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SURFACE STATES IN SEMICONDUCTORS WITH COMPLICATED BAND STRUCTURE

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In semiconductors with complicated band structure, such as GaAs, there are sections of the spectrum in which the electrons have negative effective masses. This means that the repulsion potential can lead to the formation of bound states for the electrons.

We are interested in the interface between two media with different dielectric constants, particularly the semiconductor-vacuum interface. In this case, as is well known [1], the electron in the semiconductor is acted upon by an electrostatic image force that repels it from the surface. The potential energy of the electron is of the form α/z, where $\alpha = (e^2/4\kappa)(\kappa - 1)/(\kappa + 1)$, κ is the dielectric constant of the semiconductor, and z is the distance to the surface.

We assume that the usual conditions for the applicability of the equivalent-Hamiltonian approximation are satisfied (cf., e.g., [2]). The equation for the envelope $\Psi(\vec{r})$ in the expansion of the wave function of the electron in Wannier functions takes the form ($\hbar = 1$)

$$\left[\epsilon(-i\nabla) + \frac{a}{z}\right]\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r}), \tag{1}$$

where $\varepsilon(\vec{p})$ is the law of the electron dispersion in the band. Since the potential energy depends only on z, the problem reduces to a one-dimensional one, i.e.,

$$\Psi(\mathbf{r}) = \phi(z)\exp\{ip_x x + ip_y y\},$$

where $\phi(z)$ satisfies the equation

$$\left[\epsilon\left(-i\frac{\partial}{\partial z}, p_x, p_y\right) + \frac{a}{z}\right]\phi(z) = E\,\phi(z). \tag{2}$$

Since $\phi(z)$ is an envelope function and its characteristic dimension should be much larger than the lattice period within the framework of the equivalent-Hamiltonian approximation the boundary condition for $\phi(z)$ is that it vanish at $z = 0$. It turns out that this problem has an exact solution at an arbitrary form of the dispersion $\varepsilon(\vec{p})$. We shall seek a solution in the form (for the k-th discrete level)

$$\phi(z) = e^{-\gamma_k z}(A_k z^k + A_{k-1} z^{k-1} + \ldots + A_1 z). \tag{3}$$

Expanding $\varepsilon(-i\frac{\partial}{\partial z}(p_x, p_y))$ in powers of the operator $i(\partial/\partial z)$, substituting (3), and equating coefficients of equal powers of z, we obtain an expression for the discrete levels (surface bands) $E_k(p_x, p_y)$

$$E_k = \epsilon(i\gamma_k, p_x, p_y),$$

where γ_k is the root of the equation

$$(\partial/\partial\gamma_k)\,\epsilon(i\gamma_k, p_x, p_y) = \alpha/k, \quad k = 1, 2 \ldots \qquad (4)$$

States localized on the surface correspond to those roots of Eq. (4) which satisfy the condition Re $\gamma_k > 0$. To find the energy E_k it suffices to compare the coefficients of z^k and z^{k-1} in (3). To determine the electron wave functions, it is necessary to compare the coefficients of the succeeding powers of z. We present by way of an example the expressions or the wave functions of the first and second discrete levels.

$$\Psi_1 = C_1 z e^{-\gamma_1 z}; \qquad \Psi_2 = C_2 (z - \frac{\alpha}{\epsilon''_{\gamma\gamma}(i\gamma_2)} z^2) e^{-\gamma_2 z},$$

where C_1 and C_2 are normalization constants.

By way of an example, let us consider a body-centered cubic lattice, in which $\varepsilon(p_z, p_x, p_y)$ has in the strong-coupling approximation the form

$$\epsilon(p_z, p_x, p_y) = \epsilon_0 + \Delta \cos\frac{1}{2} p_z a \cos\frac{1}{2} p_x a \cos\frac{1}{2} p_y a.$$

The expression obtained for the surface bands is

$$E_k = \epsilon_0 + \Delta\sqrt{\cos^2\frac{1}{2} p_x a \cos^2\frac{1}{2} p_y a + \left(\frac{2\alpha}{\Delta a k}\right)^2},$$

i.e., we obtain an infinite system of levels lying above the band and becoming denser towards its ceiling.

In the general case it can be stated that the roots of (4) are close to the extrema of $\varepsilon(p_z, p_x, p_y)$ as functions of p_z, since α in atomic units is approximately equal to $1/4\kappa \ll 1$. We can then expand $\varepsilon(p_z, p_x, p_y)$ near the extremum and obtain for the level E_k the unual hydrogenlike spectrum

$$E_k(p_x, p_y) = \frac{\alpha^2}{2k^2} m^*(p_x, p_y).$$

We note that the effective mass depends, generally speaking, on the position of the point in the two-dimensional Brillouin zone. Equation (4) can have in the general case also complex solutions, which correspond to quasistationary states.

The surface states described above, both stationary and quasistationary, can become manifest in non-equilibrium processes such as optical absorption. In addition, in strong electric fields the electrons can be captured by such levels, and this influences the surface mobility.

We note in conclusion that it is possible to consider in the same manner a model with two close allowed bands, for which the dispersion is of the form

$\varepsilon^2 = \Delta^2 + s^2p^2$, and the envelope function satisfies the Klein-Gordon equation. The surface levels are given by the formula

$$E_k = -(\Delta^2 + s^2p_\perp^2)^{1/2}\left[1 + \frac{\Delta a^2}{s^2k^2\sqrt{\Delta^2 + s^2p_\perp^2}}\right]^{-1/2},$$

where $p_\perp$ is the projection of the momentum on the surface of the crystal.

Thus, the system of levels lies near the ceiling of the lower band. The latter result can apparently not be applied directly to semiconductors with a narrow forbidden band. Indeed, in this case the lower band is the filled valence band of the semiconductor, and the problem assumes essentially a many-particle character. Its analysis lies beyond the scope of the present communication.

The following remark should be made concerning the calculations. They are valid if the frequency ω_e of electron motion on the surface levels is much smaller than the reciprocal relaxation time of the medium, a relaxation responsible for the establishment of κ. In this case the medium responds to the instantaneous position of the electron, and not to the averaged distribution of the charge with density $|\Psi|^2$. This is precisely why it is possible to use the usual expression for the potential of the electrostatic image. The parameter $(4\kappa)^2$ which enters in the theory is sufficiently large for both ionic (GaAs, InSb) and nonpolar (Ge, Si) semiconductors, so that ω_e turns out to be smaller than the frequency of the optical phonon, and certainly smaller than the frequencies of the bound electrons of the semiconductor.

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PLASMA HEATING BY ULTRASHORT LASER PULSES IN THE PROCESS OF ELECTRONIC HEAT CONDUCTION

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Plasma heating by focusing powerful ultrashort (10^{-11} - 10^{-12} sec) laser pulses on a solid target [1] may be accompanied by propagation of an electronic thermal wave in the interior of the target [2]. Let us consider the heating of ions in such a plasma at a laser-radiation absorbed-energy density $\varepsilon > \varepsilon_k \approx 6 \times 10^3$ J/cm^2, when heat conduction makes possible an appreciable increase of the number of heated particles. The duration τ of the ultrashort pulse turns out in this case to be shorter than the characteristic plasma times, such as the time τ_{ei} of equalization of the electron and ion temperatures, the time τ_{ac} of propagation of a rarefaction wave through the heated layer, and the time τ_m of propagation of the heat-conduction wave (calculations show that the plasma radiation has little effect on the ion heating). For example, for LiD at $\varepsilon = 10^5$ J/cm^2 we have $\tau_{ei} \sim \tau_{ac} \sim \tau_m \sim 0.5 \times 10^{-10}$ sec. Under the indicated condition, the time of spreading of the layer (the time of expansion to twice