Comment on 'Stability of the Wigner electron crystal on the perovskite lattice'

1991 J. Phys.: Condens. Matter 3 8757

(http://iopscience.iop.org/0953-8984/3/44/019)

J. Phys.: Condens. Matter 3 (1991) 8757–8758. Printed in the UK

COMMENT

Comment on 'Stability of the Wigner electron crystal on the perovskite lattice'

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Received 14 May 1991

Abstract. Using standard Ewald summation, it is found that the energy of the three-dimensional Wigner crystal on the perovskite lattice is not lower than its energy on the BCC lattice. The BCC lattice remains the most stable known arrangement for the three-dimensional Wigner crystal.

Recently, it was reported (Zucker 1991) that the three-dimensional Wigner crystal is most stable in the perovskite structure with a simple cubic unit cell and a five electron basis: $(0,0,0),(0,\frac{1}{2},\frac{1}{2}),(\frac{1}{2},0,\frac{1}{2}),(\frac{1}{2},\frac{1}{2},0),(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The method of Borwein *et al* (1988) was used.

It is also possible to calculate the potential seen by each electron via the standard Ewald sum for a three-dimensional crystal of electrons embedded in a uniform positive background (Ewald 1921)

$$\phi(i)=\frac{4\pi}{V_c}\sum_{G\neq 0}S(G)|G|^{-2}\exp\left(\frac{-|G|^2}{4\eta}-iG\cdot r_i\right)-\frac{1}{V_c}\left(\frac{\pi}{\eta}\right)S(0)$$
$$+2\sum_{j\neq i}\frac{e}{r_{ij}}\operatorname{erfc}(\sqrt{2\eta}\,r_{ij})-2e\left(\frac{\eta}{\pi}\right)^{1/2}. \tag{1}$$

Here V_c is the volume per unit cell and η is the Ewald parameter, which can be adjusted so that both sums converge rapidly. The structure factor is given by

$$S(G)=\sum_k e^{iG\cdot r_k} \tag{2}$$

where k runs over all the electrons in the basis. The Coulomb energy per electron is given by

$$\frac{E_c}{N}=\frac{e}{2M}\sum_k\phi(k) \tag{3}$$

where the sum is again over each of the M electrons in the basis.

This summation does not verify the final three energies reported in table 1 of Zucker (1991). In units of e^2/r_s, the method above gives $-1.728\,906$ for the fluorite structure, $-1.698\,535$ for the ideal spinel structure and $-1.694\,648$ for the perovskite structure. The perovskite structure is somewhat more favorable than the diamond structure, but less favorable than even the simple cubic structure. The BCC structure remains the most stable known arrangement for the three-dimensional Wigner crystal.

0953-8984/91/448757+02$03.50

Acknowledgment

This work was supported in part by the National Science Foundation.

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Reply by I J Zucker

If there is a discrepancy between the Ewald (E) and Borwein *et al* (B) evaluations of the energy of lattices of electrons compensated by a positive background, then further investigation is necessary. That a discrepancy occurs for the fluorite, spinel and perovskite lattices is surprising, since complete agreement between the two methods has always been obtained previously. However, even if no simple resolution to the conflict is forthcoming, there is no reason to assume that the E results are necessarily the correct ones. In the case of electron lattices the E method requires the subtraction of one infinite term from another infinite term—an action full of danger. On the other hand, the B technique is robust and avoids such delicate operations. Further, all the numerical work may be accomplished in a few minutes on a hand calculator.

Note added in proof. I have recently received an explanation (Baldererschi *et al*, private communication) of the differences between the reported results for the energy of the perovskite, fluorite and spinel electron structures. I did not take into account the non-eqivalence of the various sites in these structures. When this is done correctly the Borwein *et al* evaluation of the electron energy agrees precisely with the Ewald values as given by Cockayne.

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