Strong light–matter interaction in systems
described by a modified Dirac equation

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Received 22 May 2013, in final form 24 May 2013
Published 3 July 2013
Online at stacks.iop.org/JPhysCM/25/305801

Abstract

The bulk states of some materials, such as topological insulators, are described by a modified
Dirac equation. Such systems may have trivial and non-trivial phases. In this article, we show
that in the non-trivial phase a strong light–matter interaction exists in a two-dimensional
system, which leads to an optical conductivity at least one order of magnitude larger than that
of graphene.

1. Introduction

Light–matter interaction is a central research topic in atomic,
particle, and condensed matter physics. In the solid state
context [1], optical spectroscopy of materials is a powerful
method of gaining information on the dynamics of electrons
in a given material. In general, one is interested in the
optical properties of many different types of systems:
superconductors, ordinary metals, semiconductors, insulators,
two-dimensional systems, such as graphene [2, 3] and
dichalcogenides, topological insulators [4–7], and others.

Topological insulators are characterized by being
insulators in the bulk (at least ideally) and conducting at the
surface. The effective low energy Hamiltonian describing the
helical (in two dimensions) and surface (in three dimensions)
states is the massless Dirac equation [8–10]. On the other
hand, the low energy Hamiltonian of the bulk states of a
topological insulator can be approximated by a modified Dirac
equation, with a mass term that is momentum dependent.

The optical conductivity of the surface states of
topological insulators has recently been studied [11]. The optical conductivity of
bismuth-based topological insulators has been experimentally
investigated [15–17].

On the other hand, and to the best of our knowledge, the
optical conductivity of the bulk states of topological insulators
has not been studied theoretically. This is understandable,
since the focus has been on the dissipationless nature of
the edge states, which can propagate without scattering of
impurities. A topological insulator may or may not have edge
states depending on the value of the Chern number. If this
quantity is finite then there will be edge states and the system
is said to be non-trivial. On the other hand, if the Chern
number is zero there will be no edge states and the system
is said to be trivial. In what follows, we will thus consider
the contribution of the bulk states to the optical conductivity of
a topological insulator, described by a modified Dirac equation
in two dimensions. We will see that there is a regime of
parameters, where the Chern number is finite, which shows a
clear signature of the non-trivial nature of the system, in the
sense defined above.

2. The modified Dirac equation and the density of
states

The most general two-band model in two dimensions has the
form

\[ H = d_x(k)\sigma_x + d_y(k)\sigma_y + d_z(k)\sigma_z, \]

where \(\sigma_i\) is the \(i = x, y, z\) Pauli matrix. We shall consider
a particular case where \(d_x(k) = \lambda k_x\), \(d_y(k) = \lambda k_y\), and

\[ \sigma_{xx}(\omega) = \frac{\pi e^2}{2\hbar} \equiv \sigma_0. \]
\[ d_c(k) = M(k), \] that is the case of a Dirac Hamiltonian; we also assume that the mass term is momentum dependent. This model term the modified Dirac equation \[ [18] \] and applies to the bulk states of topological insulators around the \( \Gamma \)-point of the Brillouin zone. The eigenvalues of this Hamiltonian are given by

\[ E_{k,\lambda} = \lambda \sqrt{v^2 \hbar^2 k^2 + M^2(k)}, \]  

with \( k = \sqrt{k_x^2 + k_y^2} \) and \( \lambda = \pm 1 \). The normalized eigenstates are

\[ \psi_{k,+} = \frac{1}{\sqrt{2E_{k,+}}} \left( \sqrt{E_{k,+} + M(k)} e^{-\omega} \right), \]

and

\[ \psi_{k,-} = \frac{1}{\sqrt{2E_{k,+}}} \left( \sqrt{E_{k,+} - M(k)} e^{-\omega} \right), \]

where \( \theta = \arctan(k_y/k_x) \). We further consider that the mass term has the form \( M(k) = m^2 - B \hbar^2 k^2 \), with \( B \) and \( m \) constants that can be either positive or negative. This type of model appears in the theory of topological insulators \[ [10] \].

If we define the vector \( d = [d_x(k), d_y(k), d_z(k)] \), the Chern number has the form \[ [4] \]

\[ n_c = \frac{1}{4\pi} \int_{BZ} dp_x dp_y \frac{1}{E_{k,+}} \left( \frac{\partial d}{\partial p_x} \times \frac{\partial d}{\partial p_y} \right) \cdot d, \]

where \( p_y = \hbar k_y \) and the integral runs over the full Brillouin zone. For our model Hamiltonian, the Chern number acquires the form

\[ n_c = \frac{1}{2} \int_{0}^{\infty} \frac{p(Bp^2 + m^2)}{[v^2 p^2 + (m^2 - Bp^2)^2]^{3/2}} dp = \frac{1}{2} \left[ \text{sgn}(m) + \text{sgn}(B) \right]. \]

We then conclude that when \( mB > 0 \) there is a Hall current and the system is said to be topologically non-trivial; when \( mB < 0 \), \( n_c = 0 \) and the system is trivial.

In figure 1, we depict the band structure of the modified Dirac equation in the regimes \( 2Bm \leq 1 \) and \( 2Bm > 1 \) separately. It is clear in the latter case the gap is off the \( \Gamma \)-point. The band structure has, in this case, a Mexican hat shape. Then, there is a full circumference in momentum space where the group velocity is zero and this has consequences in the density of states, as we shall see below. Although we are using for the parameters \( v \hbar \) and \( B \hbar^2 \) those of HgTe quantum wells, we make no claim that our results are directly applicable to that particular system, since the value we use for \( m^2 \) is different from what is reported in the literature \[ [10] \]. We simply fix \( m^2 \) to a value that places the system in the regime \( 2Bm > 1 \).

The different behaviour of the system when \( Bm \) is either positive or negative can also be seen from the average value of the spin operator, defined as

\[ s = (\sigma_x, \sigma_y, \sigma_z). \]  

\[ \langle \psi_{k,\lambda} | \sigma_{\lambda} | \psi_{k,\lambda} \rangle = \pm \frac{v \hbar}{E_{k,+}}, \]

\[ \langle \psi_{k,\lambda} | \sigma_{\lambda} | \psi_{k,\lambda} \rangle = \pm \frac{v \hbar}{E_{k,+}}, \]

\[ \langle \psi_{k,\lambda} | \sigma_{\lambda} | \psi_{k,\lambda} \rangle = \pm \frac{m^2 - B \hbar^2 k^2}{E_{k,+}}. \]

In figure 2 we depict a vector plot of \( \langle \psi_{k,+} | \sigma_{+} | \psi_{k,+} \rangle \) and \( \langle \psi_{k,+} | \sigma_{\pm} | \psi_{k,+} \rangle \) as a function of \( k_x \) and \( k_y \), in the regime \( Bm > 0 \). At the centre of the Brillouin zone the spin points down whereas when we move off the centre the spin rotates and at large momentum it points up; in the valence band the orientation of the spin is the opposite.

The situation is different when we consider the regime \( Bm < 0 \), as shown in figure 3. In this case, the spin points along the same direction independent of the position in the Brillouin zone. The different behaviour of the spin, depending on the sign of the product \( Bm \), is a manifestation of the trivial or non-trivial nature of the system.

The density of states (DOS) of the conduction band of the topological insulator defined by Hamiltonian \( [2] \) can be easily computed. This quantity is defined by the expression

\[ \rho(\omega) = \frac{1}{A} \sum_k \delta(\hbar\omega - E_{k,+}). \]  

where \( A \) is the area of the system and \( E_{k,+} \) is given by (3) (with \( \lambda = 1 \)). Note that the expression for the DOS of the valence band can simply be obtained from the one above by replacing \( \omega \) with \( -\omega \), as \( E_{k,-} = -E_{k,+} \). Converting the summation above into an integral over the Brillouin zone in the thermodynamic limit, and performing the angular integral,
one obtains
\[ \rho(\omega) = \frac{1}{4\pi} \int_0^\infty du \delta(\hbar\omega - E_{u,+}), \] (11)
where we have performed the substitution \( u = k^2 \) in the integral over the modulus of the wavevector, and where \( E_{u,+} = \sqrt{v^2\hbar^2u + (mv^2 - B\hbar^2u)^2} \).

The computation of the explicit expression for the DOS from (11) can be performed by determining the values of \( u \) for which the argument of the delta function is zero in the expression above. Thus, we need to determine the roots of the equation \( \hbar\omega = E_{u,+} \). Such roots will only contribute to the integral in (11) if they are real and positive.

We start by noting that from equation (3) we find that the minimum of the conduction band takes place at a momentum \( k_\Delta \) given by
\[ k_\Delta = \frac{\sqrt{-1 + 2Bm}}{\sqrt{2B|h|}}, \] (12)
which implies that only for \( 2Bm > 1 \) does the minimum occur off the \( \Gamma \)-point of the Brillouin zone. In this case, the band gap is
\[ \Delta = \frac{v^2}{|B|} \sqrt{4Bm - 1}, \] (13)
and the dispersion resembles a Mexican hat, as is clearly seen in figure 1. If \( 2Bm < 1 \), the band gap occurs at the \( \Gamma \)-point and is given by \( \Delta_\Gamma = 2mv^2 \). If the condition \( 2Bm > 1 \) is met, we always have \( \Delta < \Delta_\Gamma \).

Taking into account the two different regimes \( Bm < 0 \) and \( Bm > 0 \) discussed above, and the appearance of a minimum off the \( \Gamma \)-point for \( 2Bm > 1 \), we need to consider three different cases when analysing the roots of the equation \( \hbar\omega = E_{u,+} \): (i) the trivial case, where \( Bm < 0 \); (ii) the non-trivial case, where \( Bm > 0 \) and \( 2Bm < 1 \); (iii) the non-trivial case, where \( 2Bm > 1 \). Defining \( f(u) = \hbar\omega - E_{u,+} \), the zeros of \( f(u) \), that is \( f(u_0) = 0 \), are
\[ u_0 = \begin{cases} u_- = -\frac{\sqrt{v^2(1 - 2Bm) - g(B, m, \omega)}}{2B^2\hbar^2} + \frac{g(B, m, \omega)}{2B^2\hbar^2}, \\ u_+ = \frac{\sqrt{v^2(1 - 2Bm) - g(B, m, \omega)}}{2B^2\hbar^2} + \frac{g(B, m, \omega)}{2B^2\hbar^2}, \end{cases} \] (14)
where \( g(B, m, \omega) \) is defined by
\[ g(B, m, \omega) = \sqrt{v^2(1 - 4Bm) + 4B^2\omega^2\hbar^2}. \] (15)
Since the discriminant of the square root (in \( g(B, m, \omega) \)) has to be positive, we find that \( \hbar\omega \) can have any positive value in both the trivial case and the non-trivial case if \( 4Bm < 1 \). For the non-trivial case when \( 4Bm > 1 \) we find that
\[ \hbar\omega \geq \frac{v^2}{2|B|} \frac{\sqrt{4Bm - 1}}{\Delta}. \] (16)
If \( u_- \) and \( u_+ \) are to contribute to the integration of the \( \delta \)-function, both have to be positive numbers. This imposes some restrictions on the values of \( \hbar\omega \) depending on the \( 2Bm \) parameter. A detailed analysis reveals the following conclusions. In the trivial case, only \( u_+ \) is positive and therefore \( u_- \) does not contribute to the integral. In this case, we find that \( \hbar\omega \) has to satisfy the condition \( \hbar\omega > mv^2 = \Delta_\Gamma \). In the non-trivial case, we have two regimes to consider: when (i) \( 2Bm < 1 \) and when (ii) \( 2Bm > 1 \). In case (i), only the root \( u_+ \) contributes and the frequency \( \omega \) has to satisfy the condition \( \hbar\omega > \frac{\Delta}{2} \). In case (ii), both roots contribute. The root \( u_- \) gives a contribution in the energy range \( \frac{\Delta}{2} < \hbar\omega < \frac{\Delta}{2} \), whereas...
The root $u_+$ gives a contribution in the region $\hbar \omega > \frac{v}{2}$. Taking such information into account when computing the integral in (11), we obtain, using the properties of the delta function, the result

$$
\rho(\omega) = \begin{cases} 
\frac{\omega \theta(\hbar \omega - \Delta \Gamma / 2)}{4\pi \hbar^2 v^4 (1 - 4mB) + 4B^2 \omega^2 \hbar^2} & \text{if } 2mB < 1, \\
\frac{\omega (1 + \tilde{\theta}(\Delta \Gamma / 2 - \hbar \omega)) \theta(\hbar \omega - \Delta / 2)}{4\pi \hbar^2 v^4 (1 - 4mB) + 4B^2 \omega^2 \hbar^2} & \text{if } 2mB \geq 1,
\end{cases}
$$

where $\theta(x) = 0$ if $x < 0$, $\theta(x) = 1/2$ if $x = 0$, and $\theta(x) = 1$ if $x > 0$, and where $\tilde{\theta}(x) = 0$ if $x < 0$, and $\tilde{\theta}(x) = 1$ if $x \geq 0$. A plot of this quantity for selected values of the different parameters is given in figure 4. Note the appearance of a peak and a discontinuity in the DOS, in the frequency range $\frac{v}{2} < \hbar \omega < \frac{v}{2}$, for $2mB \geq 1$, signalling the change of regime pointed out above.

3. Kubo formula: fixing the notation

From the linear response, we know that the average of the current operator is given by

$$
\langle J_\alpha \rangle = -\frac{i}{\hbar} \int_{-\infty}^{\infty} \! dt' \langle [J_\alpha(t), V(t')] \rangle,
$$

where $V(t)$ is the perturbation. We consider a Hamiltonian, $H(\hbar k)$, such that the electrons couple to the electromagnetic field through minimal coupling, that is,

$$
H = H(\hbar k - qA),
$$

where $q$ is the charge of the particles (for electrons we have $q = -e$, with $e > 0$). The current is defined as

$$
J_\gamma = -\frac{\partial H}{\partial \alpha_\gamma} = \frac{q}{\hbar} \frac{\partial H(\hbar k)}{\partial k_\gamma},
$$

and for a small $qA$ (linear response) we have

$$
H(\hbar k - qA) \approx H(\hbar k) - \sum_{\gamma} qA_\gamma \frac{\partial H(\hbar k)}{\partial k_\gamma}
$$

$$
= H(\hbar k) - \sum_{\gamma} J_\gamma A_\gamma.
$$

Thus, the perturbation reads

$$
V(t) = -\sum_{\gamma} J_\gamma A_\gamma(t),
$$

where we have assumed that $A_\gamma(t)$ is a function of time. Then, the average of the $\alpha$-component of the current is

$$
\langle J_\alpha \rangle = \sum_{\gamma} \frac{i}{\hbar} \int_{-\infty}^{t} \! dt' \langle [J_\alpha(t), J_\gamma(t')] \rangle A_\gamma(t'),
$$

where $J_\alpha(t)$ is the current operator in the interaction picture. We can now introduce a retarded function defined as

$$
\Pi^{R}_{\alpha\gamma}(t - t') = -i\theta(t - t') \langle [J_\alpha(t), J_\gamma(t')] \rangle,
$$

such that

$$
\langle J_\alpha \rangle = \frac{1}{\hbar} \sum_{\gamma} \int_{-\infty}^{\infty} \! \Pi^{R}_{\alpha\gamma}(t - t') A_\gamma(t').
$$

Fourier transforming the previous equation, we obtain

$$
\langle J_\alpha(\omega) \rangle = \frac{1}{\hbar} \sum_{\gamma} \Pi^{R}_{\alpha\gamma}(\omega) A_\gamma(\omega).
$$

If we now choose

$$
A_\gamma(t) = A_\gamma(\omega) e^{-i\omega t},
$$

$$
\Pi^{R}_{\alpha\gamma}(\omega) = \int_{0}^{\beta \hbar} \! \text{d} e^{i\omega t} \Pi_{\alpha\gamma}(t),
$$

where

$$
\Pi_{\alpha\gamma}(t) = \langle T_{\tau} J_\alpha(\tau) J_\gamma(0) \rangle,
$$

and $\beta = 1/(k_B T)$, where $k_B$ is the Boltzmann constant and $T$ the temperature.

4. Optical conductivity of a two-band Hamiltonian: formal matters

In connection with the Hamiltonian (2) let us now define creation and annihilation operators, $a^\dagger_{k,\lambda}$ and $a_{k,\lambda}$, which
create and annihilate electrons in the band $\lambda$ with momentum $\hbar k$; we denote $\lambda = +$ for the conduction band and $\lambda = -$ for the valence band. In this basis, the current operators in second quantization are defined as

\[
\hat{J}_x = \sum_{k,\lambda,\lambda'} a_{k,\lambda}^\dagger a_{k,\lambda'} \langle \psi_{k,\lambda} | \hat{J}_x | \psi_{k,\lambda'} \rangle, \\
\hat{J}_y = \sum_{k,\lambda,\lambda'} a_{k,\lambda'}^\dagger a_{k,\lambda} \langle \psi_{k,\lambda'} | \hat{J}_y | \psi_{k,\lambda} \rangle,
\]

where $J_x, (\alpha = x, y)$ is defined in equation (20).

In second quantization the Matsubara current–current correlation function is written as

\[
\Pi_{\alpha\gamma}(i\omega_n) = -\int_0^{\beta\hbar} \mathrm{d}t e^{i\omega_n t} \sum_{k_1,\lambda_1,\lambda_1'} \sum_{k_2,\lambda_2,\lambda_2'} \langle \psi_{k_1,\lambda_1} | \hat{J}_\alpha | \psi_{k_1,\lambda_1'} \rangle \times \langle \psi_{k_2,\lambda_2} | \hat{J}_\gamma | \psi_{k_2,\lambda_2'} \rangle \delta(k_1-k_2) \delta(\lambda_1-\lambda_2) \delta(\lambda_1'-\lambda_2'), \\
\times \mathcal{G}(k_1, \lambda_1, -t) \delta(k_1, \lambda_1) \delta(k_2, \lambda_2),
\]

which in terms of Green’s functions reads

\[
\Pi_{\alpha\gamma}(i\omega_n) = -\int_0^{\beta\hbar} \mathrm{d}t e^{i\omega_n t} \sum_{k_1,\lambda_1,\lambda_1'} \sum_{k_2,\lambda_2,\lambda_2'} \langle \psi_{k_1,\lambda_1} | \hat{J}_\alpha | \psi_{k_1,\lambda_1'} \rangle \times \langle \psi_{k_2,\lambda_2} | \hat{J}_\gamma | \psi_{k_2,\lambda_2'} \rangle \mathcal{G}(k_1, \lambda_1, \tau) \delta(k_1-k_2) \delta(\lambda_1'-\lambda_2),
\]

where

\[
\mathcal{G}(k, \lambda, \tau) = -(T \langle \hat{c}_{k,\lambda} \hat{c}_{k,\lambda}^\dagger \rangle (\tau)).
\]

Introducing the Fourier representation

\[
\mathcal{G}(k, \lambda, \tau) = \frac{1}{\beta \hbar} \sum_{\omega_1} e^{-i\omega_1 \tau} \mathcal{G}(k, \lambda, i\omega_1),
\]

we obtain

\[
\Pi_{\alpha\gamma}(i\omega_n) = \sum_{k,\lambda,\lambda'} \langle \psi_{k,\lambda} | \hat{J}_\alpha | \psi_{k,\lambda} \rangle \langle \psi_{k,\lambda'} | \hat{J}_\gamma | \psi_{k,\lambda'} \rangle \times \frac{1}{\beta \hbar} \sum_{\omega_1} \mathcal{G}(k, \lambda, i\omega_1 + i\omega_2) \mathcal{G}(k, \lambda', i\omega_2),
\]

which after summing over the Matsubara frequency $\omega_2$ gives

\[
\Pi_{\alpha\gamma}(i\omega_n) = \sum_{k,\lambda,\lambda'} \langle \psi_{k,\lambda} | \hat{J}_\alpha | \psi_{k,\lambda} \rangle \langle \psi_{k,\lambda'} | \hat{J}_\gamma | \psi_{k,\lambda'} \rangle \times \frac{n_{F}(k, \lambda') - n_{F}(k, \lambda)}{\omega_n + (E_{k,\lambda'} - E_{k,\lambda})/\hbar},
\]

where $n_F(x)$ is the Fermi distribution function. For $\lambda = \lambda'$ the previous result is zero due to the Fermi functions. Finally, the retarded current–current correlation function is obtained from the Matsubara one by analytical continuation, $\Pi_{\alpha\gamma}^{R}(\omega) = \Pi_{\alpha\gamma}(i\omega_n \rightarrow \omega + i0^+)$. Since

\[
\sigma_{\alpha\gamma}(\omega) = \frac{i}{\hbar \omega} \Pi_{\alpha\gamma}^{R}(\omega),
\]

the real part of the conductivity tensor is given by

\[
\text{Re} \sigma_{\alpha\gamma}(\omega) = \frac{i}{\hbar \omega} \text{Im} \Pi_{\alpha\gamma}^{R}(\omega) = -\frac{\text{Im} \Pi_{\alpha\gamma}^{R}(\omega)}{\hbar \omega}. \tag{40}
\]

From here on, we will be interested in the diagonal component of the conductivity tensor.

5. **Optical conductivity of a modified Dirac equation**

As already noted, the retarded current–current correlation function $\Pi_{xx}^{R}(\omega)$ can be obtained by analytical continuation of the Matsubara current–current correlation function, leading to an imaginary part of the form

\[
\text{Im} \Pi_{xx}^{R}(\omega) = -\frac{\pi}{\hbar} \sum_{k,\lambda,\lambda'} |\langle \psi_{k,\lambda} | J_x | \psi_{k,\lambda} \rangle|^2 \times [n_{F}(k, \lambda') - n_{F}(k, \lambda)] \delta(\omega + (E_{k,\lambda'} - E_{k,\lambda})/\hbar), \tag{41}
\]

where $A$ is the area of the system. The current operator $J_x$ is defined as

\[
J_x = -\frac{e}{\hbar} \sum_{\alpha} \partial_{x_\alpha} \bar{d}_\alpha(k) \sigma_\alpha,
\]

which we use in the calculation of the matrix elements entering in equation (41). In the thermodynamic limit, the momentum summation in equation (41) transforms into an integral in the usual way and one has to compute the angular average of the matrix elements, that is,

\[
I(k) = \int_0^{2\pi} d\theta |\langle \psi_{k,\lambda} | J_x | \psi_{k,\lambda} \rangle|^2. \tag{43}
\]

The final result is $I(k) = \mathcal{K}(k)$, where

\[
\mathcal{K}(k) = \frac{\pi \hbar^2}{E_{k,+}^2} \left[ v^2 (E_{k,+}^2 + M^2(k)) + 4BkM(k)v\sqrt{E_{k,+}^2 - M^2(k)} 
+ 4B^2 \hbar^2 k^2(E_{k,+}^2 - M^2(k)) \right]. \tag{44}
\]

The imaginary part of the current–current correlation function reads

\[
\text{Im} \Pi_{xx}^{R}(\omega) = -\frac{\pi}{\hbar} \sum_{k,\lambda,\lambda'} \frac{du}{8\pi^2} \mathcal{K}(u) \delta(\omega - 2E_{k,+}) \times [n_{F}(-\hbar\omega/2) - n_{F}(\hbar\omega/2)], \tag{45}
\]

where the change of variable $u = \lambda^2$ was again made. In what follows, we assume that the chemical potential lies in the energy gap and we take the zero temperature limit; for finite temperatures, we have to keep the Fermi functions. If we take the limit $m, B \to 0$, the real part of the conductivity reads

\[
\text{Re} \sigma_{xx}(\omega) = \frac{\sigma_0}{4}, \tag{46}
\]

which is 1/4 of the universal conductivity of neutral graphene, since we have not considered spin, and in this case there is not
Figure 5. Optical conductivity of the modified Dirac equation. The parameters used are $\hbar v = 3.65 \text{ eV } \AA$, $\hbar B = -68 \text{ eV } \AA^2$, as for HgTe quantum wells. The dashed line in the left panel is the result given by equation (46). The conductivity is in units of $\sigma_0$ and the photon energy in units of $10 = 2m^2v^2$.

In the non-trivial regime characterized by $2Bm > 1$, the density of states diverges as the energy approaches $\hbar \omega = \Delta$ and the optical conductivity is greatly enhanced relative to the case where $0 < 2Bm \ll 1$. Indeed, the divergence in the density of states also appears in the optical conductivity at photon energies close to $\Delta$. This divergence configures a strong light–matter interaction for this range of frequencies. We then expect that physical effects such as the Faraday rotation [19, 20] must exhibit dramatic results, when compared to the case of graphene, in the quantum regime dominated by inter-band transitions. Finally, we are confident that in the realm of cold atoms the parameters $B$, $m$, and $v$ can be tuned at will, making possible external tuning of the several regimes and the observation of the different effects proposed here.

Acknowledgments

JES’s work contract is financed in the framework of the Program of Recruitment of Post Doctoral Researchers for the Portuguese Scientific and Technological System, with the Operational Program Human Potential (POPH) of the QREN, participated by the European Social Fund (ESF) and national funds of the Portuguese Ministry of Education and Science.
(MEC). The authors acknowledge support provided to the current research project by FEDER through the COMPETE Program and by FCT in the framework of the Strategic Project PEST-C/FIS/UI607/2011.

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