{n=-\infty}^{+\infty} \exp(-\pi n^2 x)$ with the property that $\Theta(x) = x^{-1/2}\Theta(x^{-1})$. Further,

$$s\bar{f}_2(s) = -2\pi s \int_0^{\infty} e^{-sp} p^{1/2}\, dp = -\pi^{3/2} s^{-1/2} = -\pi^{1/2} \int_0^{\infty} \frac{dx}{(s+x)\, x^{1/2}} \tag{A.15}$$

Therefore,

$$s\,[\bar{f}_1(s) + \bar{f}_2(s)] = \pi^{-1/2} \int_0^{\infty} \left\{ \left[\Theta\left(\frac{x+s}{\pi}\right) \right]^2 - \frac{\pi}{s+x} - 1 \right\} x^{-1/2}\, dx \tag{A.16}$$

We may now take the limit $s \to 0$ and we find, applying (A.13),

$$\begin{aligned}
&\lim_{p\to\infty} \left(\sum_{n=1}^{p} \frac{g(n)}{n^{1/2}} - 2\pi p^{1/2} \right) \\
&\quad = \pi^{-1/2} \int_0^{\infty} \left\{ \left[\Theta\left(\frac{x}{\pi}\right) \right]^2 - \frac{\pi}{x} - 1 \right\} x^{-1/2}\, dx \\
&\quad = \pi^{-1/2} \int_{\pi}^{\infty} \left[\sum_{1}^{\infty} g(n)\, e^{-nx} - \frac{\pi}{x} \right] x^{-1/2}\, dx \\
&\qquad + \pi^{-1/2} \int_0^{\pi} \left[\frac{\pi}{x} \Theta^2\left(\frac{\pi}{x}\right) - \frac{\pi}{x} - 1 \right] x^{-1/2}\, dx \\
&\quad = -4 + 2 \sum_{n_1=-\infty}^{-\infty} {\sum_{n_2=-\infty}^{+\infty}}' (n_1^2 + n_2^2)^{-1/2}\, \Phi(\pi^{1/2}(n_1^2+n_2^2)^{1/2}) \\
&\quad = -4 + 0.09975 = -3.90025
\end{aligned} \tag{A.17}$$

The same result may be obtained from the general Ewald-like transformation indicated in the Introduction:

$$\begin{aligned}
&-\int \frac{1-g(\mathbf{r})}{r}\, d^2r \\
&\quad = -\int [1-g(\mathbf{r})] \frac{\Phi(\pi^{1/2}r)}{r}\, d^2r - \int [1-g(\mathbf{r})] \frac{1-\Phi(\pi^{1/2}r)}{r}\, d^2r \\
&\quad = -\int [1-g(\mathbf{r})] \frac{\Phi(\pi^{1/2}r)}{r}\, d^2r - \int [1-S(\mathbf{h})] \frac{\Phi(\pi^{1/2}h)}{h}\, d^2h \\
&\quad = -4 + 2\int g(\mathbf{r}) \frac{\Phi(\pi^{1/2}r)}{r}\, d^2r
\end{aligned} \tag{A.18}$$

The latter equality holds because the two-dimensional Fourier transform of $[1-\Phi(\pi^{1/2}r)]/r$ is $\Phi(\pi^{1/2}h)/h$ and for a simple square lattice $S(\mathbf{h}) \equiv g(\mathbf{h})$.

APPENDIX B. PROOF THAT IN THE EWALD METHOD THE AVERAGE POTENTIAL FOR THE WIGNER LATTICE IS ZERO

When the cube root of the volume per particle is taken as unit of length, the potential at an arbitrary point $\mathbf{r}$ of the central cell is given by

$$V(\mathbf{r}) = -\frac{e}{r} + e\int \frac{1-g(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|}\,d^3r' \tag{B.1}$$

Application of Parseval's theorem leads to

$$V(\mathbf{r}) = -e/r + e\int [1-S(\mathbf{h})]\exp(2\pi i\mathbf{h}\cdot\mathbf{r})\,(\pi h^2)^{-1}\,d^3h \tag{B.2}$$

Now

$$1-g(\mathbf{r}) = 1-\sum_{\mathbf{n}}{}' \delta(\mathbf{r}-\mathbf{r}_{\mathbf{n}}), \qquad 1-S(\mathbf{h}) = 1-\sum_{\lambda}{}' \delta(\mathbf{h}-\mathbf{h}_\lambda)$$

where the prime at the summation sign means that the origin is excluded. $\mathbf{h}_\lambda$ runs over the vectors of the reciprocal lattice. We now find

$$V(\mathbf{r}) = -e\sum_{\lambda}{}' \frac{\exp(2\pi i\mathbf{h}_\lambda\cdot\mathbf{r})}{\pi h_\lambda^2} \tag{B.3}$$

To obtain the average potential, this expression must be integrated over the unit cell. Now, according to a well-known theorem, $\int_{\text{cell}} \exp(2\pi i\mathbf{h}\cdot\mathbf{r})\,d^3r = 0$ for all reciprocal lattice vectors except the null vector. Hence $V_{\text{av}} = 0$.

REFERENCES

1. E. P. Wigner, *Phys. Rev.* **46**:1002 (1934); *Trans. Faraday Soc.* **34**:678 (1936).
2. K. Fuchs, *Proc. R. Soc. London* **151**:585 (1935).
3. R. A. Coldwell-Horsfall and A. A. Maradudin, *J. Math. Phys.* **1**:395 (1960).
4. L. L. Foldy, *Phys. Rev. B* **17**:4889 (1978).
5. B. R. A. Nijboer, *Philips Res. Rep.* **30**:74 (1975).
6. G. Placzek, B. R. A. Nijboer, and L. Van Hove, *Phys. Rev.* **82**:392 (1951).
7. G. L. Hall, *Phys. Rev. B* **19**:3921 (1979).
8. F. W. de Wette, *Phys. Rev. B* **21**:3751 (1980).

9. J. Ihm and M. L. Cohen, *Phys. Rev. B* **21**:3754 (1980).
10. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
11. J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).
12. G. Doetsch, *Theorie und Anwendung der Laplace-transformation* (Springer, Berlin, 1937).
13. J. L. Birman, *J. Phys. Chem. Solids* **6**:65 (1958).
14. I. S. Gradshteyn and J. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1965), formula 3.674.