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REPLY

Reply to Comment on ‘Quantum correlations between protons in potassium bicarbonate’

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Abstract

Allegations in a Comment (Fillaux and Cousson 2004 *J. Phys.: Condens. Matter* **16** 1007) that our calculation of the intensity of neutrons diffracted by potassium bicarbonate is incorrect are shown to be ill-founded. The downfall of the Comment is not to apply quantum mechanics to the calculation of scattering by indistinguishable nuclei with overlapping degrees of freedom (protons or deuterons).

We address a Comment [1] which alleges that our interpretation of total neutron scattering data for potassium bicarbonate [2] is incorrect.

The alleged ‘dramatic errors’ in our work, which are labelled (1) and (2) in [1], are dispelled by the observation that in their Comment Fillaux and Cousson adopt classical physics to interpret our quantum mechanical calculation of scattering by a dimer. The material in (1) and (2) would be appropriate if the particles (protons or deuterons) were different, as they are in classical mechanics. For in the classical case, the probability density is indeed the sum of the probabilities that one particle is around one site and the other is around the second site. The caption to figure 1 [1] explicitly states that the displayed quantities are ‘probability densities for single particles’.

Thus, the material in (1) and (2), and all that flows from it, does not apply to our interpretation, which is the intended subject of the Comment, and a wholly quantum mechanical calculation. For us the two particles in a dimer are indistinguishable and the probability density must be constructed by second quantization, or another technique, that properly handles the quantum statistics of identical particles. The correct expression for the spatial probability density, $\rho(\mathbf{R})$, which is the topic attempted in (1) and (2), is the sum of the squares of the *one-particle orbitals* and this is the expression for $\rho(\mathbf{R})$ used in section 5 of our paper. Of course, the correct expression shows interference between the particles, which is a signature of the quantum exchange process ignored by the authors of the Comment. This interference depletes $\rho(\mathbf{R})$ in the region between the most probable positions for the two nuclei and, thus,

the separation of the positions, d , exceeds the nominal separation of uncorrelated (classical) nuclei, r . Once the authors embark on their classical description they are totally divorced from our interpretation in terms of quantum-correlated particles.

Our interpretation is based on an exact expression for the total scattering of neutrons by a dimer made with identical particles (the expression is labelled (4.4) in [2]). The expression shows a purely quantum mechanical contribution to scattering and we propose that this contribution is the source of unexpected intensity from KHCO_3 in the form of rods in reciprocal space [3]. No such rods are observed with a deuterated sample. This finding is in total agreement with our proposal, because the contribution to scattering that is in question has opposite signs for protons and deuterons, on account of their different nuclear spins, and the contribution is scaled by the very different cross-sections for protons and deuterons. Thus, all other aspects being equal, a maximum in intensity from KHCO_3 , in the form of a rod of intensity, is an invisible feature in the intensity from a deuterated sample. Our success in explaining the difference in intensity distributions for the two samples escapes Fillaux and Cousson [1], who instead allege that we offer no quantitative explanation for the deuterated sample.

Diffraction by a one-dimensional object, like a dimer, produces scattered intensity in planes that are normal to the axis of the object. However, in KHCO_3 there are dimers of two types that are distinguished by opposite inclinations. (Contrary to what is implied in [1], this arrangement of the dimers is indeed possible even when the individual protons occupy crystallographically equivalent sites.) Intersections of planes of intensity from the two types generate rods of high intensity and it is these rods which are observed in total neutron scattering.

In conclusion, the allegations in [1] that our interpretation is incorrect are not relevant, because they arise from a discussion based on classical concepts whereas quantum mechanics is at the heart of everything we derive. The remaining allegations in [1] arise from misconceptions about both crystal physics and what we calculate.

References

- [1] Fillaux F and Cousson A 2004 *J. Phys.: Condens. Matter* **16** 1007
- [2] Keen D A and Lovesey S W 2003 *J. Phys.: Condens. Matter* **15** 4937
- [3] Fillaux F, Cousson C and Keen D A 2003 *Phys. Rev. B* **67** 054301
Fillaux F, Cousson C and Keen D A 2003 *Phys. Rev. B* **67** 189901 (erratum)