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2004 J. Phys.: Condens. Matter 16 1007

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COMMENT

Comment on ‘Quantum correlations between protons in potassium bicarbonate’

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Received 25 September 2003

Published 30 January 2004

Online at stacks.iop.org/JPhysCM/16/1007 (DOI: 10.1088/0953-8984/16/6/N01)

Abstract

In a recent paper, Keen and Lovesey (KL) (2003 *J. Phys.: Condens. Matter* **15** 4937) presented a theoretical model to account for lines of intensity, in addition to Bragg peaks, observed by Fillaux, Cousson and Keen (FCK) (2003 *Phys. Rev. B* **67** 054301 and 2003 *Phys. Rev. B* **67** 189901 (erratum)) in single-crystal neutron diffraction measurements on potassium hydrogen carbonate (KHCO₃). In this comment it is demonstrated that KL’s model is irrelevant and cannot account for the data under consideration.

Spatially extended and long-lived quantum entanglement of protons has been observed in the potassium hydrogen carbonate (KHCO₃) crystal [1–3]. Quantum interferences were probed with neutron scattering techniques. Depending on the coherence length of the neutron beam, interferences arising either locally from protons in centrosymmetric dimer units [1, 2] or from the extended grating-like structure of entangled protons in two dimensions [3] were observed. Keen and Lovesey (KL) questioned this latter interpretation in a subsequent paper [4] and the purpose of this comment is to emphasize some dramatic errors in their paper.

KL’s model aims to calculate the scattering function for KHCO₃ and KD₂CO₃ considering two entangled particles (protons or deuterons, respectively) whose crystallographic positions are separated by $d \approx 2.2 \text{ \AA}$ in dimer units. In equation (5.1) in [4], wavefunctions for particles separated by r , $\psi(\mathbf{R})$ and $\psi(\mathbf{r} - \mathbf{R})$ are combined as

$$\begin{aligned}\varphi_1(\mathbf{R}) &= [\psi(\mathbf{R}) + a\psi(\mathbf{r} - \mathbf{R})]/\sqrt{1 + a^2 + 2aS}, \\ \varphi_2(\mathbf{R}) &= [\psi(\mathbf{R}) - b\psi(\mathbf{r} - \mathbf{R})]/\sqrt{1 + b^2 - 2bS},\end{aligned}$$

where S is the overlap integral (referred to as the ‘mixing parameter’ in [4])

$$S = \int d\mathbf{R} \psi(\mathbf{R})\psi(\mathbf{r} - \mathbf{R}).$$

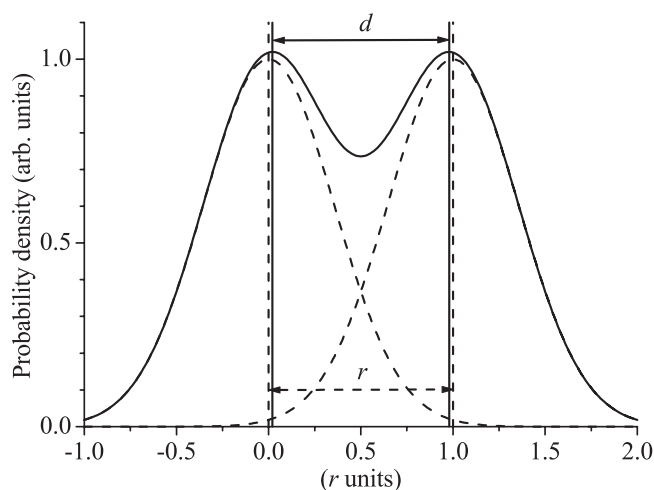


Figure 1. A schematic representation of the probability densities for single particles centred at 0 and r (dashed) and for the corresponding dimer (solid). The distance between the maxima is d for the dimer.

The calculated scattering function is isotropic (circular in shape) perpendicular to the direction \mathbf{d} defined by the two particles. The intensity varies rather slowly for $\mathbf{k} \parallel \mathbf{d}$, in marked contrast to the sharpness of the observed ridges of intensity under consideration (see figure 5 in [3]). Besides this, in order to fit the data, Keen and Lovesey arbitrarily set $r = 0.7d$, which means $S > 1/2$ (see section 6 in [4]). Then, whereas all protons (deuterons) are equivalent according to the crystal symmetry [3], they distinguish different dimers whose internuclear directions are inclined at $\pm 13^\circ$ with respect to the b crystal axis. The ridges of intensity are claimed to arise at the intercept in the (a^*, c^*) plane of discs of diffuse scattering perpendicular to these directions.

KL's model is flawed by the lack of any mechanism preventing decoherence of proton pairs, which should take place on a very short timescale via interaction with lattice dynamics. This model does not provide any sound explanation for the existence of long-lived quantum entanglement in solids. The poor agreement of the calculated maps of intensity (figure 4 in [4]) with the observed sharp ridges and the lack of quantitative analysis of the deuterated sample emphasize the imperfection of the model.

According to figure 3 in KL's paper, diffuse scattering by dimers should be observed along b^* . This is in conflict with experiments. Figure 8 in [3] shows the rather narrow width of the rods of intensity along b^* . Further examination of the data confirms the absence of unusual diffuse scattering along b^* , apart from the broad Gaussian-like profile centred at $k = 0$ due to incoherent scattering by protons. If Keen and Lovesey had not ignored the Debye–Waller factor their calculated map of intensity along b^* could have been compared with experiments.

Moreover, KL's paper is undermined by dramatic errors.

- (1) The authors claim erroneously that ' $S > 0$ leads to a separation between nuclei d which is larger than r ' (see the last paragraph of section 5). Obviously, it works the other way round: the crystallographic distance d is necessarily shorter than or, most likely, equal to the distance between the atom centres r . Consider cuts along the internuclear direction of the probability densities $|\psi(\mathbf{R})|^2$ and $|\psi(\mathbf{r} - \mathbf{R})|^2$ for particles centred at 0 and r (see the dashed curves figure 1) and the sum $|\psi(\mathbf{R})|^2 + |\psi(\mathbf{r} - \mathbf{R})|^2$ for the pair (see the solid

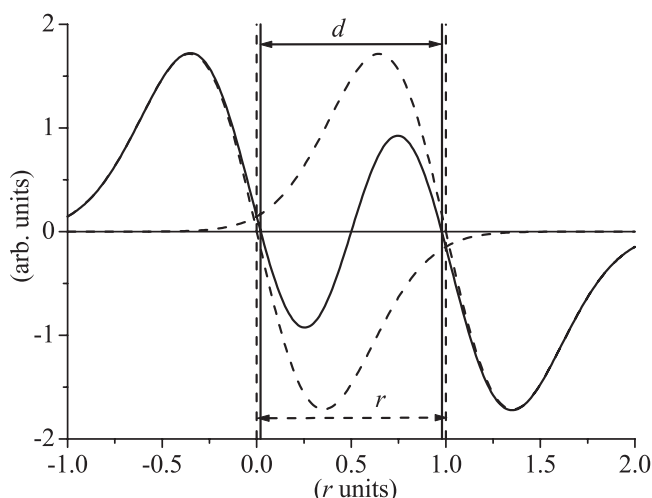


Figure 2. A schematic representation of the derivatives of the probability densities for single particles centred at 0 and r (dashed) and for the corresponding dimer (solid). The distance between the intercepts with the abscissa axis, excluding the centre, is d for the dimer.

curve figure 1). The distance d determined with the single-crystal neutron diffraction technique corresponds to the maxima of the probability density for the dimer. Plotting derivatives of the probability densities (see figure 2) gives a graphic demonstration that $d \leq r$. Therefore, the value $r = 0.7d$ used in section 6 of [4] is irrelevant. Strange as it may seem, Keen and Lovesey merely suppose that atoms are not where the crystal structure shows they are.

- (2) The overlap integral S is not an adjustable parameter. cursory examination of figure 1 in KL's paper should convince the authors that thermal ellipsoids for protons are very small compared to d and, therefore, $S \approx 0$. Needless to say, this was already emphasized in [2]. More specifically, the measured probability density of protons or deuterons can be written as

$$\rho(\mathbf{R}) \approx \rho_0 \exp(-x^2/U_{11} - y^2/U_{22} - z^2/U_{33}).$$

The U_{ii} are the experimental thermal parameters given in table IV of [3] and the coordinates are defined in figure 1 of the same paper. (In table IV off-diagonal terms U_{ij} are negligible.) y is parallel to the b crystal axis and nearly parallel to \mathbf{d} . Consequently, the overlap integral can be rewritten as

$$S \approx \rho_0 \int dy \exp[-y^2/(2U_{22}) - (y - r)^2/(2U_{22})] \sim \exp[-r^2/(4U_{22})].$$

For protons (deuterons) $U_{22} = 0.0153$ (0.0089) \AA^2 and $S \sim 10^{-35}$ (10^{-59}) must be regarded as zero. Then, $r = d$ and the scattering function for quantum entanglement in equation (5.5) in [4] is zero. The remainder of KL's paper is a meaningless discussion of a signal that cannot exist for either KHCO_3 or KDCO_3 . As a matter of fact, with the value $S \approx 0.5$ chosen by KL one can calculate the irrelevant value $r \approx 0.2 \text{\AA}$. The two maxima are no longer separated and $d = 0$.

We wish to emphasize that the narrow width of the lines of intensity under consideration, similar to those of Bragg peaks, is specific to long lived, spatially extended, quantum correlations [3]. KL's local model for diffuse scattering by protons in dimer units ignores long range correlation

and possible mechanisms preserving quantum coherence on a timescale compatible with diffraction measurements. It cannot capture the essential physics of macroscopic entanglement.

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