Supplementary material for "Three-Dimensional Icosahedral Phase Field Quasicrystal"

P. Subramanian[1], A.J. Archer[2], E. Knobloch[3] and A.M. Rucklidge,[1]
[1] *Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, United Kingdom*
[2] *Department of Mathematical Sciences, Loughborough University, Loughborough LE11 3TU, United Kingdom*
[3] *Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA*
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In this supplementary material we present two videos that explore the 3D quasicrystalline structure in more detail. We also explore the effect of different domain sizes, chosen to improve the approximation of the QC structure within a periodic domain. Both the videos present data obtained from 3D direct numerical simulations carried out in a periodic domain of size $(26 \times 2\pi)^3$, corresponding to 26 of the shorter wavelengths as defined in the main paper, as opposed to 16 wavelengths used in the paper. The system parameters are $\sigma_0 = -100$, $Q = 1$, $q = 1/\tau = 0.6180$, $\mu = -0.071$ and $\nu = -0.071$, just as in Fig. 2(c) of the main paper. In this case, the simulation was started from an initial condition where the icosahedral symmetry was imprinted in order to hasten the approach to the quasicrystalline asymptotic state, where $U(\boldsymbol{x})$ varies in the range $-0.3 \leq U(\boldsymbol{x}) \leq 1.5$.

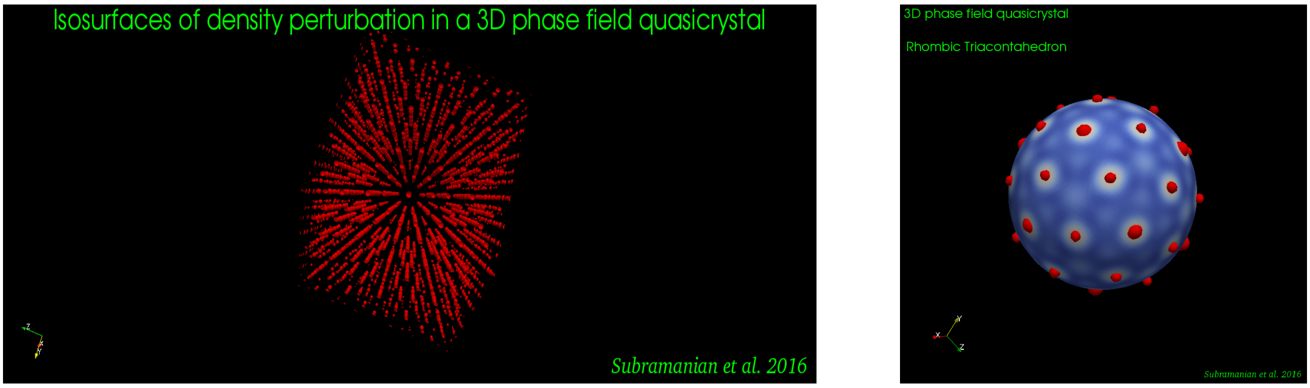

FIG. 1: Left panel: Structure of the 3D QC depicted as a contour cloud of isosurfaces of the density perturbation $U(\boldsymbol{x})$ displaying fivefold rotational symmetry. Right panel: Isosurfaces (shown as red spheres) at a chosen diameter from the center of the periodic domain are seen to form a rhombic triacontahedron with 32 vertices in this frame.

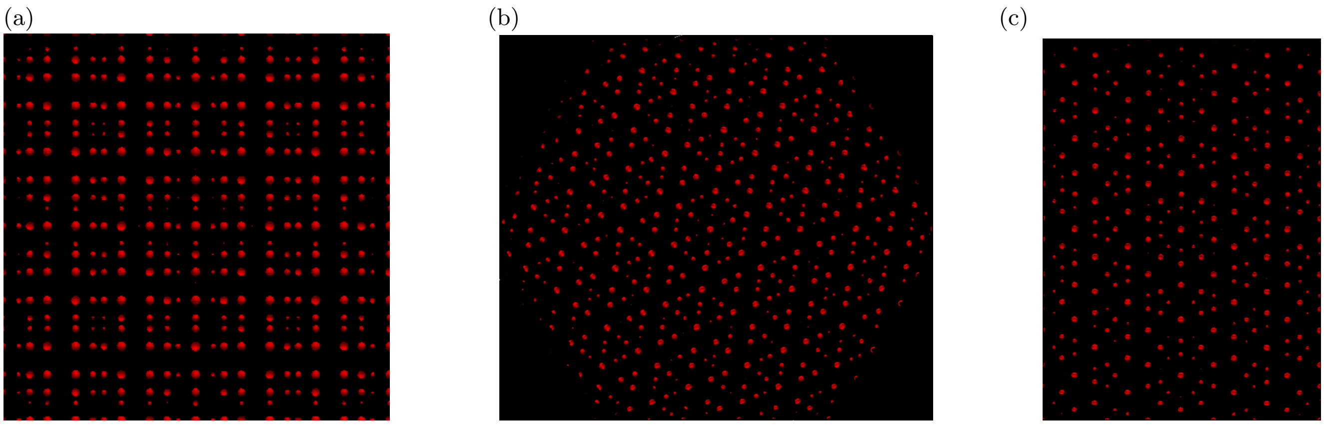

FIG. 2: Parallel projections of the contour cloud along the high symmetry directions. (a) Twofold symmetry observed in a plane perpendicular to $(1, 0, 0)$. (b) Threefold symmetry observed in a plane perpendicular to $(-1, 1, 1)$. (c) Fivefold symmetry observed in a plane perpendicular to $(\tau, -1, 0)$.

The first video displays isosurfaces in the density perturbation $U(\boldsymbol{x})$ as we revolve around the periodic domain. The red spheres represent the isosurfaces at a contour value of $U(\boldsymbol{x}) = 0.75$, and are seemingly in a non-regular arrangement or seem to possess threefold symmetry when viewed from multiple angles. The video stops at a view-point, perpendicular to the plane $(\tau, -1, 0)$, where the fivefold rotational symmetry is apparent, with ten radial lines

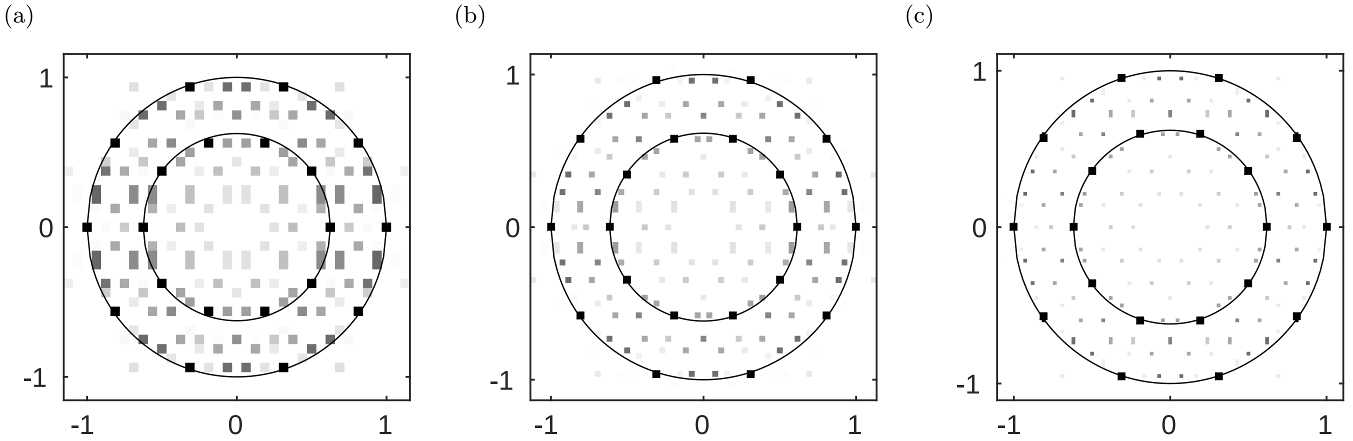

FIG. 3: Diffraction pattern taken in a plane normal to the vector $(\tau, -1, 0)$ in Fourier space. The circles of radii 1 and q are indicated. The fivefold rotation symmetry of the diffraction pattern is indicated by the 10 peaks observed on each circle. The periodic domain size is (a) 16 wavelengths, (b) 26 wavelengths and (c) 42 wavelengths.

originating from the center, as seen in the left panel of Fig. 1. In order to clarify the structure of the contour cloud, parallel projections along the twofold, threefold and fivefold symmetry axes are shown in Fig. 2. These projections are similar to Fig. 2 of [7].

In another approach to understanding the structure of this 3D QC, we start from the center of the domain, where there is a maximum of $U(\boldsymbol{x})$, and note the different polyhedral arrangements that are formed by the isosurfaces as we move radially outward. The second movie shows the first two such structures. The growing sphere displays the contours of $U(\boldsymbol{x})$ at the current radius with red and blue areas indicating positive and negative values, respectively. The first regular polyhedron, at radius $2.23 \times 2\pi$, is an icosahedron with 12 vertices, represented by the 12 red spheres. The second regular structure is a rhombic triacontahedron with 32 vertices, which is observed at a radius of $3.73 \times 2\pi$. This is shown in the right panel of Fig. 1. At larger radii, more intricate structures are observed on the surface of the growing sphere.

The effect of the size of the periodic domain in determining the QC diffraction pattern is explored in Fig. 3. We enlarge the size of the periodic domain from 16 to 26 and 42 of the shorter wavelengths. In all three cases we observe ten dominant peaks at wave numbers $k = q$ and $k = 1$, indicative of fivefold rotational symmetry. Larger domains allow a finer grid spacing in reciprocal space, so as we increase the domain size, the diffraction pattern becomes more accurate, since we are representing the irrational number $\tau = (1 + \sqrt{5})/2$ to greater precision: $\tau \approx 13/8$, $21/13$ and $34/21$, respectively, for wavevectors on the sphere $k = 1$.

The data for this paper, including a file that allows interaction with the data behind Fig. 1 through the ParaView software, is available from the Research Data Leeds repository.