Overscreening–free electron–phonon interaction in realistic materials

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State–of–the–art model Hamiltonians, like Fröhlich’s, or density functional theory approaches to electron–phonon interaction suffer from a severe overscreening error. This is due to the incorrect treatment of the screening of the ionic potential. We derive a correct formulation of the electron–phonon interaction and demonstrate its validity by numerically implementing the new scheme in a paradigmatic material: MgB$_2$, a system whose double-gap, low-$T_c$ superconductivity depends on exceptionally high phonon linewidths. We find that the present treatment enhances the linewidths by 57% with respect to what has been previously reported for the anomalous $E_{2g}$ mode. We further discover that the $A_{2u}$ mode is also anomalous (its strong coupling being completely quenched by the overscreened expression). Our results deeply question methods based on state–of–the–art approaches and impact a wide range of fields such as thermal conductivity, phononic instabilities and non–equilibrium lattice dynamics.

Introduction. The research on the physics induced by electron-phonon interaction is one of the most prolific topics in materials science and solid state physics [1–4]. The electron-phonon interaction is at the basis of the description of such disparate phenomena as BCS superconductivity [5–10], lattice thermal conductivity and transport [11–15], structural stability and phase transitions [16–19], ultrafast lattice dynamics [20–21], spectral shape of Raman, x-ray, neutron and related spectroscopies [22–25], and more. State-of-the-art methods are based either on first principles, with density functional perturbation theory (DFPT) schemes [26–29] or model electron–phonon approaches like the Fröhlich Hamiltonian [30–32]. Yet, both approaches, and more generally any approach introducing an effective electron-phonon Hamiltonian, suffer from a systematic overscreening error when computing phonon linewidths and lifetimes. This error is due to the different way electrons and phonons are affected by the electron-phonon interaction, and it has been noted by several authors [33–35]. While the role of the screening in the renormalisation of the static phonon frequencies has been recently studied [36], its relevance in the case of phonon linewidths remains underappreciated. In fact, although attempts to either overcome or minimise the overscreening error have been made [19–32], the overscreening of the phonon quasiparticle corrections has not been generally addressed in the literature, including very recent calculations [37].

In practice, the overscreening error follows from the assumption of a starting electron–phonon Hamiltonian written as

$$\hat{H} = \hat{H}_{ph} + \hat{W}_{c-ph} + \hat{H}_e,$$  

(1)

where $\hat{H}_{ph}$ is the noninteracting phonon system taken in the harmonic approximation with eigenvalues $\Omega_\nu$, $\hat{W}_{c-ph} = \sum_{ij\nu} g^{SC}_\nu \hat{\rho}_{ij} \hat{Q}_\nu$ is the electron–phonon interaction, and $\hat{H}_e$ the electronic Hamiltonian. Here, $g^{SC}_\nu$ is the screened electron–phonon matrix element between electronic states $i$ and $j$ and phonon mode $\nu$, $\hat{\rho}_{ij}$ is the electron density operator and $\hat{Q}_\nu$ the phonon displacement.

Eq. (1) is used in countless fields in physics. Its key property is that the renormalization of $\Omega_\nu$, and the screening of $g^{SC}_{\nu ij}$ appear simultaneously due to electronic correlations. The most elementary and known treatment is based on the Hartree approximation, which corresponds to the well–known Random–Phase Approximation [3,38]. Regardless of the approximation employed, it is generally not possible to obtain meaningful phonon frequencies without including screening. The problem is that physically, screening arises dynamically from the response of the electron system to the perturbation induced by lattice vibrations, while in Eq. (1) it is embedded in the approximated Hamiltonian from the start. This procedure causes any scattering event between phonons and electrons to be preemptively screened: when the dynamical response of the phonon system is computed at various orders in perturbation theory, the screening is then counted multiple times in an uncontrollable way. This implies that there is no formal way to avoid the overscreening error when Eq. (1) is used.

In this manuscript, we provide an overscreening error–free formulation of the electron-phonon interaction that avoids the use of Eq. (1). Here, by taking the paradigmatic case of MgB$_2$ as a testbed, we demonstrate that the overscreening error can lead to an underestimation of the phonon linewidths as large as 57% (the well-known $E_{2g}$ mode). At the same time we also discover instances where the overscreening error leads to a large reduction of the linewidths by more than one order of magnitude (the $A_{2u}$ mode). The present overscreening error–free approach also improves the agreement with experimental results. These results provide new theoretical insights on electron-phonon physics, while also being especially relevant to all the fields where electron-phonon interaction...
is customarily modelled with the overscreened Hamiltonian, Eq. (1).

Figure 1. Phonon linewidths in MgB$_2$ computed at the A point in the Brillouin zone. Only the relevant phonon modes are shown. Orange: overscreened (OE) linewidths. Teal: linewidths without overscreening (no OE). The full and empty bars represent the contributions to the linewidths stemming from intraband and interband processes, respectively.

The complete theoretical derivation of our proposed treatment is presented in our companion paper.

In the following, we will first explain our approach, then we will describe the results on MgB$_2$ and finally discuss the wider implications of our findings.

Screened and bare electron-phonon interaction. The phonon-related quantities appearing in Eq. (1) depend on the treatment of the electron–electron interaction, $V_{\text{e-e}}$, embodied in $H_e$. On the one hand, if $V_{\text{e-e}}$ were neglected, then the phonon quantities would be bare, i.e., unscreened: we would have $\Omega_\nu = \Omega_\nu^{\text{BARE}}$ and $g_{\nu ij}^{\text{BARE}}$, with

$$g_{\nu ij}^{\text{BARE}} = \int d^3r \, \phi_i^*(r) \partial_\nu \langle_{\text{eq}} V_{\text{e-\text{ion}}}(r) \phi_j(r).$$

Eq. (1) the $\phi_i(r)$ are eigenfunctions of $H_e$ and $V_{\text{e-\text{ion}}}$ is the electron-ion interaction. On the other hand, if the effect of $V_{\text{e-e}}$ is included by using either a fully many-body approach or any mean-field (mf) approximation, like DFPT, then the phonon frequencies, $\Omega_\nu^{\text{SCR}}$, and the electron–phonon matrix element, $g_{\nu ij}^{\text{SCR}}$, become screened. The matrix elements $g_{\nu ij}^{\text{SCR}}$ are given by:

$$g_{\nu ij}^{\text{SCR}} = \int d^3r \, d^3r' \, \epsilon^{-1}(r-r') \phi_j^*(r') \partial_\nu \langle_{\text{eq}} V_{\text{e-\text{ion}}}(r') \phi_i(r'),$$

where $\epsilon$ is the static dielectric function responsible for the screening. Since unscreened phonon frequencies are unphysical, any approach that aims at being predictive and accurate must include screening. If, however, the approach is based on Eq. (1), then the overscreening error cannot be avoided, and thus it is always present from the start when dealing with electron-phonon interactions. In the language of many-body perturbation theory, the overscreening error takes the form of a double counting of the terms originating from the perturbative expansion of $\epsilon^{-1}$.

Expression for the phonon linewidths. The phonon linewidths are given by twice the imaginary part of the retard phonon-electron self-energy evaluated at the phonon energy itself. The resulting expressions (with superscript OE denoting the overscreened case) are:

$$\gamma_{\text{OE}} = \frac{4\pi \Omega_\lambda}{N_k} \sum_{nmk} |g_{\lambda q,nmk}^{\text{SCR}}|^2 \delta(\varepsilon_{nmk}) \delta(\Omega_\lambda - \Delta^q_{nmk}),$$

and

$$\gamma_{\lambda q} = \frac{4\pi \Omega_\lambda}{N_k} \sum_{nmk} G_{nmk}^{\lambda q} \delta(\varepsilon_{nmk}) \delta(\Omega_\lambda - \Delta^q_{nmk}).$$

These expressions describe energy-conserving scatterings between phonons and electron-hole pairs. In particular, $\Omega_\lambda$ is the phonon energy of branch $\lambda$ and momentum $q$. $\Delta^q_{nmk} = \varepsilon_{nmk} - \varepsilon_{mk-q}$ is the energy of an electronic transition from band $m$ with momentum $k-q$ to band $n$ of momentum $k$, and $N_k$ is the total number of $k$-points included in the discrete $k$-integral. Eq. (4) is affected by the overscreening error while Eq. (5) is not. The difference in the two expressions is the intensity of the coupling strength, which in the overscreened case depends exclusively on the screened matrix element $g_{\lambda q,nmk}^{\text{SCR}} = 1/\sqrt{2\Omega_\lambda} \langle nk | \partial_\lambda W_{\text{e-\text{ion}}}(mk-q) | mk \rangle$ expressed in the single-particle basis with the correct energy renormalisation. The derivative of the screened interaction $W_{\text{e-\text{ion}}}$ corresponds in DFPT to the derivative of the self-consistent Kohn-Sham potential, and is equivalent to Eq. (1) when the dielectric screening is treated at the DFT level. The coupling strength which defines an overscreening–free phonon linewidth is

$$G_{nmk}^{\lambda q} = \frac{1}{2} \left\{ g_{\lambda q,nmk}^{\text{SCR}} g_{\lambda q,nmk}^{\text{BARE}} + g_{\lambda q,nmk}^{\text{SCR}} g_{\lambda q,nmk}^{\text{BARE}} \right\}.$$
Application to MgB$_2$. Magnesium diboride is a metallic layered material composed of alternating 2D sheets of boron and magnesium. It transitions to phonon-mediated superconductivity at the critical temperature $T_c = 39$ K [57–61]. This behaviour is almost entirely due to electron–phonon coupling relative to the boron atoms, whose electrons form in-plane $\sigma$ and out-of-plane $\pi$ bonds. These bonds are in turn responsible for the existence of two superconducting band gaps, with different theoretical $T_c$ [5, 61–66]. In particular, the $\sigma$ bands are considered to yield a giant “anomalous” electron–phonon coupling due to the strong orbital overlap induced by the in-plane optical phonon mode $E_{2g}$, as opposed to the $\pi$ bands undergoing a weak coupling. The calculated phonon and electron dispersions are shown in Fig. 2(a) and (b), respectively.

As they are necessary ingredients for the calculation of critical temperatures and superconducting gaps [5, 61–67], the $E_{2g}$ phonon linewidths have been extensively studied, both theoretically and experimentally, along the $\Gamma A$ [24, 68, 69] and $\Gamma M$ [70] directions in the hexagonal Brillouin zone. In these studies, the comparison is made between the full-width half-maximum of inelastic x-ray scattering spectral peaks and the results of Eq. (4), showing in general reasonable agreement, though particularly along $\Gamma A$ the linewidths are found to be larger than the theoretical results. For example, in Ref. [24] a theoretical value of 20.35 meV is found at point A, while the experimental peak width is closer to 30 meV [71].

Let us start the discussion from the calculation of the $E_{2g}$ mode. As can be seen from Fig. 1, we obtain 18.2 meV in the overscreened case, Eq. (4), in very good agreement with the same calculation in Ref. [24]. The correctly screened case, Eq. (6), gives instead the value of 28.6 meV, showing a 57% increment in the phonon linewidths. We notice that in the case of $\sigma$ bands, around 70% of the contribution comes from “intraband” terms (i.e., electron-hole pairs are formed within the same $\sigma$ subband), while the remaining 30% is due to “interband” terms involving different $\sigma$ subbands. The large 57% increase in the linewidths is also the average along the full $\Gamma A$ direction, as can be seen from Fig. 3(a), while a strong increase also appears along the $\Gamma M$ direction. Along the latter, both overscreened and overscreening–free linewidths sensibly decrease after the midpoint from $\Gamma$ to $M$ due to a sharp increase of the relative phonon energies. The comparison with experiment is difficult due to the large errorbars, but overall we do obtain a better agreement in the overscreening–free case (compare with Fig. 3 in [24] and Fig. 3 in [70] for the $\Gamma A$ and $\Gamma M$ directions, respectively).

The $E_{2g}$ mode is not the only one undergoing large changes when overscreening is removed. In fact, we see from Fig. 1 that also the acoustic $A_{2u}$ mode gains a giant linewidth increase from 1 meV (overscreened case) to 41 meV (overscreening–free case). By looking at Fig. 3(b) we realise that these giant linewidths appear along the full $\Gamma A$ direction, where the acoustic $A_{2u}$ mode maintains an average linewidth of 42 meV, and also characterise the higher-energy, optical mode of the same symmetry. Now, the infrared-active $A_{2u}$ modes involve out-of-plane oscillations of the boron atoms; furthermore, we see that the linewidth is composed by purely intraband contributions. Both these observations are consistent with the coupling of the $A_{2u}$ modes to the $\pi$ bands. Therefore, we explain the enormous difference between the overscreened and overscreening–free cases as follows. The overlap of the boron $\pi$ orbitals increases because of the $A_{2u}$ ionic oscillations; however, the effect would be weakened both by the low charge density in the overlap volume (at equilibrium, two boron atoms on different layers are separated by 3.5 Å) and especially by the electronic screening of the intervening magnesium layer. In this situation, the double counting of the screening in the calculation of the electron–phonon matrix elements then leads to a massive reduction of the coupling strength, which is not found in the correct treatment.

Our results suggest that the $\pi$-band electron–phonon
quasiparticle renormalisations and superconducting band
impact the theoretical estimates of critical temperatures,
free coupling strength, like the ones presented here, will
believe that strong variations in the overscreening error–
the theory via the Eliahsberg spectral function. We be-
error since the electron-phonon coupling strength enters
Eliahsberg theory, which is affected by the overscreening
mediated superconductivity are based on Migdal-
such cases below.

Interestingly, the acoustic $A_{2u}$ linewidths remain con-
stant along $\Gamma A$ despite strong variations in the relative
phonon energies, while the optical $A_{2u}$ linewidths de-
crease from 28 to 0.6 meV despite the phonon energies
being roughly constant. We also point out that such a
giant overscreening effect is not limited to the cou-
pling with the $\pi$ bands along $\Gamma A$, but also appears –
although to a lesser extent – in the linewidths of the in-
plane $E_{1u}$ modes, which couple with the $\sigma$ bands, along
$\Gamma M$ (here the largest effect is on the higher-energy acous-
tic $E_{1u}$ mode up to 0.5$\Gamma M$, where the overscreening–free
linewidths rise to 15 – 20 meV).

Discussion. We have studied from first-principles the
phonon linewidths of MgB$_2$ after removing the over-
screening error in the electron-phonon coupling. We
prove that in this case, this removal entails large qualita-
tive and quantitative changes with respect to the state-
of-the-art overscreened case. These findings have con-
sequences for a wide range of theoretical calculations of
phonon-related properties in crystals. We examine two
such cases below.

The current theoretical approaches around phonon-
mediated superconductivity are based on Migdal-
Eliashberg theory, which is affected by the overscreening
error since the electron-phonon coupling strength enters
the theory via the Eliashberg spectral function. We be-
lieve that strong variations in the overscreening error–
free coupling strength, like the ones presented here, will
impact the theoretical estimates of critical temperatures,
quasiparticle renormalisations and superconducting band
gaps, which in some cases show a discrepancy with the
experimental results.

The physics of out-of-equilibrium, ultrafast phenomena
related to lattice dynamics may also be very sensitive to
the overscreening error. The relaxation of the coupled
electron-lattice system is governed by differential equa-
tions in which the overscreening error is introduced at
every time step, possibly strongly affecting the result-
ning rates. In addition, the role of the time evolution
of the electronic screening out of equilibrium has to be
investigated carefully, along with the issues of total en-
ergy and particle conservations, since the overscreening
error–free treatment openly questions the standard semi-
classical Boltzmann approach based on Fermi’s golden
rule.

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[56] The computational details needed to reproduce our MgB₂ results are the following. More information about the steps and general structure of the calculations, as well as about the double grid procedure, can be found in our companion paper [39]. The input files we used for the various steps are readily available as Supplemental Material in the interest of reproducibility. The DFT steps were performed with PAW [78], scalar-relativistic pseudopotentials, available here: https://www.quantum-espresso.org/pseudopotentials We used a plane-wave cutoff of 55 Ry and a gaussian smearing of 0.025 Ry. We included 12 electronic bands in the calculations since they are enough to describe transitions within one Debye energy (∼100 meV) around the Fermi level. The electronic ground state and the derivatives of the self-consistent potential were converged with a regular k-point grid equal to 9 × 9 × 9. In order to ensure consistency between electron and phonon calculations, we used the internally relaxed lattice parameters which are equal to a = 3.074 Å and c = 3.521 Å for the in-plane and out-of-plane lattice parameters, respectively. We then used a coarse grid of 24 × 24 × 24 k-points for the electron-phonon calculations in conjunction with a fine grid of 55296 random k-points for the electronic band energies. Both these grids were converged together and along with a broadening parameter for the delta functions in Eqs. (1) and (3) equal to 5 meV. Lower values generally tended to introduce numerical noise, even for our densest coarse and fine grids.

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