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Theory of interband tunnelling in crystals with phonons

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Abstract. A general theory is presented for the interband tunnelling probability of electrons in a crystal in the presence of phonons and a strong electric field, for both the phonon-assisted and the phonon-modified-Zener tunnelling. For the case of tunnelling from a fully occupied band the dependence of the tunnelling rate on the electric field is shown in both cases to exhibit a steady term and some oscillatory terms. Similar oscillatory behaviour has been measured recently in semiconducting superlattices.

With the advent of submicron devices and semiconducting superlattices there is currently a great deal of interest in the study of all quantum mechanical aspects of the motion of electrons in crystals in a strong electric field [1–13]. We examine here the basic theory of interband tunnelling in a crystal in the presence of phonon scattering and a uniform and time-independent strong electric field. We base this theory on the equation of motion of the one-electron density operator for this system that has recently been derived [14] and the familiar Bloch representation for the crystal. We find that the interband tunnelling rate depends on the electric field through a steady term and some oscillatory terms. Such oscillatory behaviour has recently been observed [15] in semiconducting superlattices.

The interaction energy of an electron with an arbitrarily strong, uniform and time-independent electric field $\boldsymbol{E}$ is given in the scalar gauge by

$$H_f = -e\boldsymbol{E}\cdot\boldsymbol{r} = -\boldsymbol{F}\cdot\boldsymbol{r}. \tag{1}$$

The crystal Hamiltonian H_c determines the Bloch states $|nk\rangle$ of band n and wavevector k with energies $\epsilon_n^0(k)$. The effects of the electric field on the motion of the electron can be separated into intraband and interband processes as described by the matrix elements of (1) in the Bloch representation. Thus we have [6, 16]

$$\langle nk|r|n'k'\rangle = \mathrm{i}\delta_{nn'}\partial\delta_{kk'}/\partial k + R_{nn'}(k)\delta_{k,k'} \tag{2}$$

where

$$\boldsymbol{R}_{nn'}(k) = \frac{\mathrm{i}}{\Omega_0}\int_{\Omega_0} \mathrm{d}^3r\, U^*_{nk}(r)\frac{\partial U_{n'k}(r)}{\partial k} \tag{3}$$

with $U_{nk}(r)$ being the periodic part of the Bloch wavefunction $\langle r|nk\rangle$ normalized in the unit cell of volume Ω_0. In (2) and in the following $\partial/\partial k$ is a formal derivative, as discussed in detail elsewhere [17]. Now we combine the intraband elements of H_f

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with those of H_c to form the Hamiltonian H_0 to be treated exactly, and we treat the interband elements of H_t as a perturbation H' [18], i.e. we write

$$H = H_c + H_t = H_0 + H' \tag{4}$$

where

$$\langle nk|H_0|n'k'\rangle = \delta_{nn'}[\epsilon_n(k)\delta_{k,k'} - \mathrm{i}F\cdot(\partial\delta_{kk'}/\partial k)] \tag{5}$$

$$\langle nk|H'|n'k'\rangle = H'_{nn'}(k)\delta_{k,k'} = -F\cdot R_{nn'}(k)(1-\delta_{nn'})\delta_{k,k'} \tag{6}$$

with $\epsilon_n(k) = \epsilon_n^0(k) - F\cdot R_{nn}(k)$. Thus, the intraband effects of E appear as 'acceleration' whereby the crystal momentum is increased at a constant rate F. The effects of the phonons are given by the electron–phonon interaction for each electron

$$V = \sum_q v_q(b_q + b_{-q}^\dagger). \tag{7}$$

Here $q = (q,\lambda)$ denotes the phonon states of wavevector q, of branch and polarization index λ, with $-q$ standing for $(-q,\lambda)$ and of energies $\omega_q = \omega_{-q}$. The operators $b_q(b_q^\dagger)$ represent the destruction (creation) operators for the phonons in the states q and they satisfy the usual boson commutation relations. The electron operator v_q describes the interaction of an electron with the vibrating atoms of the crystal, and it must be such that $v_{-q} = v_q^\dagger$.

We have found it possible to avoid the introduction of special one-electron states, such as the Stark–Wannier or Houston states, by formulating the problem on the basis of the equation of motion of the one-electron density operator and by using only the familiar Bloch states of the unperturbed crystal.

The equation of motion for the electrons that takes into account the exchange effects can be derived from the equation of motion of the coupled system of electrons plus phonons. For weak electron–phonon interaction and under conditions of thermal equilibrium for the phonons it has been shown recently [14] that the one-electron density operator is determined by the equation (with $\hbar = 1$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}L\rho(t) + \int_0^t \mathrm{d}\tau\, C[t-\tau|\rho(\tau)] \tag{8}$$

where

$$L\rho(t) = [H,\rho(t)] = [H_0 + H',\rho(t)] = (L_0 + L')\rho(t) \tag{9}$$

and

$$C[t-\tau|\rho(\tau)] = \sum_{\eta=\pm1}\sum_q [N_q + \tfrac{1}{2}(1+\eta)]\exp[-\mathrm{i}\eta\omega_q(t-\tau)]$$
$$\times\{\exp[-\mathrm{i}L(t-\tau)][1-\rho(\tau)]v_q^\dagger\rho(\tau), v_q\} + \mathrm{HA}. \tag{10}$$

Here

$$N_q = [\exp(\beta\omega_q) - 1]^{-1} \tag{11}$$

is the average number of phonons q at temperature $(k_B\beta)^{-1}$, while the terms $\eta = +1, -1$ describe the scattering of electrons due to emission and absorption of phonons, respectively, in the Born approximation. The effects of the electron exchange on the collisions with the phonons are described by the 'exclusion factor' $[1-\rho(\tau)]$, while the effects of the electric field are given without any approximation by the time evolution Liouville operator $\exp(-iLt) = \exp[-i(L_0 + L')t]$.

Equation (8) for $\rho(t)$ is correct to all orders in H'. From equation (6) it is clear that the operator H' induces interband transitions even in the absence of phonons (*Zener tunnelling*), a much studied process [18–21]. The presence of phonons is expected on physical grounds to have two different kinds of effect on the interband tunnelling. First, the electron–phonon interaction will cause interband transitions (*phonon-assisted tunnelling*). Second, it will modify the Zener tunnelling mentioned above, because the collisions will affect the motion of the electron before and after it tunnels due to H' (*phonon-modified-Zener tunnelling*). There are, of course, additional effects due to the interference of these two tunnelling mechanisms. Here we shall consider only the simple case of the *initial* tunnelling probability from a fully occupied band to an unoccupied band in the presence of the electric field and the phonons.

We first note that in the equation of motion (8) for $\rho(t)$ the second term includes the description of interference effects between the Zener tunnelling and the phonon scattering mechanisms. As we mentioned above, we shall ignore here all effects that are of order $H'V^2$ or higher in the cross products of H' and V. We thus have for $\rho(t)$

$$\frac{d}{dt}\rho(t) = -i(L_0 + L')\rho(t) + \int_0^t d\tau\, C_0[t-\tau|\rho(\tau)] \tag{12}$$

where

$$C_0 = C\{L \longrightarrow L_0\} \tag{13}$$

i.e. C_0 is identical to C as given by (10) except that the time evolution Liouville operator $\exp(-iLt)A$ is replaced by $\exp(-iL_0t)A = \exp(-iH_0t)A\exp(iH_0t)$, where H_0, as given by (5), includes the intraband accelerating effect of the electric field exactly. This describes the tunnelling effects discussed above, since the first term in (12) includes *all* the effects of E and the second term gives *all* the effects of scattering in the lowest order in the electron–phonon interaction in the absence of any Zener tunnelling.

For the interband tunnelling phenomena we are interested in evaluating the probability of finding an electron in the state $|nk\rangle$ at time t, i.e. $\langle nk|\rho(t)|nk\rangle = f_n(k,t)$, if we know that at $t = 0$ the electrons were occupying fully a different band n_0, i.e.

$$\rho(0) = \sum_{k'} |n_0k'\rangle\langle n_0k'|. \tag{14}$$

Since the spin is conserved for all processes considered here, it is suppressed. Clearly we have $\mathrm{tr}\rho(t) = \mathrm{tr}\rho(0) = N_e$, the number of electrons.

For the *phonon-assisted tunnelling* probability we thus have, solving (12) with $L' = 0$ up to first order in C_0 and using (13) and (14),

$$f_n^{(p)}(k,t) = \langle nk| \int_0^t \mathrm{d}t_1 \exp[-\mathrm{i}L_0(t-t_1)] \int_0^{t_1} \mathrm{d}t_2 C_0[t_1 - t_2| \exp(-\mathrm{i}L_0 t_2)\rho(0)]|nk\rangle$$

$$= \sum_{k'} \sum_{q} \sum_{\eta=\pm 1} [N_q + \tfrac{1}{2}(1+\eta)] \left| \int_0^t \mathrm{d}\tau \exp(\mathrm{i}\eta\omega_q \tau) \langle nk(-t)|\hat{v}_q(\tau)|n_0 k'\rangle \right|^2 \tag{15}$$

where we have introduced the notation

$$\hat{A}(t) = \exp(\mathrm{i}L_0 t)A = \exp(\mathrm{i}H_0 t)A\exp(-\mathrm{i}H_0 t) \tag{16}$$

and

$$k(t) = k + Ft \tag{17}$$

modulo an appropriate reciprocal lattice vector so that $k(t)$ is always a vector within the Brillouin zone. Now and in the following we choose once and for all the direction of $E = F/e$ to be along any one of the reciprocal lattice vectors. The Brillouin zone can then be chosen so that the end points of $k(t)$ differ by the shortest reciprocal lattice vector $\kappa \| F$ and thus denote the same state. Thus $k(t)$ is a periodic function of t with period $T = \kappa/F$, the period of Bloch oscillations. The evaluation of the matrix element in (15) can be carried out with the use of the identity

$$\langle nk|\hat{A}(t)|n'k'\rangle = \langle nk(t)|A|n'k'(t)\rangle \exp\left(\mathrm{i}\int_0^t \mathrm{d}\tau \{\epsilon_n[k(\tau)] - \epsilon_{n'}[k'(\tau)]\}\right) \tag{18}$$

which follows from (5).

This tunnelling probability to state $|nk\rangle$ at time t starting from a full band n_0 simplifies if we consider the *average* tunnelling rate to band n for a large number of Bloch periods $T = \kappa/F$. We have thus found that the average number of electrons per unit time and unit volume that tunnel to the empty band n from the full band n_0 is

$$W_{nn_0}^{(p)} = \frac{2}{F}\frac{1}{(2\pi)^6} \sum_q \sum_{\eta=\pm 1} \left[N_q + \frac{1}{2}(1+\eta)\right] \int \mathrm{d}^2 k_\perp \int \mathrm{d}^2 k'_\perp$$

$$\times \int_{-\kappa/2}^{\kappa/2} \mathrm{d}p\, |M_{nn_0}^{(\eta)}(q,p,k_\perp,k'_\perp)|^2 \left[1 + 2\sum_{m=1}^{+\infty} \cos\left(m\frac{\Delta_{nn_0}^{(\eta)}(q,k_\perp,k'_\perp)}{F/\kappa}\right)\right] \tag{19}$$

where

$$M_{nn_0}^{(\eta)}(q,p,k_\perp,k'_\perp) = \int_{-\kappa/2}^{\kappa/2} \mathrm{d}p' \langle n, p+p', k_\perp|v_q|n_0, p', k'_\perp\rangle$$

$$\times \exp\left(\frac{\mathrm{i}}{F}\int_0^{p'} \mathrm{d}p'' [\epsilon_n(p+p'', k_\perp) - \epsilon_{n_0}(p'', k'_\perp) + \eta\omega_q]\right) \tag{20}$$

$$\Delta_{nn_0}^{(\eta)}(q,k_\perp,k'_\perp) = \frac{1}{\kappa}\int_{-\kappa/2}^{\kappa/2} \mathrm{d}p\, [\epsilon_n(p,k_\perp) - \epsilon_{n_0}(p,k'_\perp) + \eta\omega_q]. \tag{21}$$

Here we have written $k = (p, k_\perp)$, where $k_\perp$ is the component of $k \perp F$, and the two terms $\eta = +1, -1$, describe the tunnelling due to emission and absorption of phonons respectively.

For the *Zener tunnelling* probability for this case of a full band n_0 the phonons do not modify the simple interband tunnelling due to H' (in the approximation of our theory), and thus we get, from (12) with $C_0 = 0$, up to second order in L',

$$\begin{aligned} f_n^{(z)}(k,t) &= \langle nk|(-\mathrm{i})^2 \int_0^t \mathrm{d}t_1 \exp(-\mathrm{i}L_0(t-t_1)] \\ &\quad \times \int_0^{t_1} \mathrm{d}t_2\, L' \exp[-\mathrm{i}L_0(t_1-t_2)]\, L' \exp(-\mathrm{i}L_0 t_2)\rho(0)|nk\rangle \\ &= \left| \int_0^t \mathrm{d}\tau\, \hat{H}'_{nn_0}(k(-t),\tau) \right|^2 \\ &= \left| \int_0^t \mathrm{d}\tau\, F \cdot R_{nn_0}[k(\tau-t)] \exp\left(\int_0^\tau \mathrm{d}\tau'\, \epsilon_{nn_0}[k(\tau'-t)] \right) \right|^2 \end{aligned} \tag{22}$$

where we have made use of (6), (16) and (18) and $\epsilon_{nn_0}(k) = \epsilon_n(k) - \epsilon_{n_0}(k)$. An analysis of this expression, similar to that of $f_n^{(p)}(k,t)$ (15) for a large number of Bloch periods, yields for the average number of electrons per unit time and unit volume that tunnel to the empty band n from the full band n_0

$$W_{nn_0}^{(z)} = \frac{2F}{(2\pi)^3} \int \mathrm{d}^2 k_\perp\, |M_{nn_0}(k_\perp)|^2 \left(1 + 2 \sum_{m=1}^{+\infty} \cos\left(m \frac{\Delta_{nn_0}(k_\perp)}{F/\kappa} \right) \right) \tag{23}$$

where

$$M_{nn_0}(k_\perp) = \int_{-\kappa/2}^{\kappa/2} \mathrm{d}k_x\, R_{nn_0}(k_x, k_\perp) \exp\left(\frac{\mathrm{i}}{F} \int_0^{k_x} \mathrm{d}p\, \epsilon_{nn_0}(p, k_\perp) \right) \tag{24}$$

and R is the component of $\boldsymbol{R}$ in the direction of E. The first term in (23) is the standard result [18–19] obtained on the basis of various approximations. The oscillatory terms were obtained [20] some time ago for the first time on the basis of the Stark representation, i.e. the one that diagonalizes H_0.

Expressions (19) and (23) for $W_{nn_0}^{(p)}$ and $W_{nn_0}^{(z)}$ as functions of the electric field consist of a steady term and some oscillatory terms, which clearly arise from the intraband Bloch oscillations. Similar oscillations have been detected experimentally recently [15] in semiconducting superlattices. Evaluation of $W_{nn_0}^{(p)}$ and $W_{nn_0}^{(z)}$ for typical energy bands will be published elsewhere.

Most tunnelling experiments in crystals, as in a p–n tunnel diode, are performed under conditions such that only the initial tunnelling rate we discussed above is believed to be required [21]. However, with the new mesoscopic structures it will probably be necessary to consider the tunnelling processes from partially filled bands and under conditions where the depletion and replenishment of the initial states, due to the tunnelling processes, become important. These situations can be studied by constructing kinetic equations for the occupation probabilities from the basic equation of motion (8). We plan to discuss these and some elementary applications elsewhere.

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