

## Small Fermi energy, zero-point fluctuations, and nonadiabaticity in MgB<sub>2</sub>

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Small Fermi energy effects are induced in MgB<sub>2</sub> by the low hole doping in the  $\sigma$  bands which are characterized by a Fermi energy  $E_F^\sigma \sim 0.5$  eV. We show that due to the particularly strong deformation potential relative to the  $E_{2g}$  phonon mode, lattice fluctuations are reflected in strong fluctuations in the electronic band structure. Quantum fluctuations associated to the zero-point lattice motion are responsible for an uncertainty of the Fermi energy of the order of the Fermi energy itself, leading to the breakdown of the adiabatic principle underlying the Born-Oppenheimer approximation in MgB<sub>2</sub> even if  $\omega_{\text{ph}}/E_F \sim 0.1-0.2$ , where  $\omega_{\text{ph}}$  are the characteristic phonon frequencies. This amounts to a new nonadiabatic regime, which could be relevant to other unconventional superconductors.

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Four years after the discovery of superconductivity at 39 K in MgB<sub>2</sub>,<sup>1</sup> the superconducting properties of this material are still the object of investigation. One of the anomalous characteristics of MgB<sub>2</sub> with respect to conventional Migdal-Eliashberg (ME) superconductors is the remarkable smallness of the Fermi energy  $E_F^\sigma$  associated with the holelike  $\sigma$  bands, which are the most involved in the Cooper pairing. ME theory holds true indeed only if the Fermi energy  $E_F$  is much larger than any other energy scale of the system. Several analyses indicate, however, that this is not the case of MgB<sub>2</sub>. LDA calculations, for instance, estimate the energy distance between the chemical potential and the top of the  $\sigma$  bands to be  $\sim 0.4-0.6$  eV,<sup>2,3</sup> in agreement with angle-resolved photoemission spectroscopy (ARPES) measurements.<sup>4</sup> Estimates of the Fermi energy can be inferred also from penetration depth measurements giving  $E_F = 3200$  K in MgB<sub>2</sub>,<sup>5</sup> and even less in Al- and C-doped compounds.<sup>5,6</sup>

In previous studies we have analyzed some of the effects related to a small Fermi energy  $E_F^\sigma$  on different electronic and vibrational properties of MgB<sub>2</sub>. One of these effects is the breakdown of Migdal's theorem, and consequently of the Migdal-Eliashberg diagrammatic theory, which occurs when the Fermi energy  $E_F^\sigma$  and the phonon energy  $\omega_{\text{ph}}$  are comparable ( $\omega_{\text{ph}}/E_F^\sigma \lesssim 1$ ).<sup>7,8</sup> Another one is the remarkable anharmonicity of the  $E_{2g}$  phonon mode, related to the splitting in energy of the  $\sigma$  bands under the  $E_{2g}$  distortion.<sup>9</sup>

In this paper we want to discuss in greater detail new physical consequences of the comparable size of  $E_F^\sigma$  and the  $E_{2g}$  splitting energy of the  $\sigma$  bands in MgB<sub>2</sub>. In particular we review in a critical way the validity of the adiabatic Born-Oppenheimer (BO) approximation for the  $E_{2g}$  phonon, which is the most relevant to the superconducting pairing. As our main result we show that, due to the large quantum fluctuations associated with the zero point motion, the BO principle is broken down *independently* of the  $\omega_{\text{ph}}/E_F^\sigma$  ratio. This novel kind of adiabatic breakdown is thus shown to be related to the parameter  $\kappa = g_{E_{2g}}^\sigma/E_F^\sigma$ , where  $g_{E_{2g}}^\sigma$  is the electron-phonon matrix element which couples the electrons in  $\sigma$  bands to the

$E_{2g}$  phonon mode in MgB<sub>2</sub>. A simple quantum analysis gives  $\kappa \sim 0.9-1$ , strongly questioning the reliability of a Born-Oppenheimer based analysis.

The Born-Oppenheimer principle is implicitly assumed in writing down an effective electron-phonon model starting from *ab initio* techniques. In simple terms, the BO principle permits one to describe the full many-body wave function  $\Psi(\mathbf{r}; \mathbf{u})$  in terms of two separate quantum systems: a purely electronic problem, which depends parametrically on the ion variables, and an effective lattice problem, where the electronic degrees of freedom have been integrated out.<sup>10</sup> The total wave function  $\Psi(\mathbf{r}; \mathbf{u})$  can thus be written as the product of two "partial" wave functions

$$\Psi_{\alpha,n}(\mathbf{r}; \mathbf{u}) \simeq \chi_{\alpha,n}(\mathbf{u}) \varphi_n(\mathbf{r}; [u]), \quad (1)$$

where  $\mathbf{r}$  and  $\mathbf{u}$  represent the electronic and lattice degrees of freedom, respectively, and  $(\dots; [u])$  indicates a parametric (not quantum) dependence on the lattice variable. The index  $n$  identifies the quantum number of the electronic state and the label  $\alpha$  the phonon eigenstate in the effective lattice potential which depends on the electronic cloud  $\varphi_n(\mathbf{r}; [u])$ .

In the spirit of the BO approximation, the electronic ground state wave function  $\varphi(\mathbf{r}; [u])$  is obtained as the lowest energy electronic state available for fixed  $u$ . Born and Oppenheimer showed that Eq. (1) can be considered a good approximation as far as  $(-\hbar^2/M)\nabla_u^2 \varphi(\mathbf{r}; [u])$  ( $M$  being the atomic mass) is negligible. This assumption corresponds to the adiabatic hypothesis that the electronic dynamics of  $\varphi(\mathbf{r}; [u])$ , is much faster than the lattice one. In common metals a widely used parameter to evaluate this condition is the adiabatic ratio  $\omega_{\text{ph}}/E_F$ , where  $E_F$  can be estimated in the undistorted  $u=0$  ground state configuration  $E_F = E_F[u=0]$ , and  $\omega_{\text{ph}}$  is the lowest energy excitation of the  $\chi_{\alpha,n}$  phonon spectrum. However it should be noted that, in order for the adiabatic principle to apply, the condition  $(-\hbar^2/M)\nabla_u^2 \varphi(\mathbf{r}; [u]) \sim 0$  must be fulfilled in *all the region* of the  $\mathbf{u}$  space where  $\chi(\mathbf{u})$  has a sizable weight. This constraint results to be much stronger than the conventional adiabatic

condition  $\omega_{\text{ph}}/E_F \ll 1$ , since it implies the adiabatic ratio to be negligible for generic lattice distortions  $u$ , namely,  $\omega_{\text{ph}}/E_F[u] \ll 1$ , where the lattice wave function  $|\chi(\mathbf{u})|^2$  provides the range of the relevant  $u$  space. As we are going to see, the breakdown of this assumption for a relevant range of the  $E_{2g}$  lattice distortion  $u$  is expected to be responsible for the partial failure of the BO approximation in  $\text{MgB}_2$ .

In order to test the validity of the BO approximation, the example of frozen phonon techniques is particularly instructive since they are a direct implementation of the BO principle. In the frozen-phonon approach the electronic structure and the total energy of the system are calculated as a function of a static lattice distortion, in the spirit of the BO principle, providing  $\varphi(\mathbf{r};[u])$ . The frozen phonon lattice potential is therefore used to solve the lattice quantum problem and to get the ground state lattice wave function  $\chi(\mathbf{u})$ . We shall now apply the same technique to  $\text{MgB}_2$ , in order to show that, due to the small  $E_F^\sigma$  and to the strong deformation potential of the  $E_{2g}$  phonon mode, the BO approximation cannot be safely applied in this system.

As mentioned above, small Fermi energy effects in  $\text{MgB}_2$  involve the subset of the almost two-dimensional  $\sigma$  bands with a corresponding Fermi energy  $E_F^\sigma = 0.4 - 0.6$  eV,<sup>2</sup> defined as the distance in energy between the chemical potential and the edge of the  $\sigma$  band. Furthermore, the electron-phonon interaction is essentially dominated by the doubly degenerate  $E_{2g}$  phonon mode at  $\mathbf{q}=0$ ,<sup>11</sup> which gives rise to a significant  $\sigma$ - $\sigma$  band electron-phonon coupling, while the residual  $\sigma$ - $\pi$  and  $\pi$ - $\pi$  electron-phonon interaction is much weaker.<sup>12,13</sup> The effective Hamiltonian of the  $\sigma$  bands interacting with the  $E_{2g}$  phonon mode at  $\mathbf{q}=0$  can thus be written as<sup>9</sup>

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \pm I_{E_{2g}} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} u - \frac{\hbar^2 \nabla_u^2}{2M_{E_{2g}}} + V(u), \quad (2)$$

where  $u$  is the lattice displacement of the  $E_{2g}$  phonon mode and the sign  $\pm$  in the Jahn-Teller electron-phonon interaction is different for the two  $\sigma$  bands. Assuming for the moment a perfectly harmonic phonon mode with elastic constant  $a_2$ ,  $V(u) = a_2 u^2$ , we can write Eq. (2) in second quantization [ $u = (\hbar^2/4M_{E_{2g}}a_2)^{1/4}(a+a^\dagger)$ ]:

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \pm g_{E_{2g}} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} (a + a^\dagger) + \omega_{E_{2g}} a^\dagger a, \quad (3)$$

where the electron-phonon matrix element  $g_{E_{2g}} = I_{E_{2g}}(\hbar^2/4Ma_2)^{1/4}$  determines the change in the electron energy bands associated with the ground state zero point motion.

Frozen phonon calculations have been previously employed in Ref. 9 to point out the connection between small Fermi energy and anharmonic effects of the  $E_{2g}$  phonon mode in  $\text{MgB}_2$ . The appearance of anharmonic terms in the *static* phonon potential has indeed been related to a strong lattice displacement regime, namely,  $D_{E_{2g}}^\sigma = I_{E_{2g}} u \gtrsim E_F^\sigma$ . On physical grounds, we can expect that anharmonic terms will be experimentally observable only if the lattice fluctuations allowed in the system are sufficiently strong to sample regions of phase space in which the effective Fermi energy is small ( $I_{E_{2g}} u \sim E_F^\sigma$ ). We are going to show that a similar con-

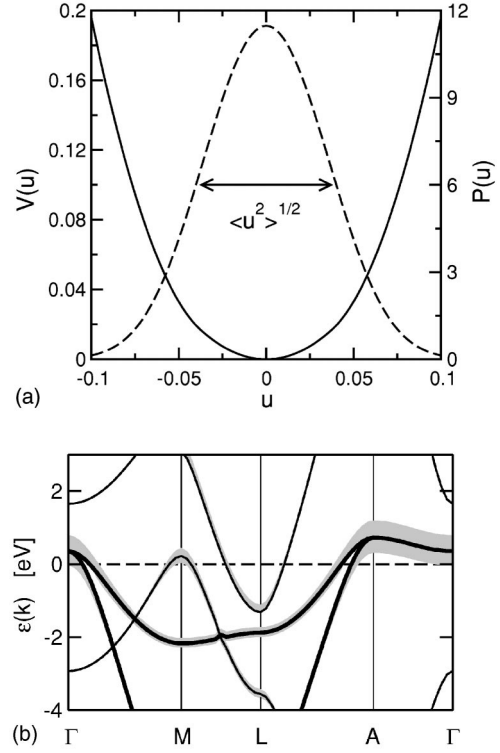


FIG. 1. (a) Frozen phonon potential  $V(u)$  for the  $E_{2g}$  mode in  $\text{MgB}_2$  (solid line, left side scale) and probability distribution function  $P(u) = |\psi_{E_{2g}}(u)|^2$  (dashed line, right side scale).  $u$  is in units of  $\text{\AA}$ ,  $V(u)$  in units of eV, and  $P(u)$  in units of  $\text{\AA}^{-1}$ . (b) Electronic structure of undistorted  $\text{MgB}_2$  (solid lines). The grey regions represent the quantum fluctuations induced by zero point lattice motion ( $|u| \leq \langle u^2 \rangle^{1/2}$ ). Bold lines represent the two  $\sigma$  bands, which are also the most affected by quantum fluctuations.

dition rules the breakdown of the adiabatic BO principle.<sup>14</sup>

In Fig. 1(a) we plot the  $E_{2g}$  frozen phonon potential  $V(u)$  obtained by local density approximation (LDA) calculations (see Ref. 9 for details). In the spirit of the BO principle we can evaluate the ground-state phonon wave function  $\chi_{E_{2g}}(u)$  by the numerical solution of the Schrödinger equation  $[-(\hbar^2/2M_{E_{2g}})\nabla_u^2 + V(u)]\chi_{E_{2g}}(u) = E_{E_{2g}}\chi_{E_{2g}}$ . We can also define a lattice probability distribution functions (PDF)  $P(u)$  through the relations  $P(u) = |\chi_{E_{2g}}(u)|^2$ , which is plotted in Fig. 1(a). In the classical (strictly adiabatic)  $M_{E_{2g}} \rightarrow \infty$  limit, and  $P(u)$  becomes a  $\delta$  function centered at  $u=0$ . The electronic structure of the undistorted lattice, which corresponds thus to the adiabatic limit, is shown in panel (b) as solid lines.

As mentioned above, there are two different sources of quantum fluctuations of the lattice configuration with respect to the classical, static limit. The first one is given by the possibility of quantum transitions between different electron and lattice eigenfunctions. This gives rise, when expanded around the lattice equilibrium position  $u=0$ , to the conventional electron-phonon scattering which leads to the *dynamical* electron-phonon renormalization of the electronic and lattice properties, usually taken into account by the corresponding self-energies. A different effect of the quantum lat-

tice fluctuations is the fact that the ground state PDF acquires a nonzero amplitude at  $u \neq 0$ , corresponding to the zero-point motion. In this framework an appropriate quantity to estimate the amplitude of the lattice quantum fluctuations is the root mean square (r.m.s.) lattice displacement

$$\langle u^2 \rangle^{1/2} = \left[ \int du u^2 P(u) \right]^{1/2}. \quad (4)$$

In the following we focus on the interesting implications of this second effect on the electronic structure. We shall show that the zero-point lattice fluctuations are unavoidably reflected, through the deformation potential, in an intrinsic source of quantum fluctuations for the electronic structure and for the Fermi energy.

A rough estimate of these effects is provided by their r.m.s. values. Applying the definition (4), we obtain for the zero-point motion of the  $E_{2g}$  phonon mode a vibrational amplitude  $\langle u^2 \rangle^{1/2} \approx 0.034 \text{ \AA}$ . The changes in the electronic structure corresponding to this lattice fluctuations are represented in Fig. 1(b) by the grey regions. The main changes of the electronic structure close to the  $\Gamma$  point  $D_{E_{2g}}^\sigma = I_{E_{2g}} \langle u^2 \rangle^{1/2}$  can be obtained from the deformation potential and roughly correspond to the thickness of the grey region at the  $\Gamma$  point. As shown in the figure, the strong quantum *lattice* fluctuations are reflected in strong *electronic* changes with a r.m.s. value of the  $\sigma$  band Fermi energy fluctuations  $\langle [E_F^\sigma(u) - E_F^\sigma(0)]^2 \rangle^{1/2} = I_{E_{2g}} \langle u^2 \rangle^{1/2} \approx 0.39 \text{ eV}$ , which is slightly smaller than the electron-phonon matrix element  $g_{E_{2g}} = 0.45 \text{ eV}$  because it includes anharmonic effects. This value is comparable to the Fermi energy of the undistorted (adiabatic) case  $E_F^\sigma = 0.45 \text{ eV}$ , resulting in a range of Fermi energy fluctuation  $0.06 \text{ eV} < E_F^\sigma < 0.84 \text{ eV}$ , and casts doubts on the usual definition of the Fermi energy, based on the BO approximation.

The relevance of this regime may be measured by the dimensionless parameter

$$\kappa = \frac{\langle [E_F^\sigma(u) - E_F^\sigma(0)]^2 \rangle^{1/2}}{E_F^\sigma} \approx \frac{I_{E_{2g}} \langle u^2 \rangle^{1/2}}{E_F^\sigma} \approx 0.91. \quad (5)$$

In common metals, although the numerator can be of the order of a fraction of eV, the denominator is usually of 5–10 eV, so that  $\kappa \ll 1$  and the role of the quantum lattice fluctuations on the electronic structure is negligible. Things are radically different for the  $E_{2g}$  phonon of  $\text{MgB}_2$ , where the large value of  $\kappa (\approx 1)$  is driven by the extremely small Fermi energy of the  $\sigma$  bands.

The sizable magnitude of the parameter  $\kappa$  calls for some physical considerations. Due to these strong quantum fluctuations, the system indeed samples, with a sizable weight, electronic configurations with zero or vanishing Fermi energy. The system thus has an intrinsic nonadiabatic character<sup>7</sup> even if the phonon frequencies  $\omega_{\text{ph}}$  are sensibly smaller than  $E_F(u=0)$ . An alternative way to understand the breakdown of the BO principle is to observe that for  $u \approx E_F^\sigma / I_{E_{2g}}$ , the electronic Fermi energy  $E_F^\sigma(u)$ , which governs the dynamics of the  $\sigma$  bands, is comparable with  $\omega_{\text{ph}}$ , which governs the lat-

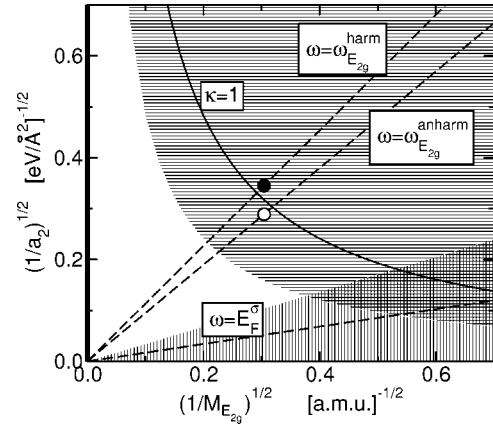


FIG. 2. Schematic phase diagram for the different kinds of nonadiabatic effects. See text for details.

tice dynamics. The variable  $u$  cannot thus be treated as a classical degree of freedom in a parametric way and  $\Psi(\mathbf{r}; \mathbf{u}) \neq \chi(\mathbf{u})\varphi(\mathbf{r}; [u])$ .

We would like to stress once more that the origin of the nonadiabatic breakdown of the BO principle stems from the strong lattice quantum fluctuations which make the electron-phonon matrix element, the *second* term in Eqs. (2) and (3), comparable with the Fermi energy. This is thus qualitatively *different* from what discussed in Refs. 7 and 8, where the nonadiabatic effects are ruled by the ratio between the energy scale of the *third* term in Eq. (3) and the Fermi energy, namely,  $\omega_{E_{2g}} / E_F^\sigma$ . Note also that the phonon frequency  $\omega_{E_{2g}}$  does *not* depend on the amplitude of the lattice fluctuations, on the contrary of the parameter  $I_{E_{2g}} \langle u^2 \rangle^{1/2} / E_F^\sigma$ . This means that the onset of one kind of nonadiabatic effects does not necessarily implies the onset of the other one, and *vice versa*.

In order to further clarify this statement let us assume for the moment a perfectly harmonic phonon mode with elastic constant  $a_2 V(u) = a_2 u^2$ . Anharmonic contributions do not play any important role in the following discussion, so we will take them into account through an “effective” elastic constant as in Ref. 15 to give the anharmonic hardening of the phonon.

The two different sources of breakdown of the BO principle are illustrated in Fig. 2 where we plot on the  $x$  axis the inverse of the square root of the phonon mass  $1/\sqrt{M_{E_{2g}}}$  and on the  $y$  axis the inverse of the square root of the elastic constant  $1/\sqrt{a_2}$ . The limit  $M_{E_{2g}} \rightarrow \infty$ , denoted by the thick line, is the strictly classical (adiabatic) case where both kinds of nonadiabatic effects are negligible. In the so-defined phase space a fixed phonon frequency is given by a straight line cutting through the origin. In Fig. 2 we show the three frequencies  $\omega_{E_{2g}} = 68 \text{ meV}$ ,  $81 \text{ meV}$ , and  $0.45 \text{ eV}$  as dashed lines, corresponding to the harmonic and anharmonic frequencies of the  $E_{2g}$  phonon, and to a hypothetical phonon in the fully nonadiabatic regime ( $\omega_{\text{ph}} = E_F^\sigma$ ), respectively. The empty (filled) circles represent, respectively, the actual position of the  $E_{2g}$  phonon of  $\text{MgB}_2$  ( $M = 10.81 \text{ a.m.u.}$ ) with (without) taking into account the anharmonic hardening. The nonadiabatic breakdown of the BO principle underlined in Ref. 7 arises in the region  $\omega_{\text{ph}} \approx E_F^\sigma$ , and is represented by the

vertically dashed area, corresponding to  $\omega_{\text{ph}}/E_F^\sigma \geq 0.5$ .

The breakdown of the BO principle due to the zero point motion, determined by the parameter  $\kappa$ , of the lattice fluctuation is also shown in Fig. 2.  $\kappa$  isolines are easily defined by the relations  $a_2 \langle u^2 \rangle^{1/2} = \hbar \omega_{\text{ph}}/2$  and  $\kappa = I_{E_{2g}} \langle u^2 \rangle^{1/2}/E_F$  using LDA values  $I_{E_{2g}} = 12 \text{ eV/\AA}$  and  $E_F^\sigma = 0.45 \text{ eV}$ . The horizontally dashed region ( $\kappa \geq 0.5$ ) represents the range of parameters where nonadiabatic effects could be triggered by the zero-point fluctuations. It is interesting to note that in this new regime nonadiabatic effects induced by lattice fluctuations can be operative even quite far from the usual “nonadiabatic” regime  $\omega_{\text{ph}} \sim E_F$ . Of course, the two sources of nonadiabaticity merge together in the highly nonadiabatic case  $M \rightarrow 0$ , where  $E_F$  is smaller than  $\omega_{\text{ph}}$  already in the absence of fluctuations. This could be the case for the cuprates and fullerene compounds since in their case  $E_F$  is smaller than in  $\text{MgB}_2$ , while the relevant phonon frequencies are comparable.

In conclusion, in this work we have pointed out the inadequacy in  $\text{MgB}_2$  of the BO approximation which is at the basis of many *ab initio* techniques, when applied to coupling between the  $E_{2g}$  phonon and the  $\sigma$  holes, which are mainly responsible for superconductivity. We have related such inadequacy to the strong lattice fluctuations of zero-point motion which, due to the large deformation potential associated with the  $E_{2g}$  phonon, induce electronic changes of the  $\sigma$  bands of the same order of magnitude of their Fermi energy ( $E_F^\sigma \approx 0.45 \text{ eV}$ ). The breakdown of the BO approximation has important consequences since it implies the failure of

many *ab initio* techniques. An appropriate inclusion of these effects is a formidable task which goes beyond the aim of this paper. We note, however, that the structural and cohesive properties of  $\text{MgB}_2$  are expected to be weakly affected by the zero-point fluctuations, both because they depend on the whole set of occupied bands (whose width is 10–20 eV), and because they involve all phonons. Its transport and superconducting properties, instead, are mainly determined from the small fraction of carriers within an energy range  $\sim \omega_{\text{ph}}$  close to the Fermi level, and which are strongly coupled to the relevant  $E_{2g}$  phonon.

As a last remark, it is interesting to remind the reader that the nonadiabatic effects induced by lattice fluctuations are increased as the force constant decreases. Electron-phonon systems with incipient lattice instabilities (corresponding to flattening of the lattice potential) could thus be good candidates for the observation of similar nonadiabatic effects in other materials than  $\text{MgB}_2$ . Good candidates in this direction are bismuthates, A15 compounds and possibly monoatomic metals such as Nb or V. In particular, the important role of the lattice fluctuations in A15 compounds, which was already pointed out by Anderson in Ref. 16, could provide the basis to investigate some interesting similarities between A15 and diborides systems.

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