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FINITE DIFFERENCE METHOD DETERMINATION OF THE NANO-HETERO-INTERFACE WAVE-FUNCTION ENGINEERING OF INTER-SUBBAND LASER FUNCTIONALITY

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Abstract: A novel LASER action nano-hetero-structure of the inter-subband, mid-infrared functionality type is designed on the basis of optically pumped dual resonant tunnelling of conductivity electrons within an appropriately energetically determined scheme of five subbands hosted by two communicating asymmetric, approximately rectangular quantum wells (QWs).

The upper LASER action level employed is the second excited subband of the nanostructure's back, wider QW and is provided with electrons via resonant tunnelling from the first excited subband of the nanostructure's front QW populated through remotely ignited optical pumping out of the local fundamental subband.

The first excited back QW subband functions as the lower LASER action level, directly delivering the received electrons to the local fundamental subband – via fast vertical longitudinal optical phonon scattering – wherefrom they are being recycled back to the nanostructure's front QW fundamental subband by virtue of a second-reverse sense-resonant tunnelling-mediated normal charge transport mechanism.

The handling of the de Broglie wave-function problem evolves into a numerical calculation of a Sturm-Liouville eigensystem solved by means of a finite difference method employing an appropriate tridiagonal coefficient matrix.

Keywords: finite difference method, Sturm-Liouville eigensystem, nano-hetero-interface wave-function

1. Introduction

The investigation of semiconductor hetero-interfaces is a prominent subject of ongoing research in view of their crucial importance for the functionality of numerous optoelectronic microdevices [1–6].

For more than two decades, the designing strategy of band gap engineering [7] or, conformally, wave-function engineering has systematically yielded an admirable

wealth of innovative semiconductor devices offering a high degree of tunability of their optoelectronic performance.

The most celebrated pioneering microelectronic hetero-structures of the kind have been the Bloch oscillator [8, 9], the resonant tunnelling double hetero-diode [10], the hot electron tunnelling transistor [11], and the revolutionary LASER quantum cascade [12, 13].

In the present paper, the principle of operation of an inter-subband, far mid-infrared unipolar LASER action hetero-structure based on optically pumped dual resonant tunnelling between two, both spatially and energetically depth-wise, asymmetric quantum wells (QWs) is outlined in terms of wave-function engineering and quantum mechanical conductivity electron vertical transport and local energetic transition functionality.

The handling of the de Broglie wave-function problem evolves into a numerical calculation of a Sturm-Liouville eigensystem solved by means of a finite difference method employing an appropriate tridiagonal coefficient matrix.

2. Proposed nano-hetero-interface wave-function engineering for inter-subband LASER functionality

The present paper aims at proposing a novel LASER action nano-hetero-structure [14] operational principle, based on a remotely optically pumped [15, 16] dual resonant tunnelling (OPRT) unipolar change transport mechanism that can be materialized within the framework of two communicating quantum wells (CQWs), asymmetric *both* in their spatial extension *and* energetic barrier height aspects, hosting a total of five partially localised subbands: two (the fundamental $\mathbf{If}\rangle$ and the first excited $\mathbf{If'}\rangle$) on the part of the envisaged device's front [**F**] QW and the remaining three (the fundamental $\mathbf{Ib}\rangle$, the first excited $\mathbf{Ib'}\rangle$ and the second excited $\mathbf{Ib''}\rangle$) on the other part, of the OPRT device back [**B**] QW. This is a band gap engineering design meant to establish two selective energy matches, achievable by a nanostructure's respective growth procedure: one between the uppermost subbands $\mathbf{If'}\rangle$ and $\mathbf{Ib''}\rangle$ of the two CQWs and the other concerning the two neighbouring QWs innermost fundamental sublevels $\mathbf{If}\rangle$ and $\mathbf{Ib}\rangle$ (Figure 1).

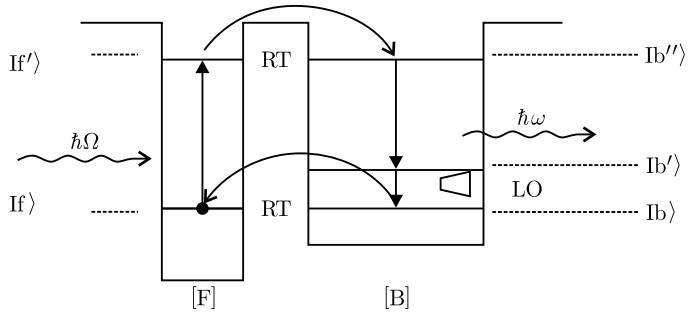

Figure 1. Band gap engineering of the proposed OPRT LASER nano-hetero-device

The two LASER action OPRT nanodevice levels are designed to be the second excited $\mathbf{Ib''}\rangle$ back [**B**] QW subband and the local next-lower first-excited $\mathbf{Ib'}\rangle$ one.

The upper OPRT LASER action level is predicted to be provided with conductivity electrons resonantly tunnelling [17, 18] into it out of its energetically matched device front [**F**] QW first excited $\mathbf{If'}\rangle$ subband, populated through remotely ignited optical inter-subband pumping from its local fundamental $\mathbf{If}\rangle$, front QW, subband. The lower OPRT nanostructure's LASER action level is expected to be directly delivering its radiatively de-excited electrons to the local device back [**B**] QW, fundamental $\mathbf{Ib}\rangle$ subband via particularly fast longitudinal optical (LO) phonon scattering, almost vertical in the reciprocal space and favoured by a band gap-engineered energetic proximity of the entailed $\mathbf{Ib'}\rangle \leftrightarrow \mathbf{Ib}\rangle$ inter-subband separation with the characteristic LO phonon energy valid under the device's operational conditions entailed by the [**B**] QW semiconductor material.

The considered OPRT LASER nanostructure resonant microcavity functionality [19–21] is further determined by the above LO phonon scattering of radiatively down-converted conductivity electrons (from the LASER action lower level to the local [**B**] QW fundamental subband) being succeeded by their recycling back to the OPRT LASER nanostructure's [**F**] QW fundamental $\mathbf{If}\rangle$ subband by virtue of a second-reverse sense-resonant tunnelling-mediated normal charge transport mechanism.

The rate equation modelling of the LASER action functionality of subband levels $\mathbf{Ib''}\rangle$ and $\mathbf{Ib'}\rangle$ is taken in the following form:

$$\frac{dN_{\mathbf{Ib''}\rangle}}{dt} = \frac{1}{T_{\mathbf{FB}}} N_{\mathbf{If'}\rangle} - \frac{1}{\tau_{\mathbf{Ib''}\rangle}} N_{\mathbf{Ib''}\rangle}, \tag{1}$$

$$\frac{dN_{\mathbf{Ib'}\rangle}}{dt} = \frac{1}{\tau} N_{\mathbf{Ib''}\rangle} - \frac{1}{\tau_{\mathbf{Ib'}\rangle}} N_{\mathbf{Ib'}\rangle}, \tag{2}$$

with $N_{\mathbf{If'}\rangle}$, $N_{\mathbf{Ib'}\rangle}$ and $N_{\mathbf{Ib''}\rangle}$ being the sheet electron concentration of nanostructure resonator levels $\mathbf{If'}\rangle$, $\mathbf{Ib'}\rangle$ and $\mathbf{Ib''}\rangle$, respectively, $\frac{1}{T_{\mathbf{FB}}}$ being the temporal rate of achieving the resonant tunnelling charge transport from the [**F**] QW first excited subband $\mathbf{If'}\rangle$ onto the energetically commensurate [**B**] QW second excited subband $\mathbf{Ib''}\rangle$, and $\tau_{\mathbf{Ib''}\rangle}$ being the total lifetime of the upper LASER action level $\mathbf{Ib''}\rangle$, expressible by means of the combined radiative and non-radiative $\mathbf{Ib''}\rangle \rightarrow \mathbf{Ib'}\rangle$ down-conversion rate $\frac{1}{\tau}$ and the non-radiative direct $\mathbf{Ib''}\rangle \rightarrow \mathbf{Ib}\rangle$ relaxation rate $\frac{1}{\tau_{\mathbf{Ib''}\rangle \rightarrow \mathbf{Ib}\rangle}}$ as follows:

$$\frac{1}{\tau_{\mathbf{Ib''}\rangle}} = \frac{1}{\tau} + \frac{1}{\tau_{\mathbf{Ib''}\rangle \rightarrow \mathbf{Ib}\rangle}}, \tag{3}$$

$\frac{1}{\tau_{\mathbf{Ib'}\rangle}}$ being the non-radiative, fast vertical longitudinal optical phonon scattering rate of electrons received by the lower LASER action subband $\mathbf{Ib'}\rangle$ to the local, [**B**] QW, fundamental subband $\mathbf{Ib}\rangle$.

Equations (1) and (2) form a system with five unknowns, namely $N_{\mathbf{Ic}\rangle}$ ($\mathbf{c} = \mathbf{f}, \mathbf{f'}, \mathbf{b}, \mathbf{b'}, \mathbf{b''}$) – the areal electron densities of the five nanostructure resonator levels $\mathbf{Ic}\rangle$ – along with the following equations:

$$\frac{dN_{\mathbf{If}\rangle}}{dt} = \frac{1}{T_{\mathbf{BF}}} N_{\mathbf{Ib}\rangle} - \frac{I\Sigma}{\hbar\Omega} N_{\mathbf{If}\rangle}, \tag{4}$$

$$\frac{dN_{\mathbf{If'}\rangle}}{dt} = \frac{I\Sigma}{\hbar\Omega} N_{\mathbf{If}\rangle} - \frac{1}{T_{\mathbf{FB}}} N_{\mathbf{If'}\rangle}, \tag{5}$$

$$\frac{dN_{\mathbf{Ib}\rangle}}{dt} = \frac{1}{\tau_{\mathbf{Ib}''\rangle\rightarrow\mathbf{Ib}\rangle}} N_{\mathbf{Ib}''\rangle} + \frac{1}{\tau_{\mathbf{Ib}'\rangle}} N_{\mathbf{Ib}'\rangle} - \frac{1}{T_{\mathbf{BF}}} N_{\mathbf{Ib}\rangle}, \tag{6}$$

where $\frac{1}{T_{\mathbf{BF}}}$ denotes the temporal rate at which the (reverse-sense) $\mathbf{Ib}\rangle \rightarrow \mathbf{If}\rangle$ resonant electron tunnelling is effected within the CQWs, I – the optical pumping intensity, Ω – the pumping photon cyclic frequency, and Σ – the optical absorption cross-section exhibited by electrons initially resting upon the [**F**] QW fundamental subband level $\mathbf{If}\rangle$ to incoming pumping photons.

The aforementioned model formalism employed – based upon the rate equation monitoring of the proposed OPRT LASER action level population evolution and inversion – incorporates determination of the transmission coefficient [14, 17] for the resonant tunnelling inter-QW communication mechanism's consecutive steps.

3. Finite difference algorithm for resolving the nano-hetero-interface wave-function eigensystem

To study the applicability of the proposed optically-pumped dual-resonant tunnelling LASER action unipolar charge transport mechanism we have already considered an indicative generic semiconductor nano-hetero-structure based on the conventional $Al_xGa_{1-x}As/GaAs$ material system [22].

In particular, we have employed two totally asymmetric – both in their spatial width and energetic barrier height approximately rectangular quantum wells, communicating through an intervening barrier layer both formulated within (different portions of) the GaAs semiconductor: the front QW [**F**] of spatial width of 96 Å and energetic barrier height of 221 meV, contained between a surface $Al_{0.3}Ga_{0.7}As$ slab and the inter-QW communication barrier layer, and the back QW [**B**] of growth axis extension of 162 Å and an energetic confinement hill of 204 meV, spanning the region between the inter-QW communication barrier layer and a bottom $Al_{0.33}Ga_{0.67}As$ slab. The intervening inter-QW communication barrier layer has been regarded as a succession of two sublayers of $Al_{0.3}GA_{0.7}As$ and $Al_{0.33}Ga_{0.67}As$, of similar thickness.

The Sturm-Liouville eigenvalue system comprising the quantum mechanical Schrödinger differential equation for the nano-hetero-interface wave-function and the appropriate asymptotic boundary conditions is treated below according to the finite difference method, after the employment of an independent variable transformation restricting the integration domain to a universal dimensionless interval. The handling of the problem evolves into numerical calculation of the eigenvectors and the respective eigenvalues of a specific tridiagonal matrix hosting the three successions of coefficients appearing in the kind of finite difference equations selected to convergently approach the initial Sturm-Liouville differential equation.

With respect to the generic situation of a conductivity electron being hosted by the quantum well (QW) of potential energy profile $U(x)$ against the growth axis coordinate x within a conventional semiconductor nanodevice hetero-interface, the pertinent Schrödinger equation, concerning the electron's de Boglie time-independent wave-function $\psi(x)$ and taking into account the spatial variation $m^*(x)$ of the carrier effective mass, reads as follows:

$$-\frac{d}{dx}\left[\frac{\hbar^2}{2m^*(x)}\frac{d\psi(x)}{dx}\right] + U(x)\psi(x) = E\psi(x), \tag{7}$$

where E is the allowed energy eignevalue conjugate to each physically meaningful wave-function $\psi(x)$, solving Equation (7) and vanishing asymptotically at infinities, *i.e.*

$$\psi(\pm\infty)=0 \tag{8}$$

and $\hbar$ is Planck's action constant divided by 2π.

Performing now an independent variable transformation, namely:

$$x\equiv\alpha x^{*}\operatorname{arctanh}(\xi)\leftrightarrow\varphi(\xi)\equiv\psi[x(\xi)], \tag{9}$$

we obtain, instead of Equation (7), the Sturm-Liouville differential equation:

$$\frac{d}{d\xi}\left[\mu(\xi)\frac{d\varphi(\xi)}{d\xi}\right]-v(\xi)\varphi(\xi)+\lambda\sigma(\xi)\varphi(\xi)=0, \tag{10}$$

under the following boundary conditions:

$$\varphi(-1)=0 \qquad \text{and} \qquad \varphi(+1)=0, \tag{11}$$

with functions $\mu(\xi)$, $v(\xi)$ and$\sigma(\xi)$ of the new dimensionless variable ξ (belonging to the universal interval $[-1,+1]$) defined as:

$$\mu(\xi)\equiv\frac{1}{\alpha}(1-\xi^{2})\frac{m_0}{m^{*}[x(\xi)]}, \tag{12}$$

$$v(\xi)\equiv\frac{2\alpha}{1-\xi^{2}}\frac{U[x(\xi)]}{E^{*}}, \tag{13}$$

$$\sigma(\xi)\equiv\frac{2\alpha}{1-\xi^{2}}, \tag{14}$$

and a new dimensionless, "reduced energy" eigenvalue λ defined as:

$$\lambda=\frac{E}{E^{*}}, \tag{15}$$

where E^{*} denotes a convenient energy scale,

$$E^{*}\equiv\frac{\hbar^{2}}{m_0 x^{*2}}\equiv 1\text{eV}, \tag{16}$$

rendering the characteristic confinement length, x^{*}, entering the independent variable transformation (9) after the dimensionless scale factor α equal to 2.76043 Å, m_o giving the electron rest mass.

To convert the Sturm-Liouville differential equation concerning the nano-hetero-interface two-dimensional electron gas (2 DEG) transformed wave-function $\varphi(\xi)$ into a linearized system of difference equations, we employ the following numerical approximation:

$$\frac{d}{d\xi}\left[\mu(\xi)\frac{d\phi(\xi)}{d\xi}\right]\rightarrow\frac{1}{k}\left[\mu_{i+\frac{1}{2}}\left(\frac{\phi_{i+1}-\phi_i}{k}\right)-\mu_{i-\frac{1}{2}}\left(\frac{\phi_i-\phi_{i-1}}{k}\right)\right], \tag{17}$$

in which the computational (nodal and interstitial) grid points ξ_n (whence $f_n\equiv f(\xi_n)$, with f standing for function φ, μ, v or σ, as the case may be) are chosen as follows:

$$\xi_i=-1+ik \quad (i=0,1,2,\ldots,N+1), \quad \xi_{i\pm\frac{1}{2}}=\xi_i\pm\frac{k}{2} \quad (i=0,1,2,\ldots,N+1), \tag{18}$$

for uniform grid spacing:

$$k=\frac{1-(-1)}{N+1}=\frac{2}{N+1}, \tag{19}$$

and for which the adjoining boundary conditions become, after Equations (11) and (18):

$$\begin{gathered}\phi_0=\phi(\xi_0)=\phi(-1)=0, \quad \text{and} \\ \phi_{N+1}=\phi(\xi_{N+1})=\phi\left(-1+(N+1)\frac{2}{N+1}\right)=\phi(+1)=0.\end{gathered} \tag{20}$$

The Schrödinger equation eigenvalue problem is thus approximated by the following system of difference equations:

$$\{\alpha_i\phi_{i-1}+\beta_i\phi_i+\gamma_i\phi_{i+1}=-k^2\Lambda\phi_i; \quad i=1,2,\ldots,N\} \tag{21}$$

or, equivalently, in the tridiagonal matrix row form:

$$\left\{\sum_{j=1}^{N}\{[\alpha_i\delta_{i-1,j}+\beta_i\delta_{i,j}+\gamma_i\delta_{i+1,j}]\phi_j\}=-k^2\Lambda\phi_i; \quad i=1,2,\ldots,N\right\}, \tag{22}$$

($\delta_{i,j}$ – the Kronecker delta), with the sets of coefficients α_i, β_i, γ_i defined as:

$$\alpha_i\equiv\frac{\mu_{i-\frac{1}{2}}}{\sigma_i}, \quad \gamma_i\equiv\frac{\mu_{i+\frac{1}{2}}}{\sigma_i}, \quad \beta_i\equiv-\left(\alpha_i+\gamma_i+\frac{k^2v_i}{\sigma_i}\right), \quad i=1,2,\ldots,N \tag{23}$$

and Λ denoting an approximation to the exact reduced energy eigenvalue λ (see Equation (15)), produced by the constructed numerical algorithm and expected to converge with it more closely with the increasing number N of utilised nodal points ξ_i of the computational grid.

The treatment has thus evolved into a matrix eigenvalue problem:

$$\left\{\sum_{j=1}^{N}\{\Lambda_{i,j}\phi_j\}=-k^2\Lambda\phi_i; \quad i=1,2,\ldots,N\right\} \tag{24}$$

with an N^{th} order square tridiagonal matrix $\{(\Lambda_{i,j};\ j=1,2,\ldots,N);\ i=1,2,\ldots,N\}$ defined by:

$$\Lambda_{i,j}\equiv\alpha_i\delta_{i-1,j}+\beta_i\delta_{i,j}+\gamma_i\delta_{i+1,j}. \tag{25}$$

Indeed, the opposites of the eignvalues of matrix $\{\Lambda_{i,j}\}$ divided by k^2 give Λ, the approximations of the hetero-interface wave-function exact reduced energy eigenvalues λ, thus computing (Equation (15)) the allowed QW 2DEG subband energies $E=\lambda E^*$. Obviously, given that the general Sturm-Liouville system (Equation (10)) may admit an infinite sequence of eigenvalues λ, the finite succession of N eigenvalues Λ for the algorithmic matrix $\{\Lambda_{i,j}\}$ provides numerical approximations of only the N lowest true reduced-energy eigenvalues λ, a slightly reduced approximation sufficiency for the last higher order computed eigenvalues being algorithmically probable. At the same time, the N-determined Sturm-Liouville eigenvectors $|\varphi(\xi)\rangle$ conjugate to these numerical eigenvalues Λ unveil through transformation (Equation (9)) the quantum-mechanically allowed wave-functions $\psi(x)$ for the 2DEG dwelling within the nanodevice's hetero-interface QW and underlying the crucial optoelectronic effects exhibited by the generic semiconductor nanostructure.

In this application, the partially localised conductivity electron eigenstates accommodated by the couple of communicating QWs have been computed (after an appropriate treatment of the rate equation system of Section 2) [22] to correspond

to the energy eigenvalues $E(\mathbf{If}\rangle) = 32\,\mathrm{meV}$, $E(\mathbf{If}'\rangle) = 136\,\mathrm{meV}$ (measured within each QW from its energetic bottom upwards) for the front QW fundamental and first excited bound state, respectively, and $E(\mathbf{Ib}\rangle) = 14\,\mathrm{meV}$, $E(\mathbf{Ib}'\rangle) = 55\,\mathrm{meV}$, $E(\mathbf{Ib}''\rangle) = 121\,\mathrm{meV}$ for the back QW fundamental, first-excited and second-excited bound state, respectively.

Notably, against this predicted energy eigenvalue configuration, the fundamental back QW eigenstate $\mathbf{Ib}\rangle$ elevated by 14meV over the back QW energetic bottom is well aligned with the conjugate fundamental eigenstate $\mathbf{If}\rangle$ of the front QW raised above its QW energetic bottom by an amount corresponding to the inter-QW energetic bottom discrepancy plus approximately the former fundamental eigenstate $\mathbf{Ib}\rangle$ height over its local QW bottom.

Likewise, the uppermost bound eigenstates of the two communicating QW emerge aligned, as the difference in the height of each of them over its local QW bottom almost cancels the energetic height asymmetry of the two QW bottoms.

Ultimately, in application [22], a LASER far mid-infrared emission OPRT functionality in the $19\,\mu$m band has been reached.

4. Conclusion

A novel principle for nano-hetero-interface inter-subband LASER functionality has been outlined with the pertinent wave-function engineering determined through a finite difference method algorithm concerning the entailed Sturm-Liouville eigensystem. The synergy of the algorithm with the LASER rate equation model solution proves satisfactory by virtue of an already treated application.

References

[1] Harris J J, Murray R and Foxon C T 1993 *Semicond. Sci. Technol.* **8** 31
[2] Shengs S Li, Chuang M Y and Yu L S 1993 *Semicond. Sci. Technol.* **8** S406
[3] Logansen L V, Malov V V and Xu J M 1993 *Semicond. Sci. Technol.* **8** 568
[4] Juang C 1991 *Phys. Rev.* **B 44** 10706
[5] Asbel M Ya 1992 *Phys. Rev. Lett.* **68** 98
[6] Papadopoulos G J 1997 *J. Phys.* **A 30** 5497
[7] Capasso F and Cho A Y 1994 *Surf. Sci.* **299/300** 878
[8] Grondin R O, Porod W, Ho J, Ferry D K and Iafrate G J 1985 *Superlattices and Microstructures* **1** 183
[9] Churchill J N and Holmstrom F E 1981 *Phys. Lett.* **A 85** 453
[10] Sollner T C L G, Goodhue W D, Tannenwald P E, Parker C D and Peck D D 1983 *Appl. Phys. Lett.* **43** 588
[11] Yokoyama N, Imamura K, Oshima T, Nishi H, Muto S, Kondo K and Hiyamizu S 1984 *Japan J. Appl. Phys.* **23 L** 311
[12] Faist J, Capasso F, Sivco D, Sirtori D, Hutchinson A L, Chu S N G and Cho A Y 1994 *Science* **264** 553
[13] Faist J, Capasso F, Sirtori C, Sivco D L, Hutchinson A L and Cho A Y 1996 *Electron. Lett.* **32** 560
[14] Jasprit Singh 1995 *Semiconductor Optoelectronics*, McGraw-Hill, New York, Chapter 10
[15] Julien G H, Gauthier-Lafaye O, Boucaud P, Sauvage S, Lourtioz J-M, Thierry-Mieg V and Phanel R 1998 *Inter-subband Transitions in Quantum Wells: Physics and Devices*, Kluwer Academic Publishers, Boston, Chapter 1, Paper 2nd
[16] Anagnostakis E A 1994 *Phys. Stat. Sol.* **B 181** K15

[17] Bastard G 1987 *Wave Mechanics Applied to Semiconductor Hetero-structures*, Les Edition de Physique, Les Ulis Cedex – France, Chapters IV, VI
[18] Chiou W H, Pan H J, Liu R C, Chen C Y, Wang C K, Chuang H M and Liu W C 2002 *Semicond. Sci. Technol.* **17** 87
[19] Pessa M, Guina M, Dumitrescu M, Hirvonen I, Saarinen M, Toikkanen L and Xiang N 2002 *Semicond. Sci. Technol.* **17** R1
[20] Buldu J M, Trull J, Torrent M C, Garcia-Ojalvo J and Mirasso C R 2002 *J. Opt. B: Quantum Semiclass. Opt.* **4** L1
[21] Kulakovskii V D, Tartakovskii A I, Krizhanovskii D N, Gippius N A, Skolnick M S and Roberts J S 2001 *Nanotechnology* **12** 475
[22] Anagnostakis E A 2003 *Proc. 2003 Atomic Level Characterisation of New Materials and Devices, ALC'03*, Hawaii, USA, p. 27