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On the Green function of periodic Coulomb systems

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In honor of Emanuel Mooser's 60th birthday

Abstract. An analysis of real space representations of the Green function of neutral and periodic Coulomb systems is presented. It is shown how to represent this Green function, generally known through its Fourier representation, in terms of absolutely convergent Poisson sums of auxiliary potential functions. Explicit representations are constructed to treat problems of Electrostatics which occur in periodic systems composed of cells possessing a quadrupole moment.

I. Introduction

The Fourier representation of the Green function of a periodic and neutral Coulomb system in the three dimensional space $\mathbb{R}^3$ is given by

$$G(r) = \sum_K{}' \frac{4\pi}{|\Lambda| K^2} e^{iKr} \tag{1.1}$$

where Λ is the basic cell of the periodic system, $|\Lambda|$ is the volume of the cell, r is a vector in $\Lambda \neq 0$, $|r|$ is its euclidean norm, K is a vector in the reciprocal space and Kr is the ordinary scalar product. The $'$ indicates that the term $K = 0$ is omitted from the sum. This restriction expresses the condition of charge neutrality that the r.h.s. of the Poisson equation (2.4) associated with (1.1) must satisfy. This is so because there is no Green function for the bare Coulomb potential (c.f. [1], p. 98).

The potential energy of a periodic, neutral and dipole-free assembly of any number of charged particles with position vectors $\{r_i\}$ in Λ and charges $\{e_i\}$ is given by

$$V = \tfrac{1}{2} \sum_{i \neq j} e_i e_j G(r_i - r_j) + \sum_i e_i^2 U \tag{1.2}$$

where the shape-dependent constant U is defined by

$$U = \lim_{r \to 0} \frac{1}{2}\left(G(r) - \frac{1}{|r|}\right) \tag{1.3}$$

In Section 4 of this Note, we shall return to (1.3).

If the assembly of charges possesses a non vanishing polarisation, then, (1.2) must be supplemented by a quadratic form in the components of the polarisation as shown particularly clearly by S. W. de Leeuw, J. W. Perram and E. R. Smith in their first paper on the 'Simulation of Electrostatic Systems In Periodic Boundary Conditions' [2].

The purpose of this note is to investigate real space representations of $G(\mathbf{r})$. This means that we are interested in finding representations of $G(\mathbf{r})$ as Poisson sums of auxiliary potential functions centered in the cells of the periodic system, integrable at infinity and with zero mean values. If $g(\mathbf{r})$ is such a function, then

$$G(\mathbf{r})=\sum_{\mathbf{R}} g(\mathbf{r}+\mathbf{R}) \tag{1.4}$$

will be absolutely convergent and defined for all $\mathbf{r}$ in $\mathbb{R}^3 \neq \{\mathbf{R}\}$ where $\{\mathbf{R}\}$ is the set of the centers of the cells $\Lambda(\mathbf{R})$ which cover $\mathbb{R}^3$. We shall often write $\Lambda(0)=\Lambda$ for simplicity.

In the following sections, we shall introduce a certain class of functions $g(\mathbf{r})$ satisfying the requirements listed above and we shall discuss the application of specific representations to problems of Electrostatics which occur when Λ possesses a quadrupole moment. Indeed, for cells without quadrupole moment, E. H. Lieb and B. Simon have solved (1.4) within a constant (given by (3.5)), in Sections VI.2 and VI.3 of their fundamental paper on 'The Thomas–Fermi Theory of Atoms, Molecules and Solids' (c.f. [1], p. 98, 100 and 101). In fact, the content of these sections has stimulated the development of the present investigations.

II. The auxiliary potential functions

We establish here the conditions which have to be fulfilled by the admissible $g(\mathbf{r})$. Let us set $|\Lambda|^{-1}=\rho$ and let $\bar{g}(\mathbf{q})$ be ρ times the Fourier transform of $g(\mathbf{r})$. Unless otherwise specified, all the integrals are carried over $\mathbb{R}^3$. With these conventions we have

$$\bar{g}(\mathbf{q})=\rho\int d^3r e^{-i\mathbf{q}\mathbf{r}} g(\mathbf{r}) \tag{2.1}$$

and

$$g(\mathbf{r})=|\Lambda|\int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\mathbf{r}} \bar{g}(\mathbf{q}) \tag{2.1'}$$

Let us calculate $\bar{G}(\mathbf{K})$ from (2.1). Using the property that $\exp i\mathbf{K}\mathbf{R}=1$, $\forall \mathbf{K}$ and $\mathbf{R}$ defined in Section 1, we find:

$$\begin{aligned}\bar{G}(\mathbf{K})&=\rho\int_{\Lambda(0)} d^3r e^{-i\mathbf{K}\mathbf{r}} G(\mathbf{r})=\frac{4\pi\rho}{K^2}\\ &=\sum_{\mathbf{R}}\rho\int_{\Lambda(0)} d^3r e^{-i\mathbf{K}\mathbf{r}} g(\mathbf{r}+\mathbf{R})=\sum_{\mathbf{R}}\rho\int_{\Lambda(\mathbf{R})} d^3r' e^{-i\mathbf{K}\mathbf{r}'+i\mathbf{K}\mathbf{R}} g(\mathbf{r}')\\ &=\rho\int d^3r' e^{-i\mathbf{K}\mathbf{r}'} g(\mathbf{r}')\\ &=\bar{g}(\mathbf{K})\end{aligned}$$

The first condition is accordingly

$$\bar{g}(q)|_{q=K} = \bar{G}(K) = \frac{4\pi\rho}{K^2}; \qquad K \neq 0 \tag{2.2}$$

and the second condition is

$$\lim_{q\to 0} \bar{g}(q) = \bar{G}(0) = 0 \tag{2.3}$$

which is sufficient to guarantee the integrability of $g(r)$ at infinity.

We proceed by examining the Poisson equation satisfied by $G(r)$. We have

$$\begin{aligned} -\Delta G(r) &= \sum_K{}' 4\pi\rho e^{iKr} = \sum_K 4\pi\rho e^{iKr} - 4\pi\rho \\ &= 4\pi(\delta_\Lambda(r) - \rho) \end{aligned} \tag{2.4}$$

where $\delta_\Lambda(r)$ is the periodic Dirac δ distribution, i.e.

$$\delta_\Lambda(r) = \sum_R \delta(r+R) \tag{2.5}$$

If we introduce (1.4) and (2.5) into (2.4), we get

$$\sum_R -\Delta g(r+R) = 4\pi\left(\sum_R \delta(r+R) - \rho\right) \tag{2.6}$$

Then, the question is: which Poisson equation should $g(r)$ satisfy? Since (2.6) represents a sum rule, the most general answer is provided by a resolution of the constant term in (2.6), trivialy periodic in Λ, in terms of piece-wise continuous source functions $f_c(r)$, the subscript c standing for 'candidate' such that

$$\begin{aligned} 1 &= \sum_R f_c(r+R) \\ &= \sum_K \bar{f}_c(K) e^{iKr} \end{aligned} \tag{2.7}$$

with $\bar{f}_c(0) = 1$ and zero otherwise. The candidate functions $g_c(r)$, is then chosen to be the inhomogeneous solution in $\mathbb{R}^3$ of the Poisson equation

$$-\Delta g_c(r) = 4\pi(\delta(r) - \rho f_c(r)) \tag{2.8}$$

which, in Fourier space, becomes

$$q^2 \bar{g}_c(q) = 4\pi\rho(1 - \bar{f}_c(q)) \tag{2.9}$$

We observe that for $q = K \neq 0$

$$\bar{g}_c(K) = \frac{4\pi\rho}{K^2} \tag{2.10}$$

and the condition (2.2) is satisfied for any f_c solution of (2.7). For $K = 0$ however, (2.3) restricts the choice of $f_c(r)$ to that class $\{f\} \subset \{f_c\}$ for which

$$\lim_{q\to 0} \bar{g}(q) = \lim_{q\to 0} \frac{4\pi\rho}{q^2}(1 - \bar{f}(q)) = 0 \tag{2.11}$$

Since $f(r)$ is symmetric (2.11) means that, for small q

$$\bar{f}(q)=1+O(q^4) \tag{2.12}$$

In real space (2.12) means that

$$\rho\int d^3r f(r)=1 \tag{2.13}$$

and

$$\rho\int d^3r r_\alpha r_\beta f(r)\equiv I_{\alpha\beta}=0 \tag{2.14}$$

i.e. that the second moments of f vanish. The admissible $g(r)$ are furthermore given by

$$g(r)=\frac{1}{|r|}-\rho\int d^3r' f(r')\frac{1}{|r-r'|} \tag{2.15}$$

The class of source functions satisfying (2.13) and (2.14) must be further restricted. Considerations of physical and mathematical nature, which will become obvious below, suggest considering only source functions of compact support. If so, it follows from (2.13), (2.14) and (2.15) that, for large $|r|$, outside the support of $f(r)$, the potential function decays as $1/|r|^5$ for all shapes of Λ.

In summary, the problem of defining the admissible potential functions has been formulated as follows: we look for identity resolving, piece-wise continuous, even source functions $f(r)$ of compact support, normalized to unity and with vanishing second moments. Then $g(r)$ is given by (2.15).

III. Auxiliary source functions

We develop here an operational procedure for constructing source functions $f(r)$ belonging to the class defined above. We shall proceed inductively and begin with the construction, in two steps, of the simplest possible $f(r)$ for a cubic cell $\Lambda=c$. First, (2.2) will be satisfied but not (2.3) and then, (2.2) and (2.3).

In Section 2, we have learned that any solution of (2.7) satisfies (2.2). The simplest of these solutions is certainly the characteristic function $\chi(r)$ which is one for r in Λ and zero otherwise. For a cubic cell of linear dimension a we have

$$\bar{\chi}(q)=\prod_{\alpha=1}^{3}\frac{\sin(q_\alpha a/2)}{(q_\alpha a/2)} \tag{3.1}$$

The potential function, say $\gamma(r)$, associated with this source function satisfies the Poisson equation

$$-\Delta\gamma(r)=4\pi(\delta(r)-\rho\chi(r)) \tag{3.2}$$

and becomes

$$\gamma(r)=\frac{1}{|r|}-\rho\int_c d^3r'\frac{1}{|r-r'|} \tag{3.3}$$

This is precisely the potential function considered by Lieb and Simon ([1] Eq. 119). Since the second moments of the charge distribution of 3.2 are diagonal and isotropic, $\gamma(r)$ falls off as $1/|r|^5$ for large $|r|$ and the Poisson sum $\sum_R \gamma(r+R)$ is absolutely convergent. This sum represents the electrostatic potential produced at the point r from an infinite cubic array of point charges immersed in uniform background of opposite charge. This system is readily identfied as a Wigner lattice. The Fourier transform of (3.3) is

$$\bar{\gamma}(q)=\frac{4\pi\rho}{q^2}\left(1-\prod_{\alpha=1}^{3}\frac{\sin(q_\alpha a/2)}{(q_\alpha a/2)}\right) \tag{3.4}$$

For $K \neq 0$ we have evidently

$$\bar{\gamma}(K)=\frac{4\pi\rho}{K^2}$$

whereas $\bar{\gamma}(0)$ is not zero. We have instead

$$\begin{aligned}\lim_{q\to 0}\bar{\gamma}(q)&=\lim_{q\to 0}\frac{4\pi\rho}{q^2}\left(\frac{a^2}{3!\,4}\sum_\alpha q_\alpha^2\right)=\frac{4\pi\rho}{24}a^2\\ &=\rho\int d^3r\gamma(r)\end{aligned} \tag{3.5}$$

However, since $\bar{\gamma}(0)$ is a well defined non vanishing constant, it is easy to carry out the second step. The simplest way of implementing (2.3) is indeed to write

$$\begin{aligned}g(r)&=\gamma(r)-\frac{4\pi}{24a}\chi(r)\\ &=\gamma(r)-\rho\int d^3r'\gamma(r')\cdot\chi(r)\end{aligned} \tag{3.6}$$

The Fourier transform of this $g(r)$ is

$$\bar{g}(q)=4\pi\rho\left(\frac{1-\bar{x}(q)}{q^2}-\frac{a^2}{24}\bar{\chi}(q)\right) \tag{3.7}$$

with the property $\bar{g}(0)=0$. Notice however that the above choice makes $g(r)$ discontinuous at the surface of the cube. We shall return to this point in Section 4.

The above exercise tells us that the characteristic function of the cell is manifestly useful in that it is the simplest function which fulfills (2.2). This fact suggests constructing an admissible $\bar{f}(q)$ for the general case with the Ansatz

$$\bar{f}(q)=\bar{f}_0(q)\bar{f}_1(q) \tag{3.8}$$

where

$$\bar{f}_0(q)=\bar{\chi}(q) \tag{3.9}$$

and where $\bar{f}_1(q)$ is chosen to fulfill (3.2), i.e. to cancel the quadratic q dependence of $\bar{\chi}(q)$ for small q as required by (2.12). For the cubic case discussed above, we might choose $\bar{f}_1(q)=1+\frac{1}{24}a^2q^2$ since $\bar{\chi}(q)\cong 1-\frac{1}{24}a^2q^2$ and obtain

$$\bar{g}(q)=\frac{4\pi\rho}{q^2}(1-\bar{\chi}(q)(1+\tfrac{1}{24}\partial^2q^2)) \tag{3.10}$$

We notice that (3.10) is exactly (3.7)!

We proceed with the characterization of the admissible source functions in real space. From the Ansatz (3.8), we have in the general case

$$
\begin{aligned}
f(r) &= \rho \int d^3r' f_0(r') f_1(r-r') \\
&= \rho \int_\Lambda d^3r' f_1(r-r')
\end{aligned}
\tag{3.11}
$$

The function $f_1(r)$ is still unknown apart from the fact that it is of compact support. In addition, we know its mean value

$$
\rho \int d^3r f_1(r) = 1 \tag{3.12}
$$

since $\bar{f}(0) = 1$ and $\bar{f}_0(0) = 1$ and its second moments from (2.14) and (3.11)

$$
\begin{aligned}
\rho \int d^3r r_\alpha r_\beta f(r) = 0 &= \rho \int d^3r' r'_\alpha r'_\beta f_0(r') \\
&\quad + \rho \int d^3r'' r''_\alpha r''_\beta f_1(r'') \\
0 &= I_{0\alpha\beta} + I_{1\alpha\beta}
\end{aligned}
\tag{3.13}
$$

We are left with the question of finding the most convenient function $f_1(r)$ for a given situation. A few examples are treated in the next Section.

IV. Applications

We develop here two specific representations of $G(r)$: the first one with the purpose of giving a precise meaning to the shape-dependent constant U defined by (1.3), the second one, with the purpose of examining the source function of smallest support in real space.

As a preamble to the first application we return for a moment to the cubic case in order to interpret U on the basis of the potential functions $g(r)$ given by (3.5). As expected, we shall find that U is the Madelung energy of the simple cubic Wigner lattice. The demonstration is based on an appropriate decomposition and re-arrangements of the terms contributing to U. We have

$$
\begin{aligned}
2U &= \lim_{r\to 0}\left(G(r) - \frac{1}{|r|}\right) = \lim_{r\to 0}\left(\sum_R g(r+R) - \frac{1}{|r|}\right) \\
&= \lim_{r\to 0}\left(\sum_R \left(\gamma(r+R) - \chi(r+R)\rho \int d^3r' \gamma(r')\right) - \frac{1}{|r|}\right) \\
&= -\rho \int_c \frac{d^3r}{|r|} + \sum_{R\neq 0} \gamma(R) - \rho \int d^3r \gamma(r) \\
&= -\rho \int_c \frac{d^3r}{|r|} + \sum_{R\neq 0} \gamma(R) - \sum_R \int_c d^3r \gamma(r+R) \\
&= -2\rho \int_c \frac{d^3r}{|r|} + \rho^2 \int_c d^3r\, d^3r' \frac{1}{|r-r'|} \\
&\quad + \sum_{R\neq 0} \left\{\frac{1}{|R|} - \rho \int_c d^3r \frac{1}{|R+r|} - \rho \int_c d^3r' \frac{1}{|R-r'|} + \rho^2 \int_c d^3r\, d^3r' \frac{1}{|R+r-r'|}\right\}
\end{aligned}
\tag{4.1}
$$

The first term is twice the attractive interaction between the particle located at $r=0$ and the cell $c(0)$, the second term is the self-energy of $c(0)$, and the terms in parentheses represent the interaction potential between the two cells $c(0)$ and $c(R)$. Half of (4.1) is precisely the Madelung energy or ground state energy of the cubic Wigner lattice.

After this useful little exercise, we consider the general case and we look for a simple function $f_1(r)$ satisfying (3.12) and (3.13). Inspection of these conditions suggests choosing

$$\rho f_1(r)=2\delta(r)-\rho\chi(r) \tag{4.2}$$

We verify indeed that

$$\rho\int d^3r f_1(r)=1$$

and that

$$\rho\int d^3r r_\alpha r_\beta f_1(r)=I_{1\alpha\beta}=-I_{0\alpha\beta}$$

for all Λ. With (4.2) the source function becomes

$$\begin{aligned}f(r)&=\rho\int d^3r' f_0(r')f_1(r-r')\\&=2\chi(r)-\Delta(r)\end{aligned} \tag{4.3}$$

where

$$\Delta(r)=\rho\int d^3r'\chi(r')\chi(r-r') \tag{4.4}$$

is ρ times the overlapping volume between the characteristic functions separated by the vector r. For instance, for an orthorhombic cell of linear dimension a_1, a_2, a_3

$$\Delta=\prod_{\alpha=1}^{3}\left(1-\frac{|r_\alpha|}{a_\alpha}\right) \tag{4.5}$$

It follows from (4.4) that the support of (4.3) is a cell of the same shape as Λ but with linear dimensions twice those of Λ. With (4.3), Poisson's equation for $g(r)$ becomes

$$-\Delta g(r)=4\pi(\delta(r)-2\rho\chi(r)+\rho\,\Delta(r)) \tag{4.6}$$

and in Fourier space it reads

$$q^2\bar{g}(q)=4\pi\rho(1-2\bar{x}(q)+\bar{x}^2(q)) \tag{4.7}$$

The inhomogeneous solution of (4.6) can be written in the form

$$\begin{aligned}g(r)&=\frac{1}{|r|}-\rho\int d^3r'\frac{1}{|r+r'|}-\rho\int d^3r''\frac{1}{|r-r''|}\\&\quad+\rho^2\int_\Lambda d^3r'\,d^3r''\frac{1}{|r+r'-r''|}\end{aligned} \tag{4.8}$$

It follows from (4.8) that $g(r)$ can be interpreted as the interaction potential between two neutral and dipole-free cells separated by the vector r. The constant U is then given by

$$2U = \lim_{r\to 0}\left(\sum_R g(r+R) - \frac{1}{|r|}\right)$$

$$= \lim_{r\to 0}\left(g(r) - \frac{1}{|r|}\right) + \sum_{r\neq 0} g(R)$$

$$= -2\rho\int_\Lambda d^3r \frac{1}{|r|} + \rho^2\int_\Lambda d^3r\, d^3r' \frac{1}{|r-r'|} + \sum_{R\neq 0} g(R) \tag{4.9}$$

which proves unambiguously that U is the ground state energy of a Wigner lattice with unit cell Λ of any shape.

We have just given a useful interpretation of $g(r)$. However, we can give another interpretation of $g(r)$ in writing the source function (4.3)

$$f(r) = f_0(r) + f_2(r) \tag{4.10}$$

with

$$f_0(r) = \chi(r)$$

as before and

$$f_2(r) = \chi(r) - \Delta(r)$$

than, with

$$\gamma(r) = \frac{1}{|r|} - \rho\int_\Lambda d^3r' \frac{1}{|r-r'|} \tag{4.11}$$

the potential $g(r)$ becomes

$$g(r) = \gamma(r) - \rho\int d^3r' f_2(r') \frac{1}{|r-r'|} \tag{4.12}$$

In Fourier space this way of writing $g(r)$ becomes

$$\bar{g}(q) = \frac{4\pi\rho}{q^2}(1-\bar{\chi}(q)) - \frac{4\pi}{q^2}(\bar{\chi}(q) - \bar{\chi}^2(q))$$

$$= \bar{\gamma}(q) - \bar{\chi}(q)\bar{\gamma}(q)$$

Now it is clear that for a non-cubic cell $\bar{\gamma}(0)$ is not defined. We have indeed

$$\lim_{q\to 0}\gamma(q) = \lim_{q\to 0}\frac{4\pi}{q^2}\left(1-\rho\int_\Lambda d^3r e^{iqr}\right) = \lim_{q\to 0}\frac{4\pi}{2} I_{0\alpha\beta}\frac{q_\alpha q_\beta}{q^2} = ?$$

Nevertheless, $\gamma(r)$, the first term of (4.12) can be viewed as the potential produced by the 'real' charge density of the cell Λ, namely $\delta(r) - \rho\chi(r)$. As to the second term, it can be viewed as being produced by a 'fictituous', symmetric charge density $f_2(r)$, of zero mean value, changing sign at the surface $\partial\Lambda$ of Λ, decreasing linearly to zero on both sides of $\partial\Lambda$, positive inside Λ and negative outside and with second moments

$$I_{2\alpha\beta} = \rho\int d^3r r_\alpha r_\beta f_2(r) = 0 - I_{0\alpha\beta} \tag{4.13}$$

which compensate exactly the second moments of the real charge density. This interpretation immediately suggests the question: can we squeeze $f_2(r)$ into a surface charge double layer? The answer is yes in the sense of distributions. The result is very simple, and will be given without proof. Consider

$$\begin{aligned}\bar{f}_2 &= \bar{\chi}(q) - \bar{\chi}^2(q)\\ &= \bar{\chi}(q)(1-\bar{\chi}(q))\end{aligned}$$

expand

$$\begin{aligned}1-\bar{\chi}(q) &= 1-\rho\int d^3 r e^{iqr}\\ &= \sum_{\alpha,\beta} \tfrac{1}{2} I_{0\alpha\beta} q_\alpha q_\beta + \cdots\end{aligned}$$

and retain only the quadratic terms of the expansion. The function $\bar{f}(q)$ becomes

$$\bar{f}^*(q) = \bar{\chi}(q) + \bar{\chi}(q)\tfrac{1}{2} I_{0\alpha\beta} q_\alpha q_\beta \tag{4.14}$$

and thus

$$\bar{g}^*(q) = \frac{4\pi\rho}{q^2}(1-\bar{\chi}(q)(1+\tfrac{1}{2} I_{0\alpha\beta} q_\alpha q_\beta)) \tag{4.15}$$

appear to be the natural generalization of (3.10). The corresponding auxiliary potential function becomes

$$g^*(r) = \frac{1}{|r|} - \rho\int_\Lambda d^3 r' \frac{1}{|r-r'|} + \tfrac{1}{2} I_{0\alpha\beta} D_\alpha D_\beta \rho \int_\Lambda d^3 r' \frac{1}{|r-r'|} \tag{4.16}$$

where $D_\alpha = \partial/\partial r_\alpha$. It is apparent that among all admissible $g(r)$, (4.16) is that of smallest support. This property is of theoretical interest and may also prove useful for determining $G(r)$ quantitatively and efficiently from (1.4).

If Λ is cubic then $I_{0\alpha\beta} = \frac{1}{12} a^2 \rho\, \delta_{\alpha\beta}$ and the last term of (4.16) becomes

$$\begin{aligned}\tfrac{1}{24} a^2 \rho\, \delta_{\alpha\beta} D_\alpha D_\beta \int_c d^3 r' \frac{1}{|r-r'|} &= -\frac{4\pi}{24a}\int_c d^3 r'\, \delta(r-r')\\ &= -\frac{4\pi}{24a}\chi(r)\end{aligned}$$

which is exactly the last term of g given by (3.5). This shows a posteriori that the choice of (3.5) was not artificial and that the jump of g at the surface of the cube results from the effect of the surface charge double layer.

As a closing point, we note that for finite r and, while keeping its shape, the size of the cell $\to\infty$, the tensor

$$-\frac{1}{4\pi} D_\alpha D_\beta \int_\Lambda f^3 r' \frac{1}{|r-r'|}$$

becomes the well-known depolarization tensor of the theory of polarizable media.

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