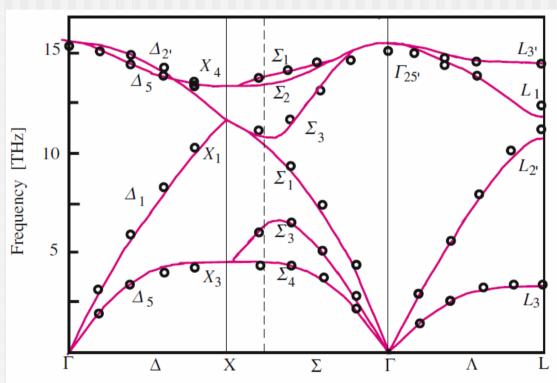
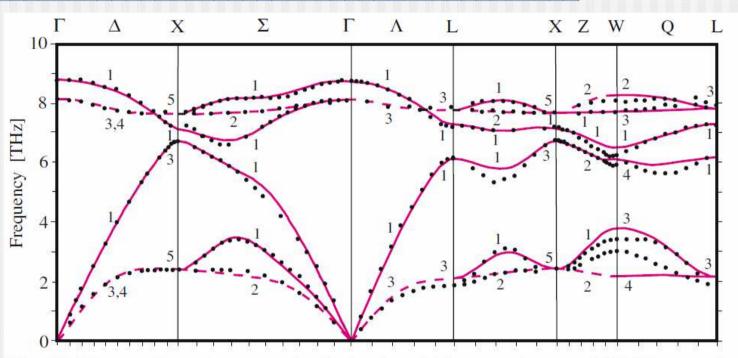


# Relaciones de dispersión de fonones: (Caso Si).



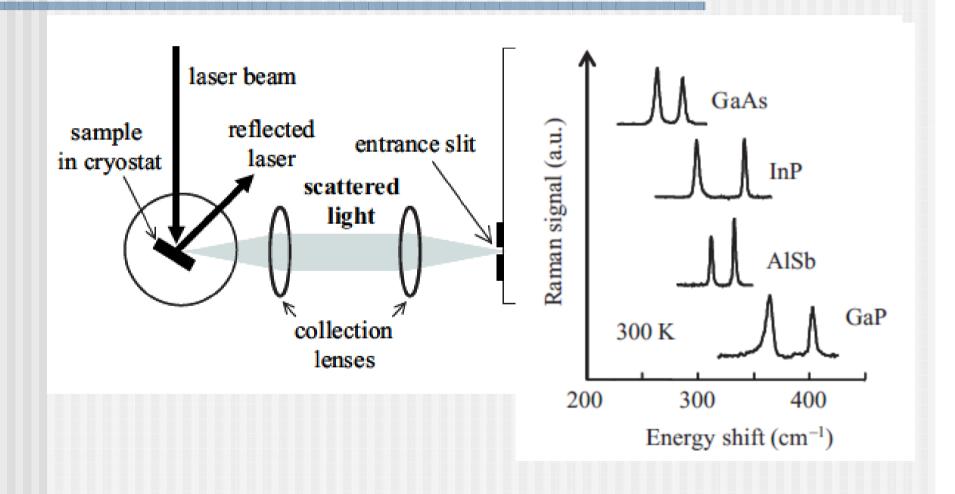
**Fig. 3.1.** Phonon dispersion curves in Si along high-symmetry axes. The *circles* are data points from [3.4]. The continuous curves are calculated with the adiabatic bond charge model of *Weber* [3.5]

# Relaciones de dispersión de fonones: (Caso GaAs).



**Fig. 3.2.** Phonon dispersion curves in GaAs along high-symmetry axes [3.6]. The experimental data points were measured at 12 K. The *continuous lines* were calculated with an 11-parameter rigid-ion model. The numbers next to the phonon branches label the corresponding irreducible representations

#### Raman



#### Función de Bloch

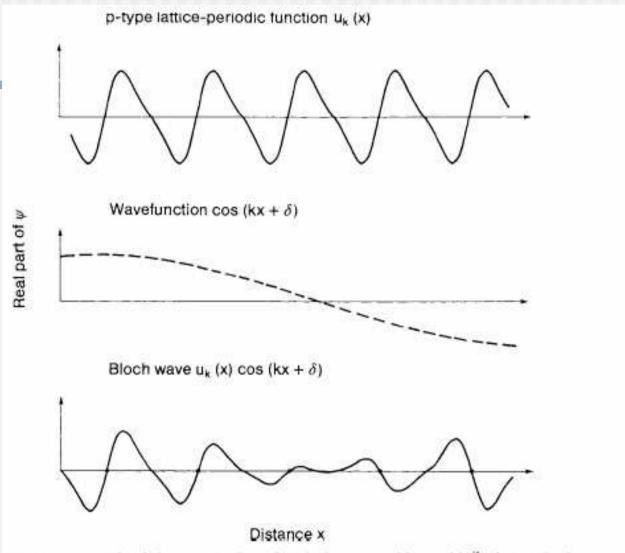


Fig. 7.1. Example of the construction of a Bloch wave  $\psi_k(r) = u_k(r)e^{ikr}$  from a lattice-periodic function  $u_k(r)$  with p-type bonding character and a plane wave

# Acoplamiento en Ecuación Central de Teoría de Bandas

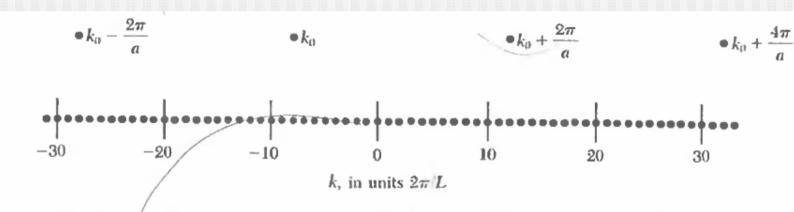


Figure 7 The lower points represent values of the wavevector  $k = 2\pi n/L$  allowed by the periodic boundary condition on the wavefunction over a ring of circumference L composed of 20 primitive cells. The allowed values continue to  $\pm \infty$ . The upper points represent the first few wavevectors which may enter into the Fourier expansion of a wavefunction  $\psi(x)$ , starting from a particular wavevector  $k = k_0 = -8(2\pi/L)$ . The shortest reciprocal lattice vector is  $2\pi/a = 20(2\pi/L)$ .

#### Mezcla Estados en 1D

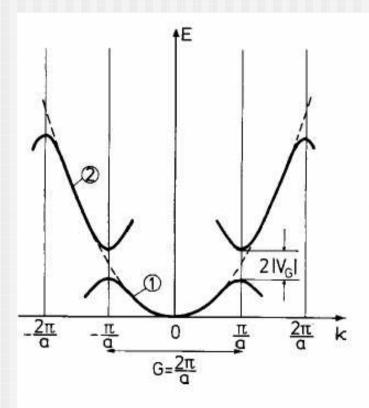


Fig. 7.5. Splitting of the energy parabola of the free electron (---) at the edges of the first Brillouin zone  $\mathbf{k} = \pm \pi/a$  in the one-dimensional case). To a first approximation the gap is given by twice the corresponding Fourier coefficient  $V_G$  of the potential. Periodic continuation over the whole of  $\mathbf{k}$ -space gives rise to continuous bands  $\mathbb O$  and  $\mathbb O$ , shown here only in the vicinity of the original energy parabola

#### Red Vacía 1D

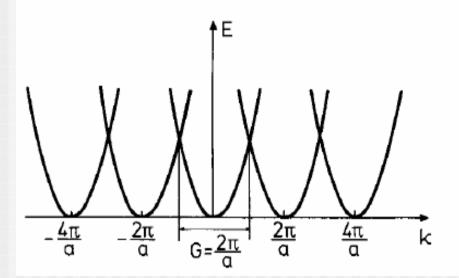


Fig. 7.2. The parabolic energy curves of a free electron in one dimension, periodically continued in reciprocal space. The periodicity in real space is a. This E(k) dependence corresponds to a periodic lattice with a vanishing potential ("empty" lattice)

### Periodicidad de la Estructura Electrónica en Red Recíproca

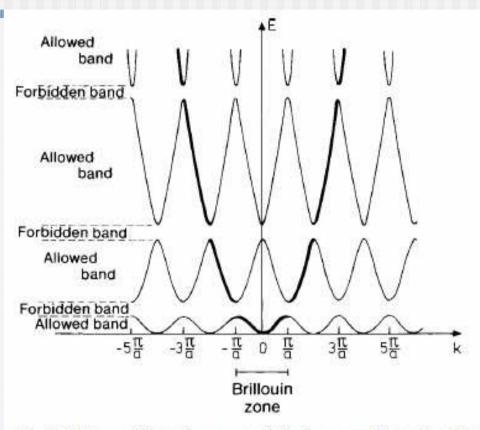
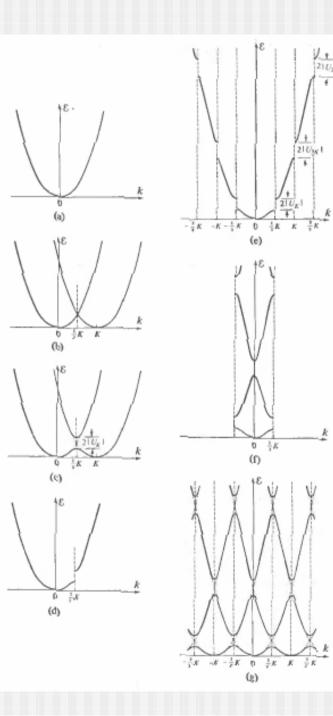


Fig. 7.6. Energy dispersion curves E(k) for a one-dimensional lattice (lattice constant a) in the extended zone scheme. As can be seen, the quasi-free-electron approximation gives rise to forbidden and allowed energy regions due to the opening of band gaps, as shown in Fig. 7.5 (cf. the vanishing potential case of Fig. 7.2). The parts of the bands corresponding to the free-electron parabola are indicated by the thick lines



(b) Step 1 in the construction to determine the distortion Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to deter-"plane." The degeneracy of the two parabolas at K/2is split. (d) Those portions of part (c) corresponding to the original free electron parabola given in (a). (e) Effect of all additional Bragg "planes" on the free electron parabola. This particular way of displaying the electronic levels in a periodic potential is known as the extended-zone scheme. (f) The levels of (e), displayed in a reduced-zone scheme, (g) Free electron levels of (e) or (f) in a repeated-zone scheme.

# (a) The free electron 8 vs. k parabola in one dimension. in the free electron parabola in the neighborhood of a Bragg "plane," due to a weak mine the distortion in the free electron parabola in the neighborhood of a Bragg Permitida Prohibida

# Red Vacía Estructura Cúbica Simple

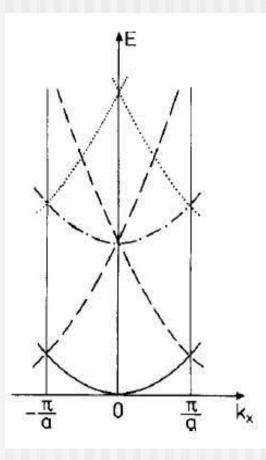


Fig. 7.3. Bandstructure for a free electron gas in a primitive cubic lattice (lattice constant a), represented on a section along  $k_x$  in the first Brillouin zone. The periodic potential is assumed to be vanishing ("empty" lattice). The various branches stem from parabolas whose origin in reciprocal space is given by the Miller indices hkl. (—) 000; (——) 100,  $\bar{1}00$ ; (——) 010,  $0\bar{1}0$ , 001,  $00\bar{1}$ ; (——) 110,  $10\bar{1}$ ,  $10\bar{1}$ , 10

# Red Vacía Diamante (fcc) vs. Estructura Electrónica Si

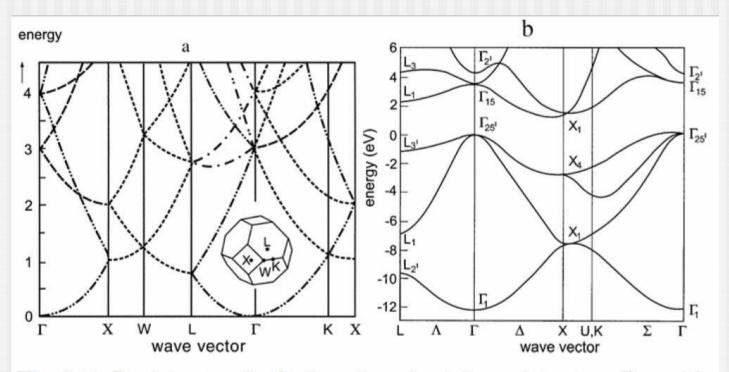


Fig. 8.12. Band structure for the three dimensional diamond structure. For vanishing potential (a) and a realistic band structure calculation for Si (b). The numbers at  $\Gamma$  give the irreducible representations (see Sect. 26.4 to 6), still neglecting spin: According to [76A1,81M1,96Y1] of Chap. 1

### Potencial Periódico Unidimensional

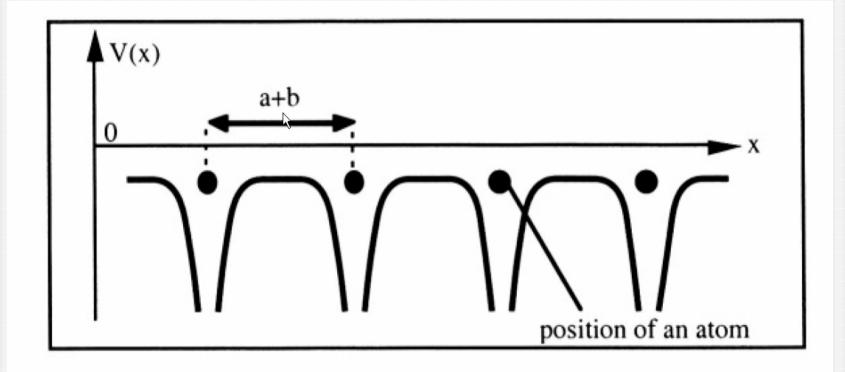


Figure 1.6: Periodic potential in a one-dimensional crystal.

### Potencial Krönig Penney

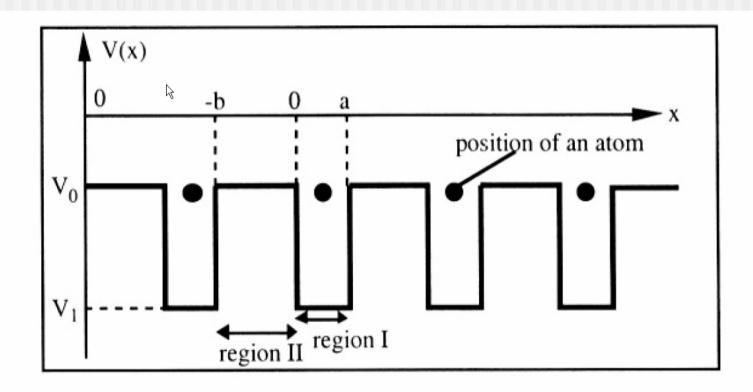
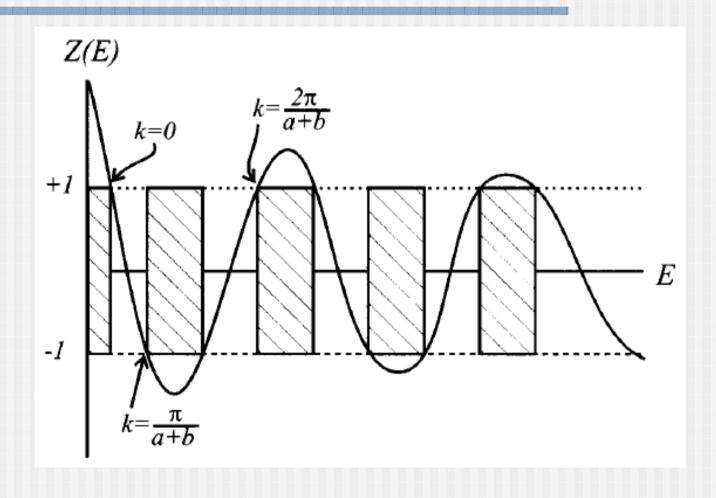


Figure 1.7: Periodic potential of the Krönig and Penney model.

## Regiones de Energía Permitida y Regiones de Energía Prohibida



## Regiones de Energía Permitida y Regiones de Energía Prohibida

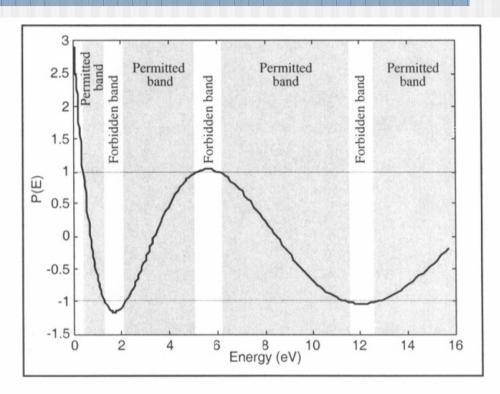


Figure 1.8: P(E) as a function of the electron energy, E, for silicon. The shaded areas correspond to the permitted energy bands, where there is a solution to Equation 1.1.29.

#### Relaciones de Dispersión

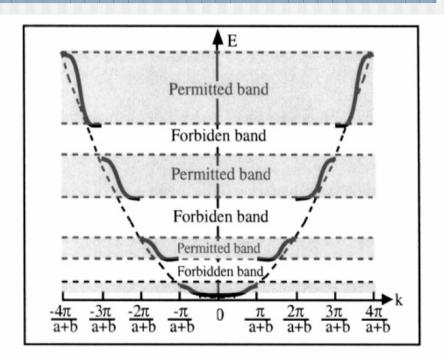


Figure 1.9: Energy versus k in a one-dimension crystal. The dotted line parabola represents the E(k) relationship for a free electron (from Figure 1.1).

### Zona Extendida vs. Zona Reducida

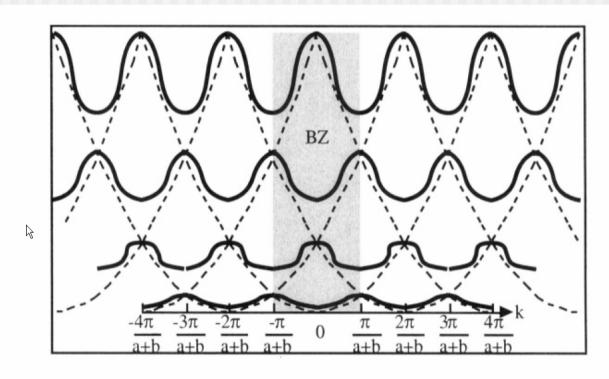
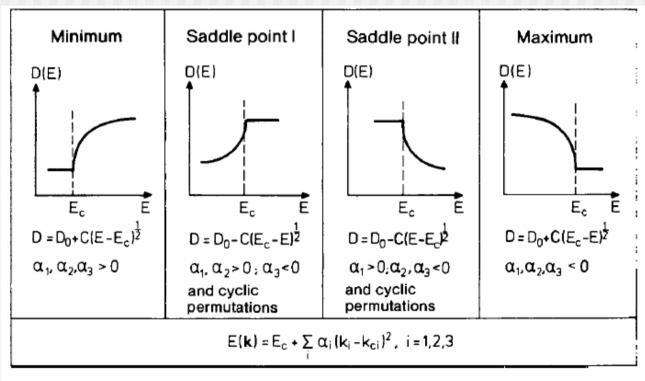


Figure 1.10: E(k) diagram of Figure 1.9, repeated with a  $2\pi/(a+b)$  period. The shaded area highlights the first Brillouin zone (BZ).[5]

#### Densidad de Estados



**Fig. 7.14.** Form of the density of states D(E) in the vicinity of the four possible types of critical point in three dimensions. The energy of the critical points is denoted by  $E_c$  and the corresponding k-space position by  $k_{ci}$  (i = 1, 2, 3). In the parabolic approximation, the energy band has the form  $E(k) = E_c + \sum_i \alpha_i \cdot (k_i - k_{ci})^2$  in the vicinity of a critical point, where  $\alpha_i = \text{const.}$  The quantities  $D_0$  and C in the figure are also constants

### Estructura Electrónica y Densidad de Estados del Cu

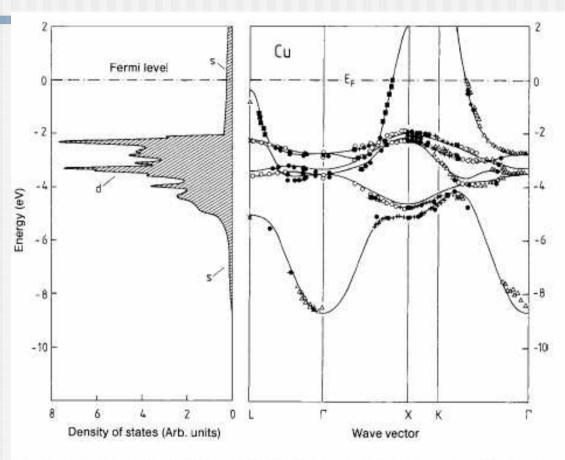


Fig. 7.12. Bandstructure E(k) for copper along directions of high crystal symmetry (right). The experimental data were measured by various authors and were presented collectively by Courths and Hüfner [7.4]. The full lines showing the calculated energy bands and the density of states (left) are from [7.5]. The experimental data agree very well, not only among themselves, but also with the calculation

### Estructura Electrónica y Densidad de Estados del Ge

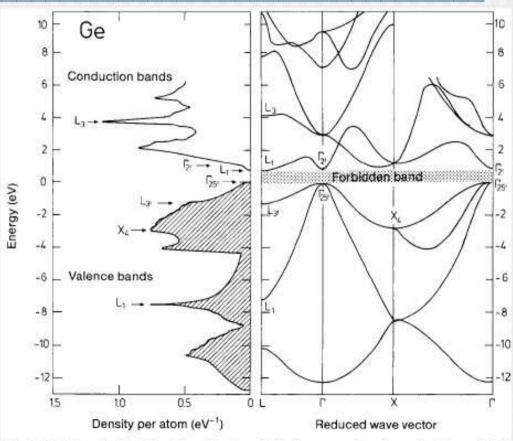


Fig. 7.13. Theoretically derived bandstructure E(k) for germanium along directions of high symmetry (right), and the corresponding electronic density of states (left). A number of critical points, denoted according to their position in the Brillouin zone  $(\Gamma, X, L)$ , can be seen to be associated with regions of the bandstructure where E(k) has a horizontal tangent. The shaded region of the density of states corresponds to the states occupied by electrons [7.6]

#### Paquete de Onda Electrónico

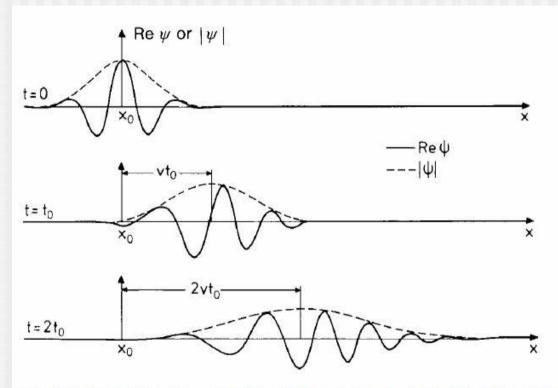


Fig. 9.1. Real space representation of the wave packet describing the motion of a spatially localized free electron at times  $t = 0, t_0, 2t_0...$  (Re  $\{\psi\}$ : —;  $|\psi|$ : ——). The center of the wave packet, i.e., in the particle picture the electron itself, moves with the group velocity  $v = \partial \omega / \partial k$ . The halfwidth of the envelope increases with time. As the wave packet spreads, the wavelength of the oscillations of Re  $\{\psi\}$  becomes smaller at the front and larger at the rear

#### Masa Efectiva

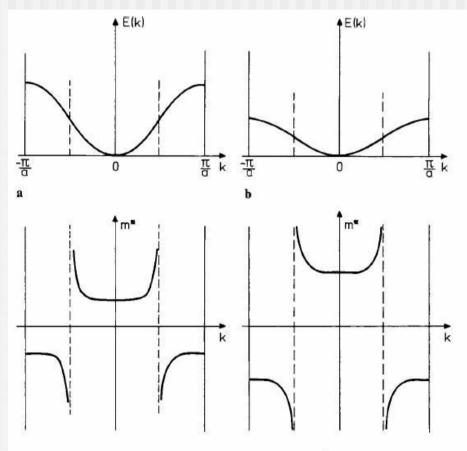


Fig. 9.2a,b. Schematic behavior of the effective mass  $m^*(k)$  for a one-dimensional bandstructure E(k): (a) for strong curvature of the bands, i.e., small effective masses; (b) for weak curvature, i.e., large effective masses. The dashed lines denote the points of inflection of E(k)

# Polarón: Interacción Electrón-Fonón Longitudinal Óptico

