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LETTER TO THE EDITOR

Stability of the Wigner electron crystal on the perovskite lattice

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Abstract. Wigner condensation is found to have lowest energy on the perovskite lattice structure. It is suggested that this may be of relevance for studies of high-temperature superconductivity.

Wigner (1934) showed that an electron gas bathed in a compensating background of positive charge would crystallize. Since then a considerable body of work—Fuchs (1935), Wigner (1938), Coldwell-Horsfall and Maradudin (1960)—has shown that if an electron gas were to crystallize, the most stable of the three common cubic structures from energy considerations would be the BCC lattice. Other structures such as the diamond lattice and the HCP structure were investigated by Foldy (1978), but the BCC structure was still found to be the one energetically preferred, albeit by a very small margin.

In 1988, Borwein and co-workers proposed a new and very rapid method of determining the lattice energy of any Wigner lattice. Using this method several other common cubic structures have been investigated, namely the fluorite (F), perovskite (P) and spinel (S) lattices. The results are displayed in table 1 along with those from previous calculations.

The results show clearly that the BCC lattice is no longer the most stable energetically, but that now it is the P lattice, and by quite a large margin. It is to be noted that the recently discovered high-temperature superconductors have the P structure, and the fact that the P lattice is the most stable Wigner crystal may have some bearing on this.

Table 1.

Structure	Electrons/ unit cell	$U/(e^2/a)$	$U/(e^2/r_s)$
SC	1	−2.837297	−1.760119
FCC	4	−4.584875	−1.791753
BCC	2	−3.639240	−1.791860
Diamond	8	−5.386798	−1.670851
HCP	6	−3.241859	−1.791676
Simple hexagonal (axial ratio 1)	3	−2.995772	−1.771389
Fluorite	12	−6.188734	−1.676918
Spinel	56	−10,326163	−1.674352
Perovskite	5	−5.386798	−1.954240

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The calculation for the P lattice is now detailed, following the method of Borwein *et al* (1988). The perovskite structure is made up of *five* interpenetrating simple cubic (SC) lattices of side a. Taking any lattice site as an origin of a coordinate system, the P lattice may be described as

$$\mathrm{SC}(0,0,0) + \mathrm{SC}(0,\tfrac{1}{2},\tfrac{1}{2}) + \mathrm{SC}(\tfrac{1}{2},0,\tfrac{1}{2}) + \mathrm{SC}(\tfrac{1}{2},\tfrac{1}{2},0) + \mathrm{SC}(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})$$

where $\mathrm{SC}(x,y,z)$ is the notation for a SC lattice based on the coordinates (x,y,z) relative to the origin $(0,0,0)$. Assuming that electrons on these sites interact with a Coulomb potential in a background of positive compensating charge, following Borwein *et al* (1988) and Zucker (1975), the energy, $U(\mathrm{P})$ of the electron P crystal may be expressed in terms of e^2/a as

$$U(\mathrm{P}) = a(1) + d(1) + (3c(1) - a(1))/2 \tag{1}$$

where

$$a(1) = \sum{}' (m^2 + n^2 + p^2)^{-1/2} \qquad b(1) = \sum{}' (-1)^m (m^2 + n^2 + p^2)^{-1/2}$$

$$c(1) = \sum{}' (-1)^{m+n} (m^2 + n^2 + p^2)^{-1/2} \qquad d(1) = \sum{}' (-1)^{m+n+p} (m^2 + n^2 + p^2)^{-1/2}.$$

The prime on the summation sign implies that the summation over all the indices m, n, p from $-\infty$ to ∞ excludes the case where m, n, p are simultaneously zero. $a(1)$ as given above is divergent, but by writing

$$a(2s) = \sum{}' (m^2 + n^2 + p^2)^{-s}$$

a functional equation for $a(2s)$ may be found that enables $a(1)$ to be evaluated as $b(1) + c(1) + d(1)/3$. The values of $b(1) - d(1)$ may be calculated using transformations that convert the slowly conditionally convergent sums given above into rapidly absolutely convergent sums—see Zucker (1976). With the figures given there, the value of $U(\mathrm{P})$ in terms of e^2/a is $-5.386\,798\,044$. There are five electrons per unit cube of volume a^3. If r_s is the radius of a sphere of volume equal to the volume per electron, we have

$$\tfrac{1}{5}a^3 = \tfrac{4}{3}\pi r_s^3. \tag{2}$$

Thus in terms of e^2/r_s, $U(\mathrm{P})$ is $-1.954\,239\,66$, which is considerably greater than the value for $U(\mathrm{BCC})$. The values given in table 1 have been obtained in a similar fashion.

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