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# Elementary excitations in uranium dioxide: Unravelling the tangle

## *Excitations élémentaires dans le dioxyde d'uranium : un écheveau à démêler*

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ABSTRACT

In solids with d- and f-electrons, under certain conditions the orbitals align to form an ordered structure. Collective excitations breaking this arrangement can take the form of oscillations of electric quadrupoles, the so-called quadrupolar waves. These represent a propagating pattern of charge densities implying a modulation of quadrupolar moments. Quadrupolar waves constitute a major component of the dynamics of uranium dioxide in its magneto-quadrupolar ordered phase. Together with spin-waves and phonons, these produce a very complex spectrum of elementary excitations having hybrid character over most of the Brillouin zone. Although neutron scattering spectra only reveal the tip of the iceberg of this spectrum, its complete and detailed modelling is needed to understand such experiments. Distinct roles of Jahn–Teller and superexchange mechanisms as sources of quadrupolar interactions can be clearly identified by such modelling.



RÉSUMÉ

Dans les solides contenant des électrons f ou d, les orbitales s'alignent sous certaines conditions pour former une structure ordonnée. Les excitations collectives qui brisent cet alignement peuvent prendre la forme d'oscillations des quadrupôles électriques, appelées ondes quadrupolaires. Celles-ci représentent une modulation de la densité de charge, qui se propage en produisant une modulation des moments de quadrupôle des ions. Les ondes quadrupolaires sont une des composantes principales dans la dynamique du dioxyde d'uranium dans sa phase ordonnée magneto-quadrupolaire. Avec les ondes de spin et les phonons, elles produisent un spectre très complexe d'excitations élémentaires qui ont un caractère hybride sur la plus grande partie de la zone de Brillouin. Bien que les mesures de diffusion inélastique de neutrons ne dévoilent que la pointe de l'iceberg de ce spectre, sa modélisation complète et détaillée est nécessaire pour comprendre ces mesures. Ceci permet aussi d'identifier de manière claire les rôles distincts des mécanismes de superéchange et Jahn–Teller comme sources d'interactions quadrupolaires.



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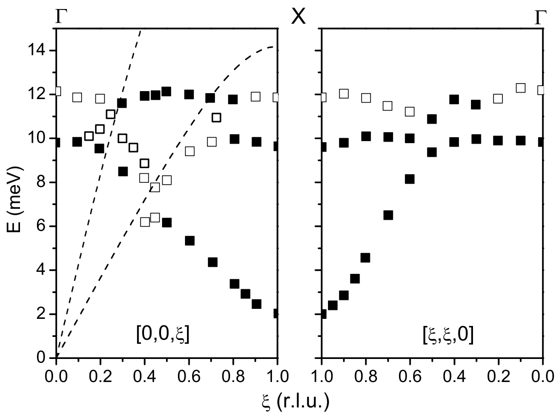


**Fig. 1.** Dispersion of the excitations observed by inelastic neutron scattering in the low-temperature phase of $UO_2$ [4,6,8–10]. Open symbols indicate qualitatively smaller intensity than the black symbols. The broken lines indicate acoustic phonon branches measured at high temperature (Ref. [14]). Excitations around 12 meV correspond to an optical quadrupolar branch, which is absent within spin-wave theories.

## 1. Introduction

Uranium dioxide is one of the most investigated actinide compounds and it has long been considered as an archetype for multi-**k** structures [1,2] and magnetoelastic phenomena [3–7]. In spite of this, the nature of elementary excitations in its antiferromagnetic phase has been debated since their first investigations by inelastic neutron scattering (INS) [4,8]. These experiments evidenced well-defined magnetic and vibrational modes whose complex dispersion relations suggested large mutual interactions with resulting hybrid magnon–phonon modes. Subsequent INS experiments [9,6,10], including measurements with neutron polarisation analysis, provided a detailed picture of the low-energy dynamics (Fig. 1). The most astonishing aspect is the presence of qualitative features in the dispersion relations which cannot be explained in terms of spin-wave theories. In particular, an entire optical branch of excitations observed in INS should not exist within such theories, and its nature has been unknown for several decades.

The ultimate cause of the peculiarities of $UO_2$ is the large orbital component of its ionic states. In the parent $NpO_2$ compound, this originates striking static properties, with a non-dipolar phase transition characterised by a triple-**k** ordering of electric quadrupoles and magnetic triakontadipoles [11,12]. The observed excitations fit theoretical expectations, although the lack of large-enough single-crystals makes a detailed analysis non yet possible [13]. In $UO_2$ the static order is still complex, even if not as peculiar as in $NpO_2$. Yet, a large amount of high-quality single-crystal data evidenced an intricate spectrum of low-energy collective excitations with impressive orbital effects. These show up in two aspects which concur in making the dynamics particularly complex: on the one hand, collective oscillations of the charge density of U ions are driven by two-ion quadrupolar couplings associated with superexchange and virtual-phonon mechanisms. These dispersive *quadrupolar waves* (QWs) are an essential ingredient of the dynamics [15,16]. On the other hand, the different types of elementary excitations, i.e., QWs, magnons and phonons, strongly mix and produce hybrid modes over most of the Brillouin zone. The result is a "tangle" of dispersive modes whose understanding and identification is possible only by an accurate modelling where all relevant degrees of freedom are included on the same footing (Fig. 2).

QWs are similar to the so-called *orbitons* in 3*d* systems [17,18], where a flip of the 3*d* orbital state, with the associated magnetic and/or quadrupolar moments, propagates along the lattice. Yet, being spin and orbital degrees of freedom nearly decoupled, the energy-scale of orbitons is usually very different (and larger) than that of spin waves, whereas in the present case the large spin–orbit interaction yields spin and quadrupole fluctuations in the same energy window, below 15 meV. The resulting hybridisation of QWs with magnons and phonons makes them detectable by conventional INS techniques. The identification and modelling of these collective excitations sheds light onto the scarcely known world of multipolar two-ion interactions, the nature and form of which usually remain elusive. Indeed, static properties are typically affected by only a few of the many possible microscopic couplings between active quadrupoles/multipoles. In particular, when quadrupoles are order parameters in a phase transition, the relative importance of phonons (Jahn–Teller) and exchange (electronic) mechanisms in the phase transition cannot be inferred from static properties alone. Conversely, in the dynamics, many active multipoles and the detailed microscopic interactions among them play a role, and much more information can be extracted by modelling experimental data on multipolar dynamics, in much the same way as the detailed form of spin exchange couplings can be extracted by modelling spin-wave spectra.

## 2. Theoretical model

Uranium dioxide undergoes a first-order phase transition at $T_N = 30.8$ K to a triple-**k** transverse type-I AF state, accompanied by a Jahn–Teller (JT) distortion of the oxygen sublattice [7]. The ordering corresponds to a noncollinear arrangement with four sublattices, where magnetic moments point along the four inequivalent $\langle 111 \rangle$ directions. The charge density dis-

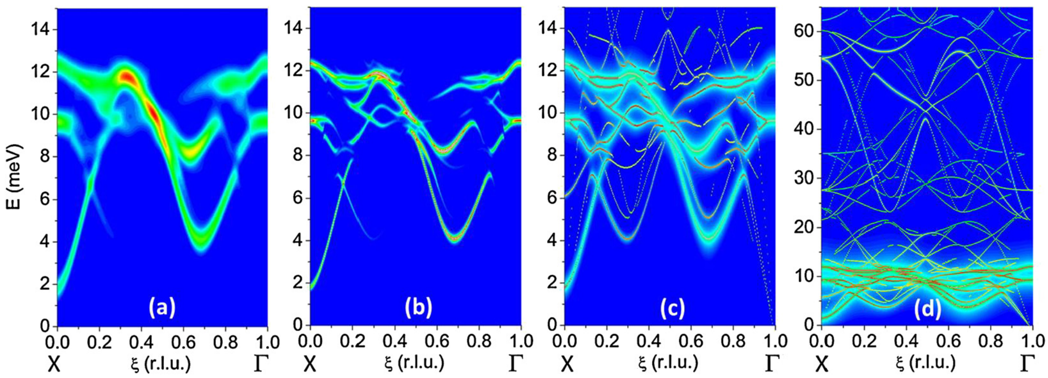


**Fig. 2.** (Colour online.) The complexity of elementary excitations in $UO_2$ fully emerges in these figures that report the calculated magnetic-dipole INS cross-section along $(1+3\xi, 1-\xi, 0)$, a non-symmetry direction connecting $X$ and $\Gamma$ points. The colour scale represents intensity in arbitrary units. Panel (a) shows what would be seen in an actual experiment with typical resolution (FWHM = 0.75 meV). Panel (b) displays magnetic modes with high resolution. In panel (c) the colour scale maps intensity logarithmically to enhance modes with low or tiny cross-section. It is evident that the few peaks observed in an experiment are just the tip of the iceberg of a tangle of mixed modes which need to be modelled in detail to understand the observed spectra. Spins, quadrupoles and acoustical phonons are involved. Panel (d) shows how mode mixing yields a small magnetic cross-section in optical phonons too.

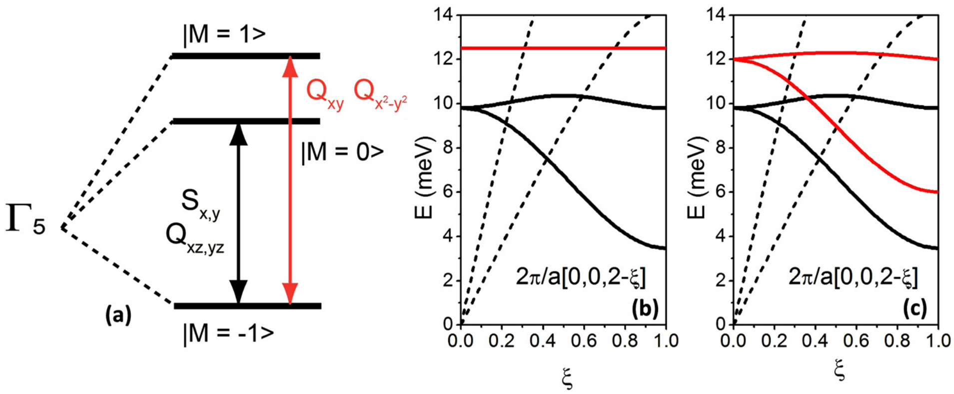


**Fig. 3.** (Colour online.) (a) Splitting of the $\Gamma_5$ ground triplet of the CF Hamiltonian (pseudo-spin $S=1$) in presence of the MF of Eq. (2). Vertical arrows indicate nonvanishing matrix elements for the corresponding operators. (b) Qualitative dispersion of spin waves along the $\Gamma X$ direction (black curves) within a customary spin-wave theory. Dashed lines represent acoustical phonons, whereas the red line represents the atomic-like quadrupolar branch associated with the $\Delta M = 2$ transition in panel (a). (c) Two-ion quadrupolar interactions make this branch dispersive and split it into acoustical and optical components. In this qualitative illustration mixing effects with spin-waves and phonons are absent.

tribution is oblate with respect to the moment direction, corresponding to a triple-**k** electric-quadrupole order. Quadrupoles are secondary-order parameters of the primary AF order, thus they do not drive the phase transition. However, even if their mutual interactions are not large enough to produce a purely quadrupolar first-order state, they play an important role, being responsible for the first-order character of the phase transition [19].

The U ions in $UO_2$ are tetravalent, with a $5f^2$ electronic configuration and $J=4$ ground multiplet. The large crystal field (CF) ($\sim 200$ meV) isolates a $\Gamma_5$ ground triplet, whose eight active degrees of freedom are a triplet of $\Gamma_4$ magnetic multipoles and the quintet of electric ones ($\Gamma_3+\Gamma_5$ in cubic symmetry). By describing the $\Gamma_5$ ground triplet in terms of a pseudospin $S=1$, the active operators are proportional to the following dipolar and quadrupolar operator equivalents:

$$\begin{aligned} &S_x, S_y, S_z \to \Gamma_4 \\ &Q_{xy} = S_xS_y + S_yS_x, \qquad Q_{xz} = S_xS_z + S_zS_x, \qquad Q_{yz} = S_zS_y + S_yS_z \to \Gamma_5 \\ &Q_{3z^2-r^2} = \big(3S_z^2 - S(S+1)\big)/\sqrt{3}, \qquad Q_{x^2-y^2} = S_x^2 - S_y^2 \to \Gamma_3 \end{aligned} \tag{1}$$

These equalities map the physical magnetic dipoles and electric quadrupoles in the first place, but also higher-rank multipoles having the same point symmetry properties (e.g., $\Gamma_4$ magnetic octupoles).

The phase transition can be modelled by a 4-sublattice mean-field (MF) approximation. By choosing the local $z$-axis to lie along the moment direction, the MF Hamiltonian is written as:

$$H_{MF} = -J S_z \langle S_z \rangle - K Q_{3z^2-r^2} \langle Q_{3z^2-r^2} \rangle \tag{2}$$

Since $S_z$ commutes with $Q_{3z^2-r^2}$, the MF eigenstates are directly $|M=1\rangle$, $|M=0\rangle$ and $|M=-1\rangle$. The presence of the quadrupolar term makes the splitting of these singlets asymmetric (see Fig. 3a). If a spin-wave calculation is built upon these MF states, the $|M=-1\rangle \rightarrow |M=0\rangle$ excitation yields spin-optical (SO) and spin-acoustical (SA) branches, where the gap of the latter at the $X$-point reflects the amount of anisotropy, associated with the static quadrupolar term of Eq. (2) (anisotropic spin exchange does not affect the $X$-point gap). Conversely, the $|M=-1\rangle \rightarrow |M=1\rangle$ excitation yields a trivial, non-dispersive quadrupolar branch, undetectable by INS due to its $\Delta M=2$ character (Fig. 3b). A comparison with Fig. 1 suggests that part of the observed peaks are likely to be associated with SA and SO states, whereas the second optical branch might be linked with the quadrupolar excitations. Indeed, if two-ion quadrupolar couplings are strong enough, the quadrupolar branch is expected to become visible in INS by mixing with the nearby SO or SA states. In addition, the branch would be dispersive and split into optical (QO) and acoustical (QA) components (Fig. 3c). However, while the QO branch might be associated with the unexplained INS peaks, no evidence was found of QA modes.

The dispersion of quadrupolar $\Delta M=2$ branches in Fig. 3c is only qualitative, as mixing effects may alter the situation considerably. Besides the mutual mixing of magnetic ($\Delta M=1$) and quadrupolar ($\Delta M=2$) modes, mixing with acoustical phonons is expected to be important. In fact, their energy window matches that of Fig. 1 and their coupling to U quadrupoles is known to be substantial by the analysis of the dynamical JT effect in Th-diluted $UO_2$ [5]. For instance, even in the lack of a model, the pair of modes at 7 meV near $[0,0,0.5]$ in Fig. 1 are strongly suggestive of an anticrossing (AC) between SA modes and TA phonons, which was indeed demonstrated by recent INS experiments with polarisation analysis [16]. Fig. 3a shows that ($\Delta M=1$) and ($\Delta M=2$) excitations are both susceptible to couple with phonons. In fact, the former is associated with fluctuations of transverse (in the local frame) components of the spin, but also of $xz$ and $yz$ electric quadrupoles, whereas in the latter $xy$ and $x^2-y^2$ quadrupoles are involved. These four quadrupoles sense the fluctuating electric field associated with a lattice oscillation and therefore all modes of Fig. 3c are expected to experience significant mixing with phonons.

Elementary excitations in the ordered phase can be extracted by the poles of two-times Green functions for the relevant low-$T$ observables, i.e., the set of all $A_{\mathbf{R},d}$, where $A$ is one of the operators in Eq. (1) and $\mathbf{R}, d$ label U ions, $\mathbf{R}$ being a cell index and $d=1-4$ an index for the 4 sublattices in the 3$\mathbf{k}$ structure. In the presence of magnetoelastic coupling, lattice deformations must be added to the set of relevant observables. The INS cross section is obtained from the absorptive part of the dynamical magnetic susceptibility, which is linked to the spin–spin Green functions. The most general form of the Hamiltonian is:

$$H = H_{SS} + H_{QQ} + H_P + H_{ME} \tag{3}$$

where $H_{SS}$ and $H_{QQ}$ are superexchange spin–spin and quadrupole–quadrupole interactions, respectively, $H_P$ describes free phonons, and $H_{ME}$ the magnetoelastic couplings. Spin-quadrupole terms are forbidden by time-reversal invariance. Consistency of (3) with (2) has to be ensured. Generic two-times retarded Green functions of the form

$$\langle\langle A_{\mathbf{R},d}; A_{\mathbf{R}',d'}\rangle\rangle = -\frac{\mathrm{i}}{\hbar}\theta\left(t-t'\right)\left\langle\left[A_{\mathbf{R},d}(t), A_{\mathbf{R}',d'}\left(t'\right)\right]\right\rangle \tag{4}$$

or they Fourier transforms on $\mathbf{R}$ and $t$ can be calculated by the Random Phase Approximation [20]. In this framework, the set of all $A_{\mathbf{R},d}$ evolves under the effect of a time-dependent field generated self-consistently by the remaining $A_{\mathbf{R}',d'}$. $H_{SS}+H_{QQ}$ yield instantaneous contributions to the spin and quadrupoles effective fields, whereas the purely quadrupolar effective field associated with $H_P + H_{ME}$ displays retardation effects that are non-negligible on the timescale of the electronic dynamics. In fact, within the RPA phonons act as a transmitting medium for effective two-ion quadrupolar couplings, which can be described in terms of a long-range retarded interaction. This acts in concurrence with SE two-ion quadrupolar couplings to propagate quadrupolar fluctuations. It is important to note that the whole set of phonons (including high-energy optical ones) is considered and realistically modelled, as even strongly off-resonant phonons qualitatively influence the low-energy dynamics (see Fig. 2d).

## 3. Results

The Hamiltonian in Eq. (3) contains in principle a large number of parameters. A satisfactory fit of INS data is obtained by a minimal model with five parameters, three of which refer to $H_{SS}+H_{QQ}$ (limited to nearest-neighbours) and the remaining two to $H_{ME}$ [15,16]. For $H_P$, the rigid-ion model of Ref. [14] is adopted. The magnetic cross-section resulting from the model is shown in Fig. 4f, whereas panels (a–d) refer to models where interactions involving quadrupoles have been removed completely (a) or partially (b–d). Mutual interactions between all modes occur for most wavevectors and produce a complex spectrum of elementary excitations having mixed spin–quadrupole–phonon character. In particular, mixing with acoustical phonons causes spectacular anticrossings involving all types of electronic excitations. Fig. 4 shows that the second optical branch seen in experiments is associated with modes of predominant QO character. These are visible in INS because mixing induces a certain amount of $\Delta M=1$ component in the nominally $\Delta M=2$ excitations. As anticipated in Fig. 3, the model predicts the existence of a QA branch which had never been observed in INS experiments. Indeed, its mixing with spin-wave modes being tiny, its magnetic INS cross-section is very small.

At low energy and temperatures, the number of independent elementary excitations at each wavevector is as large as 20: 4 spin-wave-like and 4 quadrupole-like ($\Delta M=1$ and $\Delta M=2$ in Fig. 3, times 4 sublattices) and 12 phonon-like (3 acoustical branches and their foldings, accounting for the 4 sublattices). The richness and complexity of the spectrum are even more

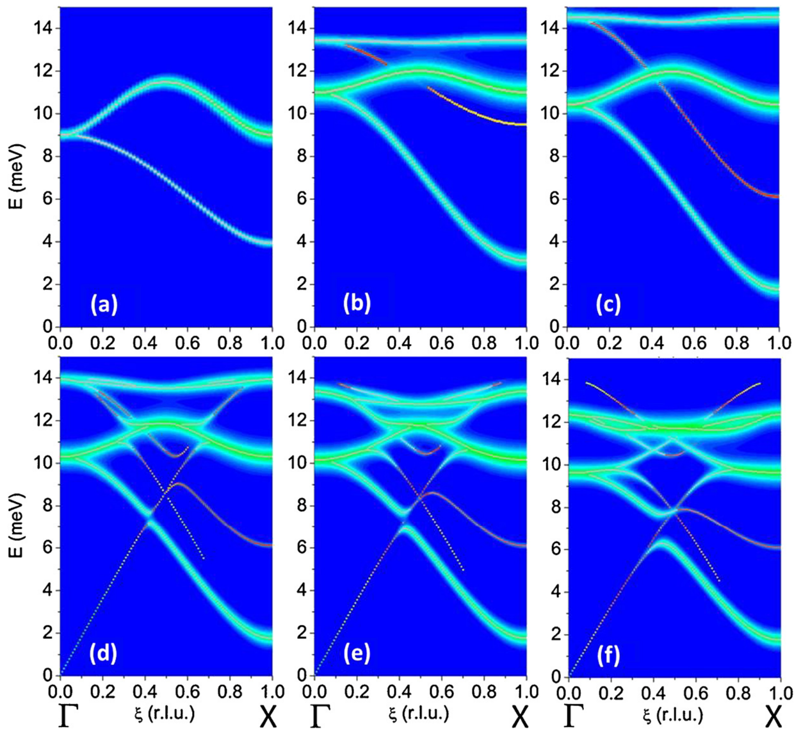


**Fig. 4.** (Colour online.) Dipolar magnetic INS cross section along $[1, 1, 1-\xi]$, calculated with the model discussed in this paper. The colour scale represents intensity in arbitrary units. The whole model corresponds to panel (f), whereas panels (a)–(e) correspond to intermediate models and are shown to clarify the origin of the modes: (a) $H = H_{SS}$: this corresponds to the standard spin-wave theory. Quadrupolar modes are invisible. (b) $H = H_{SS} + H_{QQ}/2$. (c) $H = H_{SS} + H_{QQ}$. Quadrupolar modes become visible by mixing with spin waves, and split in QO and QA branches, the latter carrying tiny magnetic component. (d) $H = H_{SS} + H_{QQ} + H_P + H_{ME}/3$. Anticrossings involving phonons are well visible already for an ME coupling reduced to one third: $\xi \simeq 0.35$, $E \simeq 11$ meV (AC between SO and folded TA modes); $\xi \simeq 0.4$, $E \simeq 7$ meV (AC between SA and TA modes); the largest AC is at $\xi \simeq 0.6$, $E \simeq 9.5$ meV (AC between QA and TA modes). (e) $H = H_{SS} + H_{QQ} + H_P + H_{ME}/2$. The size of the ACs of panel (d) increases roughly linearly in $H_{ME}$. (f) $H = H_{SS} + H_{QQ} + H_P + H_{ME}$. This is the full model, where complex mutual interactions between all modes occur for most wavevectors. Note how the second-order mixing with high-energy optical phonons produces a downward shift of the excitations, most evident for the QO branches.

evident if one moves away from a symmetry direction in reciprocal space. For instance, Fig. 2 shows how the relatively simple spectrum that would be inferred from a real INS experiment actually hides a tangle of a large number of hybrid modes if analysed in detail. It is interesting to observe how the second-order mixing of electronic modes with high-energy optical phonons produces a downward shift of the low-energy excitations (Fig. 4). At the same time, optical phonons acquire a small magnetic component (Fig. 2d), but since this component is scattered over a large number of modes, the shift of their energies is negligible. This is consistent with the results of Ref. [9], where no significant shift of optical phonon frequencies was observed in INS.

## 4. Evidence of the QA branch

The mixing of the QA branch with spin-wave modes is tiny, hence its magnetic INS cross-section is very small. However, the presence of these hidden quadrupolar excitations can be indirectly proved by exploiting the predicted huge anticrossing between QA and phonon TA modes (see Fig. 4). For reduced wavevectors $\xi$ close to 0.6, the mixing is maximal and results in two modes:

$$\psi_1 \simeq \frac{1}{\sqrt{2}}[\mathrm{QA}+\mathrm{TA}] \qquad \psi_2 \simeq \frac{1}{\sqrt{2}}[\mathrm{QA}-\mathrm{TA}] \tag{5}$$

This implies that two peaks in the vibrational INS cross-section should be present in an energy-window where a single peak (bare TA phonon) would be expected. New INS experiments were recently performed targeting mixed electron–phonon modes along $\Gamma X$ [16]. Triple-axis spectrometers were used to compare neutron scattering intensities at equivalent points in different Brillouin zones and in different polarisation channels. In this way, magnetic and phonon characters in excitations were unambiguously identified. These experiments revealed the presence of two additional modes with vibrational character for reduced wavevectors close to 0.6, thus confirming the prediction of the model of a hidden QA branch (see Fig. 5). The measured energies are slightly larger than calculated, but such minor discrepancies are to be expected in view of the minimal set of free parameters in the theoretical model.

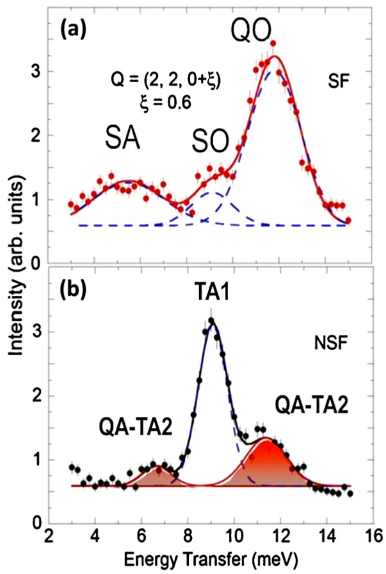


**Fig. 5.** (Colour online.) Constant-Q energy scan recorded with the triple-axis spectrometer IN22 (ILL) at $\mathbf{Q} = (2,2,0) + (0,0,0.6)$ (polarisation $\mathbf{P} \| \mathbf{Q}$; $T = 2$ K). (a) Neutron counts in the spin-flip channel; individual components of the spectrum are shown by dashed lines. (b) Non-spin-flip (NSF) neutron counts. The central peak at $\sim 9$ meV is a transverse acoustic phonon, whereas the weaker peaks at $\sim 6.6$ meV and $\sim 11.4$ meV correspond to mixed TA–QA modes (Eq. (5)).

## 5. Conclusions

The behaviour of elementary excitations resulting from this analysis poses strict constraints on the form of the Hamiltonian in Eq. (3). In particular, we can unequivocally quantify the role of Jahn–Teller and superexchange mechanisms in the behaviour of quadrupolar degrees of freedom. Surprisingly (in view of the large anticrossings involving phonons), it turns out that as far as the static quadrupolar order is concerned, SE plays the leading role. In fact, at the wavevector describing this ordering [$X$-point] JT interactions appear to be nearly vanishing and hence the order is stabilised by SE quadrupolar interactions alone. However, JT interactions are very important both in the dynamics away from $X$ and in static properties near $\Gamma$ (macroscopic quadrupolar response) [15].

To conclude, elementary excitations in $UO_2$ are a tangle of modes with hybrid spin, quadrupole and phonon character. These modes result from a complex interplay between superexchange and magnetoelastic interactions, and their modelling provides an exceedingly detailed picture of the role of quadrupoles in the physical properties. A similar complex role is expected in other systems with unquenched orbital degrees of freedom, notably in actinide compounds with high symmetry. However, additional complications (e.g., conduction electrons or lack of mixing with visible modes) may render the identification of elementary excitations and their theoretical modelling even more problematic than in $UO_2$.

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