Direct current photoexcitation: Could it be relevant for QWIPs?

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We examine the possibility of direct current photoexcitation (DCPE) across a semiconductor heterostructure. After reviewing the quantum-mechanical limitations on the elementary processes imposed by T-invariance and the canonical commutation rules, we use inverse methods to generate some encouraging examples, whose DCPE rates are close to the obtained bounds. July 10, 2001

The current generation quantum well infrared photodetectors (QWIPs) are based on photoexcitation of carriers from a quantum well of some shape, followed by their thermalization and transport across the device by an applied external bias field. The main parasitic effect limiting their sensitivity is the dark current, which is significantly increased by the applied bias field. Photovoltaic detectors, with non-zero response at zero bias, have also been considered [1]. These work on an essentially three level asymmetric scheme. At equilibrium in the dark, only the first (ground) state is populated. A second excited state is longer lived than the photoexcited third, which decays (mostly nonradiatively).Some fraction of the photoexcited carriers gets trapped in the second, wherefrom it can be extracted by a smaller bias field. Alternatively, the nonzero dipole moment of the resulting nonequilibrium steady state generates a potential difference across the device. In both cases the device's response depends on difficultly controllable ratios of life and relaxation times. To our knowledge, no attempts have been made to explore the possibility of generating a strong photocurrent in an asymmetric system of quantum wells at zero bias by *direct photoexcitation* of the current carrying states.

We will consider a simple model for the conduction electron dynamics in the semiconductor heterostructure: the potential depends only on one coordinate (x). Then, the transverse motion (in planes perpendicular to the growth direction) degrees of freedom separate. The longitudinal part of the electron's wave function satisfies the (constant) effective mass Schrödinger equation [2]

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + U(x)\psi(x) = E\psi(x) \qquad (1)$$

The spectrum of (1) with potentials which are fast decaying at infinity consists of the continuum ($E = \hbar^2k^2/2m \geq 0$, with $k \geq 0$) and the (possibly empty) set of negative eigenvalues. The scattering matrix

$$S(k) = \begin{pmatrix} T(k) & R_-(k) \\ R_+(k) & T(k) \end{pmatrix} \qquad (2)$$

connects the *in* states (asymptotically ingoing plane waves, $\mathrm{e}^{\pm ikx}$ near $x = \mp\infty$) with the *out* ones (behaving like $\mathrm{e}^{\pm ikx}$ near $x = \pm\infty$). Here $T(k)$ and $R_\pm(k)$ are the complex transmission and reflection to the right/left coefficients. [3]

Since the potential in (1) is real, the eigenfunctions asscociated to the (non-degenerate) eigenvalues are always real (apart for an irrelevant global phase) and cannot carry a current. The scattering states in the continuum are doubly degenerate, and their "wave functions" can be chosen current carrying, $\langle x|\pm, k\rangle = \phi_\pm(x;k)$, like the plane waves in the absence of a potential. Their asymptotic behavior at $\pm\infty$ is

$$\langle x|+,k\rangle \approx \frac{1}{\sqrt{2\pi}}\begin{cases} \mathrm{e}^{ikx} + R_-(k)\mathrm{e}^{-ikx}; & x \to -\infty \\ T(k)\mathrm{e}^{ikx}; & x \to +\infty \end{cases} \qquad (3)$$

$$\langle x|-,k\rangle \approx \frac{1}{\sqrt{2\pi}}\begin{cases} T(k)\mathrm{e}^{-ikx}; & x \to -\infty \\ \mathrm{e}^{-ikx} + R_+(k)\mathrm{e}^{ikx}; & x \to +\infty \end{cases} \qquad (4)$$

The states (3)-(4) are normalized was chosen in the wavenumber scale [4],

$$\langle \alpha, k|\alpha', k'\rangle = \delta_{\alpha\alpha'}\delta(k-k'). \qquad (5)$$

The (one-dimensional) current density of the state $|\pm, k\rangle$ is $j_\pm(k) = \pm e|T(k)|^2\hbar k/2\pi m$. This is $|T(k)|^2$ times smaller than the one of a plane wave with the same wavenumber.

The left/right currents carried by the $|\pm, k\rangle$ states with k in an interval of width $2\delta k$ around k_0 are

$$I_\pm = \mathcal{A}\int_{k_0-\delta k}^{k_0+\delta k} \mathrm{d}k N_\pm(k) j_\pm(k) = \pm\frac{2e\mathcal{A}\delta E}{h}\{N_\pm\mathcal{T}\}_{E_0} \qquad (6)$$

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Here $\mathcal{A}$ is the area of the device, $N_\pm$ are the surface densities of right/left moving electrons in the interval, $E_0 = \hbar^2 k_0^2/2m$, δE is the halfwidth of the interval in the energy scale, $\mathcal{T}(E) = |T(k)|^2$ is the transmittance, and $\{\ \}_{E_0}$ denotes averaging on the interval.

The values of the currents appearing in (6) can be quite respectable. Indeed, taking an average surface density of $\{N_\pm \mathcal{T}\}_{E_0} = 10^8 cm^{-2}$ and a width $2\delta E = 10 meV$ we obtain about $100 Acm^{-2}$. The total current is zero if the surface densities are equal, $N_+ = N_-$, as in the case of a symmetric well. On the other hand, if the surface densities of left/right moving electrons are different, the currents no longer compensate.

Consider a quantum well/barrier system of some yet unprecised shape, having only one bound state with energy $E_\text{b} = -\hbar^2\kappa^2/2m$, doped to a surface density N_s. The length of the structure should not exceeed ℓ - the mean free path of the electrons (say 1000Å), so that the movement across it can be considered ballistic. The electrons are photoexcited by photons of energy $\hbar\omega$ (wavelength $\lambda = 2\pi c/\omega\sqrt{\epsilon}$) polarized along the growth direction. The intensity of the photon field can be characterized by $\mathcal{N}_{\lambda^3}$ — the number of fertile photons in a cube of size λ [5],

Let τ_l be the lifetime of the final photoexcited states in an interval of width $2\delta k$ around $k_\omega = \sqrt{2m\omega/\hbar - \kappa^2}$ by all processes excepting direct radiative recombination to the bound state. Assuming a steady state, the numbers of right/left moving photoelectrons are

$$\mathcal{A}N_\pm = (2\pi)^2 \omega \tau_l \mathcal{N}_{\lambda^3} N_s \frac{\mathcal{A}}{\epsilon\lambda^2} \frac{e^2}{\hbar v(k_\omega)} \frac{|\langle \pm, k_\omega | x | \text{b} \rangle|^2}{\lambda} \quad (7)$$

Here, $v(k_\omega)$ is the velocity of electrons with wavenumber k_ω, and $\langle \pm, k|x|\text{b}\rangle$ are the bound-to-continuum dipole matrix elements. We neglected the thermal ionization of the electrons bound by the heterostructure, assumed $N_s \gg N_\pm$, and that the lifetime and the energy width $\delta E = \hbar^2 k_\omega\, \delta k/m$ satisfy $\tau_l \delta E > \hbar$.

Being real, the bound states of (1) are invariant under time-reversal, while the continuum ones change into their complex conjugates, $\phi_\pm(x; -k)$. Since (1) is a second order linear differential equation, it has only two linearly independent solutions. Thus, the four solutions $\phi_\pm(x; \pm k)$ satisfy 2 relations which can be written as [6]

$$T(-k)\phi_\pm(x;k) = \phi_\mp(x;-k) - R_\pm(-k)\phi_\mp(x;k). \quad (8)$$

Multiplying the complex conjugate of the upper sign eq. (8) by $x\phi_\text{b}(x)$ and integrating with respect to x, we obtain

$$TM_+ = \overline{M_-} - \overline{R_+} M_-, \quad (9)$$

where we set $M_\pm(k) = \langle \pm, k|x|\text{b}\rangle$, and omitted the k dependences.

Apparently, we have four homogeneous linear constraints for four unknowns (the real and imaginary parts of $M_\pm$): the complex eq. (9), and the one obtained by reversing all the signs in the indices. But only two of them are independent. Indeed, the latter relation becomes an identity if we substitute the real and imaginary parts of M_+ from (9) into it. Thus, there are only two independent constraints on the phases and the absolute values of the matrix elements $M_\pm$:

$$\left|\frac{M_+}{M_-}\right|^2 = \frac{1 + |R|^2 - 2|R|\cos(2\chi_-)}{1 - |R|^2} \quad (10)$$

$$\tan(\chi_-)\tan(\chi_+) = \frac{1 - |R|}{1 + |R|} \quad (11)$$

Here, the phases $\chi_\pm = \arg(M_\pm) - \frac{1}{2}\arg(R_\mp)$, $|R| = |R_\pm|$, and we used eqs. (21)-(23) of Ref. [3].

A glance at (10) tells us that the excitation is symmetric at full trasmission resonances ($|R| = 0$), even for non-symmetric potentials. The asymmetry will be quite small for $|R| \ll 1$. In the other limiting case, $|R| \to 1$, the asymmetry could be quite large, depending on whether one or both the arguments of the tangents in (11) approaches zero (mod π). Nevertheless, the carried current will be small, since the current density is proportional to the transmittance, $|T|^2$.

In the latter case, the photoexcited electrons will be localized mostly to one side of the device, but their chance of tunneling through the before thermalization and recombination in the well is small. A nonequilibrium charge distribution with a non-zero electric dipolar moment can be generated, inducing a voltage difference across the device, which will act as a bound-to-continuum photovoltaic detector. Here, we will not pursue this further, but will concentrate on direct current photoexcitation (DCPE).

Assuming that the argument of the cosine in (10) can attain the optimal value ($2\chi_- = \pi$), we find that the maximum asymmetry that can be achieved by photoexcitation is bounded by

$$|M_+|^2 - |M_-|^2 < |R| \left(|M_+|^2 + |M_-|^2\right). \quad (12)$$

At intermediate values of $|R|$, the total photoexcited current might be a significant fraction of the values predicted by (6).

Substituting (7) into (6) and subtracting, the directly photoexcited current across the plane of the structure is

$$I = I_+ - I_- = C \int_{k_\omega - \delta k}^{k_\omega + \delta k} \mathrm{d}k \quad (13)$$

where we set

$$C = \quad (14)$$

and assumed that the difference of the matrix elements is slowly varying on the interval.

Substituting the bound (12) into (13), we get

$$I < C \int_{k_\omega - \delta k}^{k_\omega + \delta k} \mathrm{d}k |T(k)||R(k)| \left(|M_+(k)|^2 + |M_-(k)|^2 \right). \tag{15}$$

Here, we used the f-sum rule,

$$\int_0^{+\infty} \mathrm{d}k (k^2 + \kappa^2) \left(|M_+(k)|^2 + |M_-(k)|^2 \right) = 1. \tag{16}$$

to estimate from above the integral in (15).

To get results close to the estimate (15) the error we make by extending the integral to $(0, +\infty)$ must be minimal. This means that *a)* The reflectance $|R(k_\omega)|^2 \approx 1/3$, which maximizes the product $|RT^2|$; *b)* The f-sum rule must be close to saturation on the inteval $(k_\omega - \delta k, k_\omega + \delta k)$.

Having failed to detect strong limitations imposed by the basic laws of quantum mechanics on direct current photoexcitation (DCPE), the next question is if potentials with such rates of DCPE *exist*, and whether they are *realisable* as heterostructures. We will employ inverse scattering techniques towards this end.

It is well known (see *e.g.* [6]) that in the absence of bound states, the inverse scattering problem for potentials which decay sufficiently fast at infinity has an unique solution. On the other hand, if $n \geq 1$ bound states are present, there is an infinite (n-parameter) set of isospectral potentials (having the same S-matrix).

The construction of one-parameter subsets of the isospectral manifold is particularly simple using the so-called double Darboux transformation [7]. Let E_b , and $\phi_\mathrm{b}(x)$ be an eigenvalue and the corresponding normalized bound state of (1). Then, the family of Schrödinger equations with potentials

$$U_\tau(x) = V(x) - \frac{\hbar^2}{m} [\ln \Omega_\tau(x)]'' \tag{17}$$

where

$$\Omega_\tau(x) = 1 + (\mathrm{e}^{2\tau} - 1) \int_{-\infty}^{x} \phi_b^2(y) \mathrm{d}y \tag{18}$$

is *isospectral* for any value of the *deformation parameter* $-\infty < \tau < +\infty$. One can readily check by direct substitution that for any $E \neq E_\mathrm{b}$ and $\psi_E(x)$ a solution of (1), the function

$$\tilde{\psi}_E(x;\tau) = \left[E_\mathrm{b} - E + \frac{\Omega_\tau''}{2\Omega_\tau} \right] \psi_E - \frac{\Omega_\tau'}{\Omega_\tau} \psi_E' \tag{19}$$

satisfies (1) with the potential U_τ. Since $\phi_\mathrm{b}(x)$ decays exponentially at infinity, the the leading order asymptotic behavior at infinity of the transforms of bounded solutions (continuous spectrum) is unchanged after renormalization by the τ independent constant $E_\mathrm{b} - E$. This ensures the coincidence of the S-matrices. Finally, the normalized bound state at energy E_b, which has no precursor among the solutions of (1), is

$$\tilde{\phi}_\mathrm{b}(x) = \frac{\mathrm{e}^\tau \phi_\mathrm{b}(x)}{\Omega_\tau(x)} \tag{20}$$

Taking a simple possible realistic example, a square well having only one bound level, we searched for the isospectral deformation which maximizes the DCPE. The wavenumber k_ω of the final state was chosen such as to maximize $|T^2(k_\omega)R(k_\omega)|$.

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[1] B.F. Levine *J. Appl. Phys.*, **74**, R1 (1993); H.C. Liu and F. Capasso, editors, *Intersubband Transitions in Quantum Wells: Physics and Device Applications I, Semiconductors and Semimetals*, vol. **62**, Academic, New York, 2000; and references therein.

[2] As we have shown in [8–10] it is possible to construct Ben-Daniel and Duke (with position-dependent) effective mass hamiltonians which have the same scattering data (bound states and electron transmittance) as (1). Moreover, in [10] we have shown how to construct chemical concentration and dopant profiles for which the *self-consistent* potential coincides with a preset one in (1) or in the Ben-Daniel and Duke's equation.

[3] The reflection and trasmission coefficients satisfy

$$T(-k) = \overline{T(k)}; \quad R_\pm(-k) = \overline{R_\pm(k)} \tag{21}$$
$$|T(k)|^2 + |R_\pm(k)|^2 = 1; \tag{22}$$
$$T(k)R_+(-k) + T(-k)R_-(k) = 0. \tag{23}$$

Eq. (21) follows from time reversal invariance, while (22)-(23) express the unitarity of the S-matrix – a consequence of the conservation of probability. If the potential is reflection symmetric, then $R_+(k) = R_-(k)$. For piecewise continuous potentials, the limit $\lim_{k\to+\infty} k^2 R_\pm(k)$ is finite, see e.g. [6].

[4] L.D. Landau and E.M. Lifschitz, *Quantum Mechanics*

[5] For a running electromagnetic wave in a medium with dielectric constant ϵ, $\mathcal{N}_{\lambda^3} = 1$ corresponds to an energy flux of $2\pi\hbar c^2/\epsilon\lambda^4 \approx 2.10^4 Wcm^{-2}/\lambda_v^4[\mu]$, if we take $\epsilon = 3.4$. Here, $\lambda_v[\mu]$ is the wavelength in vacuum measured in μ.

[6] K. Chadan and P. Sabatier

[7] Apparently, transformations which can be used to generate solutions of new differential equations from known ones were first introduced by C.G.J. Jacobi, *J. Reine Angew. Math.* **17**, 68-82 (1837). In modern literature (see e.g. [6]) they are usually associated with G. Darboux, *C. R. Acad. Sci. (Paris)*, **94**, 1456-1459 (1882). The double Darboux transformation has been introduced by I.M. Gel'fand and B.M. Levitan, *Amer. Math. Transl.* Ser. 2 **1**, 253 (1955) A generalization to the variable effective mass

case appears in Gesztesy + Teschl. Subsequently, like the simple Darboux transformations, they have been repeatedly rediscovered. Recently [11] they have been applied for optimizing the second order nonlinear susceptibilities $\chi^{(2)}$ for frequency doublers.

[8] R. Balian, D. Bessis, and G.A. Mezincescu *Phys. Rev. B* (1995); *J. Physique I* (1996)

[9] D. Bessis, G.A. Mezincescu, and D. Vrinceanu, *Europhys. Lett.* (1997)

[10] D. Bessis and G.A. Mezincescu, *Microelectronics J.* (1999)

[11] Ikonic, Milanovic & al