Acoustic Plasmons in MgB$_2$

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We present strong evidence for the existence of an acoustic plasmon mode, that is, a quadrupolar charge collective mode with linear dispersion, in MgB$_2$. This mode may be responsible for the anomalously small value of the Coulomb pseudopotential required to explain the high superconducting transition temperature of 40K.

The recent discovery of superconductivity in MgB$_2$ [1] has spurred a wave of activity both on the experimental and on the theoretical side. The transition temperature of $T_c = 39.5$K is by far the highest found in any binary compound. With the exception of C$_60$, it is surpassed only by the high-temperature copper-oxide superconductors. A detailed analysis of the electron-phonon interaction finds relatively strong coupling to a high frequency phonon mode [2]. However, the observed $T_c = 39.5$K could be obtained only by assuming that the Coulomb pseudopotential takes an anomalously small value, $\mu^* \approx 0.02$ — a value roughly seven times smaller than for usual $s$-$p$ superconductors. Here, we propose that an acoustic plasmon mode exists in MgB$_2$. This leads to an attractive contribution, thereby lowering the value of the Coulomb pseudopotential.

The idea of acoustic plasmons goes back to Pines [3], and, following Fröhlich, has been considered as a mechanism for superconductivity in the transition metals in the past [4]. In the presence of two carrier species with very different effective masses, the light carriers can act to screen the Coulomb repulsion between the heavy carriers, and thereby lower the plasma frequency of the heavy carriers. The resulting plasmon mode will have a linear dispersion $\omega_a = v_a q$ (hence the term acoustic plasmon), where $v_a$ is of the order of (but somewhat higher than) the Fermi velocity of the heavy carriers. The acoustic plasmon mode is Landau damped by decay into the electron-hole continuum of the light carriers, but for small wave vectors $q$ the mode will be located within the lower range of the electron-hole continuum, so that the damping may be weak, and the acoustic plasmon may exist as a well-defined collective mode.

Since no experimental evidence of acoustic plasmons could be found, and one was able to explain superconductivity in the transition metals within the usual phonon mechanism, interest in the topic began to wane in the late 1980’s. We believe that MgB$_2$ is a good candidate for further research on acoustic plasmons and their contribution to superconductivity, due to its Fermi surface characteristics. These have been first reported in Ref. [5], and will be briefly described below:

MgB$_2$ consists of honeycomb layers of boron atoms that are stacked vertically with no displacement. The magnesium atoms are located at the center of the hexagons formed by boron, but between the boron planes. The resulting structure is called the AlB$_2$ structure. The in-plane lattice constant is $a = 3.086\,\text{Å}$, while the interlayer spacing is $c = 3.524\,\text{Å}$. Hence there is a strong anisotropy in the boron-boron bond lengths. To a good approximation, the outer shells of the Mg atoms can be assumed as being fully ionized, so that the boron system bears a certain resemblance with graphite, both structurally and electronically. The differences in the electronic properties of MgB$_2$ and graphite are mainly due to the attractive potential of the Mg ions, which enhances the dispersion of the $p_z$-orbitals parallel to the $c$-axis through hybridization with the Mg $s$-orbital.

Carriers are situated in two hole bands derived from the $\sigma$-bonding boron $p_{x,y}$-orbitals, that are essentially two-dimensional, and in one electron and one hole band derived from the $\pi$-bonding boron $p_z$-orbitals (see Fig. 1). The smaller overlap of the latter in the $x, y$-directions compensates for the larger interatomic spacing in the $z$-direction, so that the $\pi$-bands are nearly isotropic.

An essential feature of the band structure is the large difference in the $z$-components of the Fermi velocities between the $\sigma$ hole bands and the $\pi$ electron and hole bands.
As will be shown explicitly below, the existence of two different velocity scales gives rise to a weakly damped acoustic plasmon mode that corresponds to long-wavelength charge density fluctuations between these bands. While the total charge density \( \rho_\pi + \rho_\sigma \) does not fluctuate, the charge difference \( \rho_\pi - \rho_\sigma \) will vary locally. Since the \( \sigma \)-orbitals are mainly located within the Boron planes, while the charge in the \( \pi \)-orbitals is situated between the planes, this charge transfer between the orbitals gives rise to quadrupolar charge fluctuations.

We will now show the existence of a well-defined acoustic plasmon mode within the random phase approximation (RPA). For our purpose it is convenient to define the polarization insertion \( \Pi_{ab} \) for different carrier species \( a \) and \( b \) as indicated in Fig. 2. For a single carrier species, \( \Pi_{aa} \) then reduces to the standard definition [7]. The polarization insertion is related to the time-ordered density-density correlation function \( C_{ab} \) between different types of carriers as

\[
C_{ab}(r, t) = -i \langle \Delta n_a(r, t) \Delta n_b(0, 0) \rangle = \hbar \Pi_{ab}(r, t). \tag{1}
\]

Here \( q = (q, \omega) \) is a momentum four-vector, \( U_0(q) = 4\pi e^2/q^2 \) is the bare Coulomb potential, and \( n_a = n_a - \langle n_a \rangle \) denotes the fluctuations in the charge density of carrier species \( a \). Specializing to the case of two carrier species of opposite charge (electrons and holes), we can express \( \Pi_{ab} \) in the random phase approximation as

\[
\Pi_{ab}^{\text{RPA}}(q) = \frac{\delta_{ab} \Pi_0^0(q) - U_0(q) \Pi_0^0(q) \Pi_0^0(q)}{1 - U_0(q) \Pi_0^0(q) - U_0(q) \Pi_0^0(q)}, \tag{2}
\]

where the lowest-order polarization insertion \( \Pi_0^0 \) is given in terms of the non-interacting Green’s functions \( G^0_\sigma \) as

\[
\Pi_0^0(q) = \frac{2}{i\hbar} \int \frac{d^3k}{(2\pi)^3} G^0_\sigma(k) G^0_\sigma(k + q). \tag{3}
\]

We now define the total charge fluctuations \( n_+ = \hat{n}_1 - \hat{n}_2 \) and the charge transfer fluctuations \( n_- = \hat{n}_1 + \hat{n}_2 \). Then the corresponding correlation functions are given by

\[
\frac{1}{\hbar} C_-(q) = \frac{\Pi_0^0(q) + \Pi_0^0(q)}{1 - U_0(q) \Pi_0^0(q) - U_0(q) \Pi_0^0(q)}, \tag{4}
\]

and

\[
\frac{1}{\hbar} C_+(q) = \frac{\Pi_0^0(q) + \Pi_0^0(q) - 4U_0(q) \Pi_0^0(q) \Pi_0^0(q)}{1 - U_0(q) \Pi_0^0(q) - U_0(q) \Pi_0^0(q)}. \tag{5}
\]

A collective mode corresponds to a pole in the correlation function in the complex frequency plane, and can thus be identified by the condition

\[
\sum_a \Pi_0^0(q) = \frac{1}{U_0(q)}, \tag{6}
\]

which remains valid for more than two carrier species as well. For small wave vectors \( U_0(q) \) will be very large, so that we can set the left-hand side to zero instead. Inserting the above condition into the numerator of Eq. (4), we see that the pole’s residue is proportional to \( 1/U_0(q) \sim q^2 \), so that fluctuations in the total charge density are suppressed for small wavevectors. Due to the additional term in the numerator of Eq. (5) this is not the case for the charge transfer fluctuations described by \( C_+ \).

We calculated the band structure with the tight-binding linear muffin-tin orbital (TBLMTO) method [8], and used the following analytical fits for our calculations of \( \Pi^0 \): For the \( \sigma \) bands,

\[
\epsilon_\sigma(k) = \epsilon_0^{(\sigma)} + 2 \epsilon^{(\sigma)} \cos(k_z c) - \frac{\hbar^2}{2m_{e,1,2}} (k_x^2 + k_y^2), \tag{7}
\]

where \( \epsilon_0^{(\sigma)} = 0.66 \text{ eV}, \epsilon^{(\sigma)} = 0.22 \text{ eV}, m_1 = 0.27 m_e, \) and \( m_2 = 0.50 m_e, \) with \( m_e \) being the bare electron mass. For the \( \pi \) bands we used...
\[ \epsilon(k) = \epsilon_0^{(\pi)} - 2t_z^{(\pi)} \cos(k_z c) \]  
\[ \pm 2t_x \sqrt{\frac{3}{4} + \frac{1}{2} \cos(k_x a) + \cos(\frac{1}{2} k_x a) \cos(\sqrt{\frac{3}{2} k_y a})}, \]

where \( \epsilon_0^{(\pi)} = 0.16 \text{ eV}, \ t_z^{(\pi)} = 1.12 \text{ eV}, \ t_x = 1.73 \text{ eV}, \) and the positive or negative sign corresponds to the electron and hole band, respectively.

Within the approximate dispersion given by Eq. (7), the lowest-order polarization insertion of the \( \sigma \) bands can be calculated exactly for the special case where \( q \) is parallel to the \( z \)-axis:

\[ \Pi_0^{(\sigma)}(q, \omega) = \frac{m_{1,2}}{\pi \hbar^2 c} \left\{ \frac{\theta(1 - Y^2) - i \theta(Y^2 - 1)}{\sqrt{|1 - Y^2|}} \right\}, \]

where \( Y = 4t_z^{(\sigma)} \sin(qc/2)/\hbar \omega, \) and \( \theta(x) \) is the Heaviside step function. For \( q \) off the \( z \)-axis and for the \( \pi \)-bands we resort to numerical calculations. Results are shown in Fig. 3. From the condition (6) we can identify an acoustic plasmon mode with dispersion \( \omega_a = v_a q, \) where the plasmon velocity is \( v_a \simeq 1.78 \text{ A eV} = 2.70 \times 10^7 \text{ cm/s}. \) The acoustic plasmon mode is weakly damped by decay into the \( \pi \) electron-hole continuum. The remaining two zeroes of Re\( \Pi \) lie deep within the electron-hole continuum and correspond to overdamped modes, as can be seen from the large imaginary part of Re\( \Pi \). To estimate the damping coefficient \( \lambda \) of the weakly damped mode we assume that the contribution from the \( \pi \) carriers to the real and imaginary parts of Re\( \Pi \) is constant in the vicinity of \( \omega_a. \) Then the imaginary part of the pole’s location in the complex plane can easily be calculated from the analytic expression (9), and yields a Q-factor \( Q = \omega_a/\lambda \simeq 15. \) The acoustic plasmon mode is hence well-defined.

The above analysis leads us to propose that a well defined acoustic plasmon mode exists for small values of the transverse component \( q \perp. \) Physically this mode corresponds to quadrupolar charge fluctuations involving a local charge transfer between \( \sigma \)- and \( \pi \)-orbitals of the boron atoms. This collective mode in turn leads to an attractive retarded contribution to the Coulomb interaction in a window in \( (q, \omega) \)-space, which will modify the repulsive Coulomb pseudopotential. Further analysis is required to determine if the modification is strong enough to give the proposed reduction to a value of \( \mu^* = 0.02. \)

[1] J. Nagamatsu, N. Nakagawa, T. Muranaka, and J. Akimitsu, Nature 410, 63 (2001).
[2] Y. Kong, O. V. Dolgov, O. Jepsen, and O. K. Andersen, preprint cond-mat/0102499 (2001).