Fig. 3 Quasi-elastic broadenings ΔE^* as a function of momentum transfer k for film stack sample ($\square$) (hydration conditions as in Fig. 1), 'fluffy' sample at low ($+$) ($RH = 10\text{–}30\%$) and intermediate ($*$) ($RH = 30\text{–}50\%$) H_2O hydration levels. Resolution lines $I_r(\omega)$ (dry sample) were peak-normalised as in Fig. 2; broadened lines $I_s(\omega)$ (wet sample) were peak-normalised in the same way so that now also $I_s(0) = I_{so} = 1$ but $A_s > A_r$. Then $\Delta E^* = A_s - A_r$, and for purely Lorentzian profiles, $\Delta E^* = \pi/2(\Delta E_{\text{Lorenz}})$. Comparison with Lorentzian-fitted profiles gave values of 1.8–1.9 for the proportionality factor instead of $\pi/2$, demonstrating the presence of non-lorentzian line shape components.

Except at very low k, the film-stack broadenings agree reasonably well with an isotropic jump model for which $\Delta E \sim 1 - (\sin ka/ka)$, the jump distance $a = 5.5\text{–}6$ Å and the residence time $\tau_0 = 5\text{–}10$ ns. The broadenings measured for the fluffy sample, on the other hand, exhibit a pronounced first minimum at $k = 0.8\text{–}0.9$ Å^{-1} that cannot be modelled in any simple way. The lower curve in Fig. 3 represents a weighted superposition of $\Delta E(k)$ resulting from one- and two-dimensional CE models, the reason for this being that at lower hydration levels one might expect the migration of water molecules to proceed preferentially along polypeptide chains at the surface. Here, $a = 7\text{–}9$ Å and $\tau_0 = 15\text{–}30$ ns. This sample was hydrated continuously from the dry state at a very low rate; the hydration number at the end of the experiment, estimated from the increase in total neutron counts, was 300 ± 50 H_2O per subunit. The number N_r of amino acid residues offering primary hydration sites is difficult to assess because the surface structure and the degree of aggregation of subunits are not known in sufficient detail. Rough estimates would place this number in the range $100 < N_r < 200$ per subunit. The distances d_r corresponding to this range may be evaluated by covering the surface with a hexagonal grid and regarding each vertex point as a potential hydration site. This gives $d_r = 80 \times N_r^{-1/2}$ Å or $7.9 > d_r > 5.6$ Å, that is, a range of values that agrees well with the jump distances deduced from the broadening data by means of simple CE models.

In conclusion, we have presented the first high-resolution neutron spectra showing the interaction of water molecules with a fully covalently deuterated protein. We have observed a hydration-dependent maximum in the quasi-elastic broadening which, at sub-monolayer coverages, seems to be due to the jump-like migration of water molecules closely associated with or bound to the surface of protein molecules. Although more data need to be collected to substantiate this interpretation, as well as theoretical efforts to develop the analysis of quasi-elastic neutron scattering from biopolymers, the results given here demonstrate clearly that details of protein hydration processes down to energy changes of the order of $10^{-5} k_B T$ or 10^{-3} cm^{-1} are now within reach of neutron spectroscopic techniques. A very exciting prospect of the contrast variation method is the possibility of experiments aimed at distinguishing dynamically between the water of hydration and intramolecular fluctuations.

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Erratum

In the article 'Model of the fine-grain component of martian soil based on Viking lander data' by Nussinov *et al. Nature* **274,** 859, lines 1 and 2 on page 861 should read: 'can be suspended in the atmosphere, the fact that the mean diameter which can be obtained on this basis is 1–2 μm'. In line 11 on page 861, for 10^4 mol g^{-1} read 10^4 nmol g^{-1}.