One-Dimensional Quasicrystals from Incommensurate Charge Order

Flicker, F.; van Wezel, J.

DOI
10.1103/PhysRevLett.115.236401

Publication date
2015

Document Version
Other version

Published in
Physical Review Letters

Citation for published version (APA):
https://doi.org/10.1103/PhysRevLett.115.236401

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: https://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.

Download date: 08 Nov 2022
To bring to the fore the differences between the various charge-ordered phases discussed in the main text, it is convenient to express the modulation on top of the average charge modulation in each state as:

$$\rho(x) = \psi \cos(K \cdot x - \delta(x)).$$  \hspace{1cm} (1)

Here, $K$ is a wave vector commensurate with the lattice, which we will set to $K = 2\pi/(3a)$ from here on. The commensurate charge density wave (CCDW), incommensurate charge density wave (ICDW), discommensuration state (DC), and quasicrystalline state (QC) can then be distinguished by considering the distinct behaviour of the phase $\delta(x)$ in each. This is shown in Fig. 1 below.

![Graphs showing possible charge orderings discussed in the main text.](image-url)
For the CCDW, $\delta(x)$ is zero. For the ideal ICDW, $\delta(x)$ is the straight line $\delta(x) = (Q - K)x$, with $Q$ the incommensurate wave vector. The discommensuration phase is given by sections of zero slope connected by vertical steps at regular intervals. The height of each step is such that the density wave jumps forward by precisely one lattice spacing. For $K = 2\pi/(3a)$, the step height is thus $2\pi/3$. The width of the horizontal sections is such that the average slope of the entire stepped structure is equal to $Q$. The quasicrystal also has average slope $Q$, but consists of horizontal sections separated by sections with slope $\delta(x) = (K' - K)x$, where $K'$ is a second commensurate wave vector: in this case $2\pi/(4a)$. The sections of zero and non-zero slope in this phase form a quasiperiodic sequence.

The DC phase often arises in real materials as the most energetically-favourable way of combining electronic density modulations with a lattice coupling [1]. In practice, the discommensurations in these materials will not be perfectly sharp. Instead, they broaden slightly and the connection in $\delta(x)$ with the neighbouring horizontal regions is made smooth. We follow McMillan in accounting for this using a Fourier expansion with coefficients, controlling the discommensuration width, selected so as to minimize the free energy of the DC state. The QC phase, on the other hand, is created by starting from an ideal ICDW and then shifting the peaks of the electronic density modulation directly onto the nearest atomic position. This creates a quasiperiodic sequence consisting of sections with one of two well-defined commensurate wave vectors.

The QC phase and ICDW both have quasiperiodic elements. For the ICDW, the sequence of atomic positions and charge maxima encountered as the material is traversed is quasiperiodic. This type of ‘quasiperiodicity’, however, is generic to any superposition of two incommensurate structures, including even things like two parallel picket fences seen from a distance. In contrast, the QC phase is quasiperiodic in each of its components individually. Moreover, it also consists of precisely two unit cells. Each piece of period four within the QC state is locally indistinguishable from any other piece of period four. In the ICDW, the atomic neighbourhood of each peak in the electronic structure is perfectly unique. In that sense, it contains infinitely many unit cells, rather than two. We therefore classify the QC state as a true one-dimensional quasicrystal, in contrast to the ICDW, which is only a generic quasiperiodic sequence of charge maxima and atoms.

* Electronic address: flicker@physics.org
† Electronic address: vanwezel@uva.nl