Experimental report

31/07/2018

Proposal: **7-01-460**

Council: 4/2017

Title: Hidden nesting as origin of strongelectron-phonon-coupling

Research area: Physics

This proposal is a new proposal

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Samples: YNi2B2C

Instrument	Requested days	Allocated days	From	To
IN8 Flatcone	7	6	28/03/2018	03/04/2018

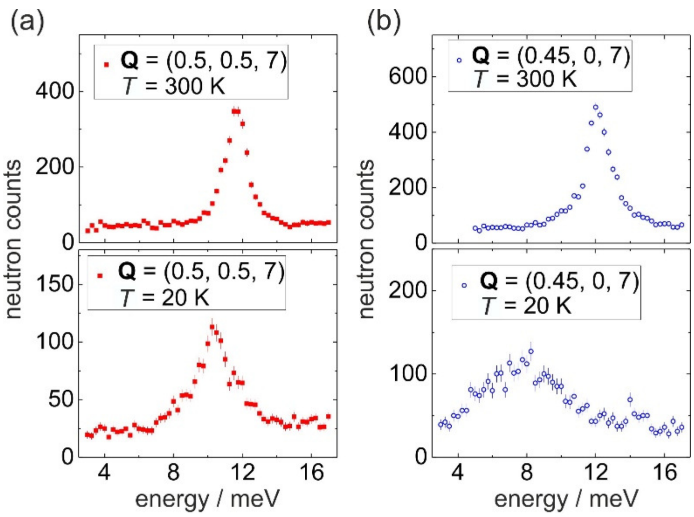
Abstract:

The interplay of complex electronic band structures and the coupling between electrons and the ionic lattice, i.e. electron-phonon-coupling (EPC), is key to an understanding of many unusual electronic band and phonon dispersions as observed, e.g., in cuprates, conventional superconductors but also magnetic metallic materials. However, recent work has shown that assuming a dominant role of the Fermi surface geometry, e.g., due to a strong nesting, is often premature. Here, we propose to perform an in-depth study of EPC as observed by measuring the phonons line width in order to determine the role of electronic band structure and EPC matrix elements. The material of choice is the strong-coupling superconductor YNi2B2C. We will investigate EPC in a volume of momentum space using the FlatCone analyzer-detector setup centered on wave vectors featuring phonons with the strongest EPC effects. We will compare our results to ab-initio lattice dynamical calculations for the phonon line width and the experimentally obtained 3D electronic band structure to determine independently the momentum-dependences of possible nesting geometries and EPC matrix elements.

We investigated the wave vector dependence of electron-phonon coupling (EPC) in the conventional superconductor YNi_2B_2C with inelastic neutron scattering (INS) on the triple-axis spectrometer IN8. The material shows strong EPC effects expressed as energy softening and linewidth broadening on cooling for two low-energy acoustic modes. This anomalous temperature dependence is usually explained by either nesting of the Fermi surface or anharmonicity, i.e. phonon-phonon scattering. However, in a previous study [1] it was found that, at first sight, both approaches are not able to explain the temperature dependence of energy and linewidth for one of the acoustic phonons. We propose an interplay of nesting of specific parts of the 3D Fermi surface and a pronounced wave vector dependence of the EPC matrix elements.

The energy scans were performed at T = 300 K and 20 K at the wave vector where the highest EPC effects are predicted by our density functional perturbation theory (DFPT) calculation and in a volume of reciprocal space to follow the evolution of the effects on changing **q**. The acoustic phonon at **q** = (0.55, 0, 0) was measured in a previous experiment in detail and hence we were mainly focusing on the acoustic phonon at and close to **q** = (0.5, 0.5, 0). Our structure factor calculations revealed that this phonon mode can be observed in the Brillouin zone adjacent to the reciprocal lattice point **τ** = (1, 0, 7) with sufficient intensity. Thus, pronounced EPC effects are expected at **Q** = (0.5, 0.5, 7). The raw data for this **Q**-point is depicted in Fig. 1 (a) at T = 300 K and T = 20 K. The energy of the phonon softens by 1.3 meV (11%) and it obtains an additional linewidth of Γ = 1.7 meV on cooling.

Respective measurements were performed along three different directions starting from **Q** = (0.5, 0.5, 7) to follow the decay of the EPC effects and to identify the wave vectors where they vanish. This resulted in large tilting angles of the whole set-up consisting of sample, sample holder and cryostat of ± 20°. This pushed the capabilities of the instrument to its limits, but still successful measurements were possible.



During the out of plane measurements we became aware that it is possible to also measure the phonon with **q** = (0.55, 0, 0) at **Q** = (0.45, 0, 7). The results of the energy scans are shown in Fig. 1 (b) and the pronounced energy softening and linewidth broadening on cooling due to

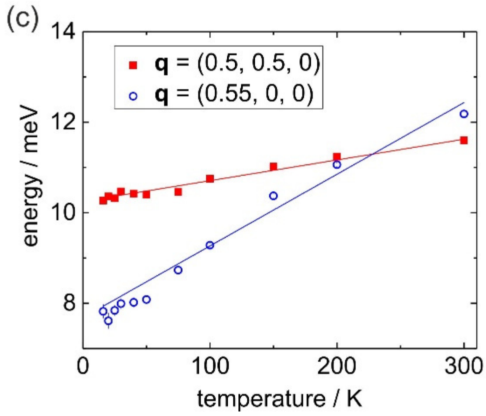


Fig. 1: (a)-(b) Raw data scans from INS at T = 300 K and 20 K for (a) **Q** = (0.5, 0.5, 7) and (b) **Q** = (0.45, 0, 7).

(c) temperature-dependence of the phonon energy of the two acoustic modes shown in (a) and (b). Straight lines are linear fits to the data points.

EPC is clearly visible. We were able to measure the temperature dependence of the phonon energy in the intermediate area between room temperature and T = 16 K (just above the superconducting transition temperature T_C = 15.2 K). The energy of both phonons shows a linear T-dependence [Fig. 1 (c)] and the softening is more pronounced for the phonon with **q** = (0.55, 0, 0) in agreement with our previous results [1].

For our measurements we employed the Cu200 monochromator/analyzer set-up due to its high energy resolution at the expense of a decreased neutron intensity. However, this is compensated by the high incoming neutron flux of the ILL reactor source and the large surface of the monochromator. The good energy resolution enabled us to resolve some mismatches between our previous INS results and the DFPT calculation. Fig. 2 (a) depicts energy scans of phonons with the wave vector **q** ≈ (0.5, 0.5, 0) conducted with a pyrolytic graphite set-up and only one broad peak is visible. The data of the IN8 measurements [Fig. 2 (b)] shows at least two peaks in the same energy range and it is even possible to distinguish between an energy hardening on cooling for a phonon with E ≈ 25 meV and a softening of a phonon with E ≈ 27 meV. This is in good agreement with our DFPT calculations.

The combined results of the calculated electronic contribution to the phonon linewidth γ_{theo} and the INS measurements are shown in Fig. 3 for the principal plane close to **q** = (0.5, 0.5, 0). The symbols represent the experimental results as indicated in the key of the figure. The size of the symbols is chosen as defined in the caption.

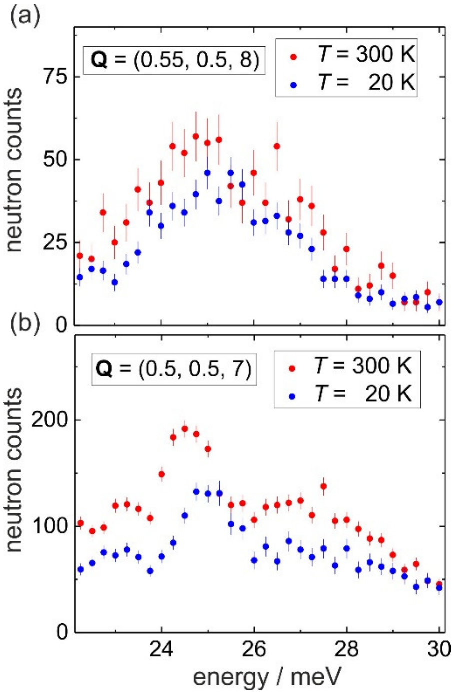


Fig. 2: Comparison of the energy resolution of two different monochromator/analyzer set-ups. (a) Raw data scans at **Q** = (0.55, 0.5, 8) at T = 300 K (red) and 20 K (blue) measured with pyrolytic graphite crystals as monochromator and analyzer, (b) respective energy scans at **Q** = (0.5, 0.5, 7) performed with a Cu200 set-up.

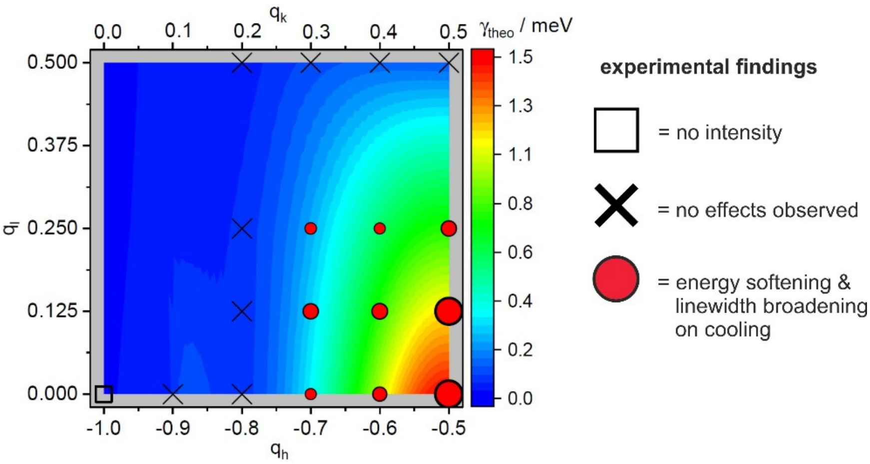


Fig. 3: Comparison of DFPT results for the electronic contribution to the phonon linewidth γ_{theo} and the INS results for energy softening and linewidth broadening on cooling for the principal plane close to **q** = (0.5, 0.5, 0). Experimental results are indicated as shown in the figure (right-hand side). The symbol for **q** = (0.5, 0.5, 0), which exhibits the largest EPC effects, has the largest size and the size of the other symbols is scaled relatively to that point.

We observe a good qualitative agreement between theory and experiment. At wave vectors with small γ_{theo} no EPC effects on cooling were measured (black crosses). Starting from **q** = (0.5, 0.5, 0) the EPC effects decrease on every direction in this plane. However, the decrease of γ_{theo} can not be connected to the reduction of the measured effects in a quantitative way for several values of **q.**

[1] F. Weber *et al.*, Phys. Rev. B **89**, 104503 (2014).