Low-Energy Charge-Density Excitations in MgB_2: Striking Interplay between Single-Particle and Collective Behavior for Large Momenta

Magnesium diboride (MgB_2), discovered in 2001 as a superconductor with a high critical temperature (T_c) of nearly 40 K [1], has been subjected to intense theoretical and experimental studies worldwide. MgB_2 is now widely accepted as a phonon-mediated conventional superconductor based on the anisotropic Eliashberg formalism. The strong electron-phonon coupling between the 2D σ bands and the in-plane vibration of the B layers dominates the superconducting properties and is largely responsible for the unusually high T_c.

Within this phonon-mediated picture of superconductivity, dynamically screened electron-electron, and electron-ion interactions play an important role. Detailed knowledge of the dielectric screening and the associated crystal potential, local-field, and exchange-correlation effects should provide further insight into the dynamical property and hence the superconducting behavior of the material. Using state-of-the-art high-resolution nonresonant inelastic X-ray scattering (NIXS) experiments performed on the Taiwan Inelastic X-ray Scattering beamline **BL12XU**, we discover that the charge response of MgB_2 is truly remarkable [2]. Indeed, as is shown in Fig. 1, a long-lived, low-energy collective excitation in MgB_2 is found to exist not only for small momentum transfer (q) as previously predicted [3], but it actually extends to higher Brillouin zones (BZ's) along the c* axis, displaying a consinelike, periodic energy dispersion with q. Experimentally, the energy dispersion can be described entirely by a simple cosine function: $\omega = \omega_0 - 2\gamma\cos(qc)$, with ω_0 = 3.55 eV, γ = 0.49 eV, and c = 0.352 nm, the lattice constant of MgB_2 along the c* axis. The enhanced scattering cross section at high q and the negligible multiple-scattering effects of the X-ray measurements play a decisive role for the clean observation of this excitation over a large momentum range.

In order to understand the physics behind the data presented in Fig. 1, we have calculated the dynamical structure factor S(q, ω) based on *ab initio* time-dependent density-functional theory (TDDFT), including fully the crystal local-field effects (CLFE). The details can be found in Ref. [2]. The calculated S(q, ω) is compared with the experiment in Fig. 2. The energy dispersion of the collective excitation (dashed curve) can be seen to agree almost perfectly with experiment throughout the four BZ's investigated. Based on the mathematical analysis of the formalism used in the calculation [2], the significance of the

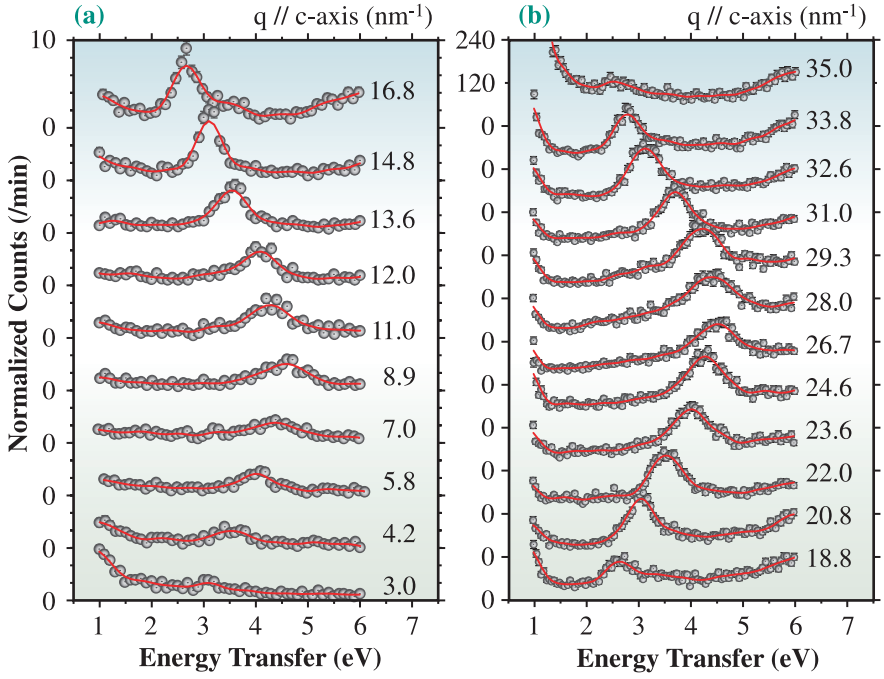

Fig. 1. NIXS spectra at various momentum transfers along the c* axis. The total energy resolution was 65 meV for **(a)** and 250 meV for **(b)**.

agreement is traced back to the fact that the dynamical response represented by S(q, ω) for q's in higher BZ's contains essentially the contribution of two terms: The first term corresponds to the response appropriate for homogeneous media and gives rise to charge fluctuations involving incoherent electron-hole pairs. The second term introduces all the CLFE in the form of a coupling function (*F*), which formally feeds the small-q charge response into charge fluctuations for large q's [2]. It should be noted that the coupling function is *material dependent*, whose actual strength determines whether such excitation can be realized in S(q, ω).

Indeed, in Fig. 3, the contribution to the S(q, ω) of MgB_2 from the first and second terms are shown for q = 32.7 nm^{-1} in the fourth BZ along the c* axis. Clearly, within the energy region of the excitation, the first term amounts only to a weak background, while the second term features a sharp peak, which is typical of the collective excitation for the reduced q (= 2.9 nm^{-1}) in the first BZ. The strength of *F* as shown in the inset of Fig. 3 is ~60 times larger in MgB_2 compared to simple metals and covalent semiconductors. Therefore, in MgB_2 *F* feeds the small-q physics into the charge fluctuation for large q's, and the collective excitation can be viewed as acting – via *F* – as a source driving the collective charge fluctuation generated in a NIXS event for large q's. It is important to notice that this process is intrinsically periodic [2].

In conclusion, the electron-hole degrees of freedom in MgB_2 lead to a novel charge response in which long-lived, collective charge-density fluctuations can be excited in a NIXS event involving large momenta. The mechanism behind the observed periodic excitation is the strong coupling between the single-particle and collective excitation channels, mediated by large CLFE due to charge inhomogeneity normal to the Mg and B layers. The impact of the CLFE on the charge response of MgB_2 rivals their importance in materials involving confined geometries such as carbon nanotubes and superlattices. Ultimately, the nature of the measured charge excitations stems from the layered electronic structure of MgB_2 and the delocalized nature of the orbitals involved in the screening. Analogous physics should be at play in other layered compounds of current interest.

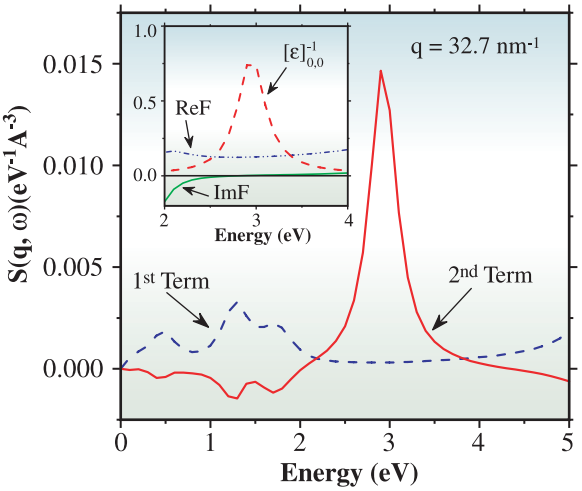

Fig. 3. Contributions from the first and second terms to S(q, ω) of MgB_2 at q = 32.7 nm^{-1} along the c* axis. The inset shows the real and imaginary parts of the coupling function (*F*) and the charge response (ε^{-1}) for q = 2.9 nm^{-1}. See Ref. [2] for further details.

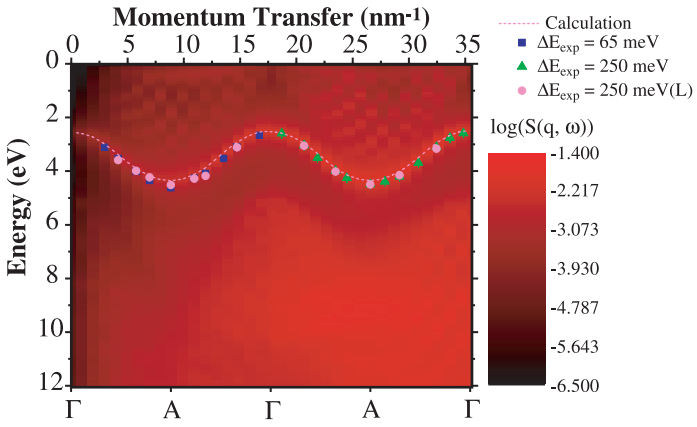

Fig. 2. Theoretical S(q, ω) in false color log scale as a function of energy and momentum transfer showing the cosine energy dispersion of the low-energy collective excitation. Filled symbols (■▲●) marks the energy positions obtained from the NIXS spectra.

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