Photonic realization of the relativistic Kronig-Penney model and relativistic Tamm surface states

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Abstract: Photonic analogues of the relativistic Kronig-Penney model and of relativistic surface Tamm states are proposed for light propagation in fibre Bragg gratings (FBGs) with phase defects. A periodic sequence of phase slips in the FBG realizes the relativistic Kronig-Penney model, the band structure of which being mapped into the spectral response of the FBG. For the semi-infinite FBG Tamm surface states can appear and can be visualized as narrow resonance peaks in the transmission spectrum of the grating.

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1. Introduction

The Kronig-Penney model for the non-relativistic Schrödinger equation [1] is a well-known model in solid-state physics that describes the electronic band structure of an idealized one-dimensional crystal. The Kronig-Penney model has served on many occasions as a paradigmatic model to study a wide variety of physical phenomena, including band structure properties, localization effects in disordered lattices, electronic properties of superlattices, Peierls transitions and quark tunnelling in one-dimensional nuclear models. Relativistic extensions of the Kronig-Penney model (also referred to as the Dirac-Kronig-Penney model) have been discussed by several authors (see, for instance, [2–13] and references therein), and the impact of relativity on the band structure and localization, such as shrinkage of the bulk bands with increasing band number, have been highlighted on many occasions. In earlier studies, the Dirac-Kronig-Penney model also attracted some attention and caused a lively debate about the existence of so-called Dirac surface states, i.e. relativistic surface Tamm states which disappear in the non-relativistic limit [3, 7, 14–19]. In recent years, there has been an increased interest in simulations of relativistic quantum effects using different physical set-ups, and analogues of such fundamental phenomena as Zitterbewegung

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and Klein tunnelling -rooted in the Dirac equation- have been proposed and demonstrated for electrons in graphene [20, 21] and for matter waves using trapped cold atoms [22]. Light propagation in guiding optical structures has been also shown to provide a beautiful laboratory system to investigate the classical analogous of a wide variety of coherent non-relativistic [23] and relativistic [24–28] quantum phenomena. In particular, it was recently shown that light propagation in fibre Bragg gratings (FBGs), i.e. optical fibres with a superimposed modulation of the refractive index profile, provides an experimentally accessible laboratory tool to simulate in optics the massive one-dimensional Dirac equation, and a photonic realization of the Dirac oscillator (i.e. the relativistic extension of the quantum harmonic oscillator) has been proposed [29].

In this work we propose a photonic realization of the relativistic Kronig-Penney model and relativistic surface Tamm states based on light propagation in FBGs with phase defects. Light propagation in a FBG with a periodic sequence of phase slips is shown to simulate the relativistic Kronig-Penney model, the relativistic band structure of which being mapped into the spectral transmission of the FBG. Similarly, a semi-infinite FBG with phase defects interfaced with a uniform FBG with a different modulation period is shown to support Tamm surface states analogous to the relativistic Tamm states. Such surface states are responsible for narrow resonance peaks in the transmission spectrum of the grating. The paper is organized as follows. In Section 2, the photonic realization of the Dirac-Kronig-Penney model for an infinitely-extended crystal, based on a superstructure FBG, is presented. The photonic analogues of relativistic Tamm states in a semi-infinite lattice model are discussed in Section 3, and shown to appear as narrow resonance peaks in the spectral transmission of the FBG. Finally, the main conclusions are outlined in Section 4.

2. Photonic realization of the Dirac-Kronig-Penney model

In this section a photonic realization of the Dirac-Kronig-Penney model for an infinitely-extended lattice, based on Bragg scattering of light waves in a superstructure FBG comprising a periodic sequence of phase slips, is proposed. Let us consider light propagation in a FBG with a longitudinal effective refractive index given by

\[
 n(z) = n_0 + \Delta n m(z) \cos \left[ \frac{2\pi z}{\Lambda} + \phi(z) \right],
\]

where \( n_0 \) is the effective mode index in absence of the grating, \( \Delta n \ll n_0 \) is the peak index change of the grating, \( \Lambda \) is the nominal period of the grating defining the reference frequency \( \omega_B = \pi c / (\Lambda n_0) \) of Bragg scattering, \( c \) is the speed of light in vacuum, and \( m(z), \phi(z) \) are the slow variation, as compared to the scale of \( \Lambda \), of normalized amplitude and phase, respectively, of the index modulation. The periodic index modulation of the grating leads to Bragg scattering between two counterpropagating waves at frequencies close to \( \omega_B \). By letting

\[
 E(z, t) = \varphi_1(z, t) \exp \left[ -i\omega_B t + ik_B z + i\phi(z)/2 \right] + \varphi_2(z, t) \exp \left[ -i\omega_B t - ik_B z - i\phi(z)/2 \right] + c.c.
\]
for the longitudinal electric field amplitude in the fibre, where $k_B = \pi/\Lambda$, the slowly-varying envelopes $\varphi_1$ and $\varphi_2$ of counterpropagating waves satisfy the coupled-mode equations (see, for instance, [30])

$$
i \left[ \frac{\partial}{\partial z} + \frac{1}{v_g} \frac{\partial}{\partial t} \right] \varphi_1 = \frac{1}{2} \left( \frac{d\varphi}{dz} \right) \varphi_1 - \kappa(z) \varphi_2$$

(3)

$$
i \left[ - \frac{\partial}{\partial z} + \frac{1}{v_g} \frac{\partial}{\partial t} \right] \varphi_2 = \frac{1}{2} \left( \frac{d\varphi}{dz} \right) \varphi_2 - \kappa(z) \varphi_1$$

(4)

where we have set

$$\kappa(z) \equiv \frac{k_B m(z) \Delta n}{2n_0}$$

(5)

and $v_g \sim c/n_0$ is the group velocity at the Bragg wavelength $\lambda_B = 2\pi c/\omega_B$. The analogy between Bragg scattering of counterpropagating light waves in the FBG and the temporal evolution of two-component spinor Dirac equation in presence of an electrostatic potential is at best captured by introducing the dimensionless variables $x = z/Z$ and $\tau = t/T$, with characteristic spatial and time scales defined by

$$Z = \frac{2n_0}{k_B \Delta n}, \quad T = \frac{Z}{v_g}. \quad \text{(6)}$$

After introduction of new envelopes

$$\psi_{1,2}(z) = \frac{\varphi_1(z) \mp \varphi_2(z)}{\sqrt{2}}. \quad \text{(7)}$$

Eqs.(3) and (4) can be cast in the Dirac form

$$i \frac{\partial \psi}{\partial \tau} = -i \sigma_1 \frac{\partial \psi}{\partial x} + m(x) \sigma_3 \psi + V(x) \psi$$

(8)

for the spinor wave function $\psi = (\psi_1, \psi_2)^T$, where

$$V(x) = \frac{1}{2} \frac{d\varphi}{dx} \quad \text{(9)}$$

and $\sigma_{1,3}$ are the Pauli matrices, defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad \text{(10)}$$

In its present form, Eq.(8) is analogous to the one-dimensional Dirac equation, written in natural units $\hbar = c = 1$, in the presence of an external electrostatic potential $V(x)$, $m(x)$ playing the role of a dimensionless (and generally space-dependent) rest mass.

The Dirac-Kronig-Penney model for an infinitely-extended lattice corresponds to a constant mass $m(x) = m_0$ and to a potential $V(x)$ given by the superposition of equally-spaced $\delta$-like barriers, namely [2]

$$V(x) = V_0 \sum_{n = -\infty}^{\infty} \delta(x - na) \quad \text{(11)}$$
where $V_0 > 0$ is the area of the barrier and $a$ is the lattice period. Stationary solutions $\psi(x, \tau) = \psi_0(x) \exp(-iE\tau)$ to the Dirac equation (8) in the periodic potential (11) with energy $E$ are of Bloch-Floquet type, i.e. $\psi_0(x + a) = \psi_0(x) \exp(iqa)$, where $q$ is the Bloch wave number which varies in the first Brilloiun zone ($-\pi/a \leq q < \pi/a$). The corresponding energy spectrum is composed by a set of allowed energy bands $E = E(q)$, which are defined by the following implicit equation (see, for instance, [17])

$$\cos(qa) = \cos(V_0) \cos(\kappa a) + \frac{E}{\kappa} \sin(V_0) \sin(\kappa a),$$

(12)

where we have set

$$\kappa = \sqrt{E^2 - m_0^2}. \quad (13)$$

Equation (12) defines the dispersion relation of the relativistic Kronig-Penney model, which has been investigated by several authors (see, for instance, [2, 4, 7]). The ordinary non-relativistic limit of the Kronig-Penney model is attained from Eqs.(12) and (13) for $V_0 \ll 1$ and for energies $E$ close the $m_0$, for which the energy-momentum relation (13) reduces to the non-relativistic one $[E \simeq m_0 + \kappa^2/(2m_0)]$; in this regime, the dispersion relation (12) reduces to $\cos(qa) = \cos(\kappa a) + (m_0 V_0/\kappa) \sin(\kappa a)$, which is the ordinary dispersion relation encountered in the non-relativistic Kronig-Penney model. For larger energies $E$ but still for a low barrier area $V_0 \ll 1$, non-relativistic effects come into play as perturbative effects, which modify positions and widths of the allowed energy bands. Non-relativistic effects deeply modify the band structure of the crystal for potential strengths $V_0$ of the order $\sim 1$. In particular, if $V_0$ is an integer multiple of $\pi$, all band gaps disappear and the dispersion relation reduces to the one of a relativistic free particle [Eq.(8) with $V(x) = 0$], as if the $\delta$-barriers were absent.

In our photonic context, owing to Eq.(9) the Dirac-Kronig-Penney model simply corresponds to an infinitely-extended uniform FBG with a superimposed periodic sequence of lumped phase slips of equal amplitude $\Delta \phi = 2V_0$ and spaced by the distance $a$. The circumstance that the effects of the $\delta$ barriers disappear in the Dirac-Kronig-Penney model when $V_0$ is an integer multiple $\pi$ is simply due to the fact that, under such a condition, the phase slips are integer multiplies of $2\pi$, and thus the grating has no phase defects and mimics the dynamics of a one-dimensional free relativistic Dirac particle. It should be noticed that, in another physical context, superstructured FBGs comprising a periodic sequence of $\pi$ phase slips, corresponding to the special case $V_0 = \pi/2$, have been recently proposed and demonstrated to realize light slowing down [31, 32]; however, their connection to the Dirac-Kronig-Penney model was not noticed. It should be also noticed that any FBG structure has a finite length $L$, and thus some kind of lattice truncation should be introduced in the idealized model. As shown e.g. in [31, 32], apodization of the FBG amplitude profile $m(x)$, obtained by slowly decreasing $m(x)$ from its constant value $m(x) = m_0$ in the uniform grating region to zero at $x \rightarrow \pm \infty$, enables to adiabatically inject and eject light waves in the uniform grating region avoiding truncation effects. Correspondingly, the band structure of the Dirac-Kronig-Penney model is mapped into the alternation of stop/transmission bands observed in spectrally-resolved transmission measurements of the FBG. The spectral transmission ($t$) and reflection ($r$) coefficients for the Dirac
equation with \( m(x) \to 0 \) at \( x \to \pm \infty \), corresponding to left wave incidence, are defined from the scattering solution to (8) with the following asymptotic behavior

\[
\psi(x, \tau) \sim \begin{cases} 
\frac{1}{1} \exp[iEx - iE\tau - i\phi(x)/2] + r(E) \frac{-1}{1} \exp[-iEx - iE\tau + i\phi(x)/2] & x \to -\infty \\
t(E) \frac{1}{1} \exp[iEx - iE\tau - i\phi(x)/2] & x \to \infty
\end{cases}
\] (14)

Note that, in our photonic analogue, the energy \( E \) of the scattered waves corresponds to the (normalized) frequency detuning of light waves, propagating in the grating, from the Bragg reference frequency \( \omega_B \).

As an example, Fig.1(c) shows the numerically-computed spectral power transmission \(|t(E)|^2\) (in dB units) for a uniform FBG comprising a sequence of \( \pi \) phase slips [see Fig.1(b)] and with a super-Gaussian apodizing profile \( m(x) \) shown in Fig.1(a); parameter values are \( V_0 = \pi/2 \), \( a = 2 \), \( m_0 = 1 \) and \( L = 50 \). The power spectral transmission has been computed using a standard transfer matrix method (see, for instance, [30]). The shaded areas in Fig.1(c) indicate the stop bands of the ideal (infinitely-long) Dirac-Kronig-Penney lattice as predicted by Eq.(12). In physical units, for typical parameter values \( n_0 = 1.45 \), \( \Delta n = 1 \times 10^{-4} \), and \( \lambda_B = 1560 \) nm, which are consistent with those of Ref.[32], the spatial \( Z \) and temporal \( T \) scales for the example in Fig.1 are \( Z \simeq 5 \) mm and \( T \simeq 24 \) ps, respectively. Hence, in physical units the grating length is \( L \simeq 25 \) cm, the phase slips are separated by the distance \( aZ \simeq 1 \) cm, and the unit scale of (nonangular) frequency detuning \( E \) from the reference Bragg frequency in Fig.1(c) is \( 1/(2\pi T) \simeq 6.6 \) GHz.

3. Relativistic Tamm surface states

The existence of surface Tamm states for the relativistic Kronig-Penney model has been widely studied in earlier papers by several authors [3, 7, 14–19]. In such studies, a debate was raised about the proper boundary conditions that should be imposed to the relativistic wave function at a \( \delta \) barrier (see, for instance, [17, 34, 35]). As earlier works [3, 14–16], based on incorrect boundary conditions, suggested that the relativistic treatment yields a new class of surface states (the so-called Dirac surface states) which do not correspond to the common Tamm states [33] in the non-relativistic limit, it was subsequently realized that application of more physical boundary conditions does not yield any surface state which violates the Tamm condition in the non-relativistic limit [17]. In our photonic system, the appropriate boundary conditions in presence of discontinuities of the phase \( \phi(x) \) [and hence a \( \delta \)-like behavior of the potential \( V(x) \); see Eq.(9)] are readily obtained from Eqs.(3) and (4), and coincide with those used by Subramanian and Bhagwat in the study of relativistic Tamm states [17]. The relativistic extension of the Tamm model is defined by the potential (see, for instance, [7, 17])

\[
V(x) = \begin{cases} 
V_1 & x < 0 \\
V_0 \sum_{n=1}^{\infty} \delta(x - na) & x > 0
\end{cases}
\] (15)
Surface states are found as localized solutions to Eq.(8), near the surface $x = 0$, satisfying the appropriate boundary conditions. The energies of such states, if any, should obviously fall in a gap of the energy spectrum of the infinitely-extended Dirac-Kronig-Penney model. As in Ref. [17], we limit to consider the case $V_1 < m_0$, for which surface states occur at the energies $E$ in the interval $(m_0, m_0 + V_1)$ satisfying the equation

$$\kappa \cotg(\kappa a) = V_1 \cotg(V_0) - K$$

provided that $E - V_1 - K\cotg(V_0) > 0$ [17], where $\kappa$ is defined by Eq.(13) and

$$K = \sqrt{m_0^2 - (E - V_1)^2}.$$  

In our photonic system, the potential $V(x)$ defined by Eq.(15) and supporting the surface Tamm states at the
Figure 2. Photonic analogue of relativistic Tamm surface states in a FBG. (a) and (b): amplitude and phase profiles of the grating. (c) Numerically-computed spectral power transmission. The arrow in (c) is the spectral resonance associated to the surface Tamm state. The inset shows an enlargement of the spectral transmission spectrum near the surface-state resonance. Parameter values are given in the text.

The $x = 0$ boundary corresponds to a phase profile $\phi(x)$ of the FBG which is composed by a linearly increasing part with a slope $2V_1$ for $x < 0$, and by a staircase phase profile for $x > 0$ [see, for instance, Fig.2(b) to be commented below], as one can see after integration of Eq.(9), $\phi(x) = 2 \int x d\xi V(\xi)$. Physically, such a FBG basically corresponds to two adjacent sections of uniform grating regions but with different grating periods, with the second grating region (at $x > 0$) comprising a sequence of equally-spaced phase slips, at a distance $a$, equal to $\Delta\phi = 2V_0$. Similarly to the photonic realization of the Dirac-Kronig-Penney model discussed in the previous section, a finite grating length is introduced by apodization of the amplitude profile $m(x)$. In this case, the surface states actually become resonances of the FBG, i.e. trapped light states near $x = 0$ which are weakly coupled to the external regions of the fibre because of evanescent tunnelling (see, for instance, [29]). The existence of surface states can be thus simply recognized by the appearance of narrow resonance peaks embedded in a stop band region of the transmission spectrum of the grating. An example of the photonic analogue of relativistic...
Tamm states in a FBG is shown in Fig.2, corresponding to parameter values $V_0 = \pi/2$, $a = 2$, $m_0 = 1$, (same as in Fig.1) and $V_1 = 0.8$. For such parameter values, a numerical analysis of the Tamm condition [Eq.(16)] indicates that there exists one Tamm surface state at the energy value $E = E_0 \simeq 1.474$, and thus a resonance peak in the spectral power transmission of the grating is expected at such a detuning value. Figures 2(a) and 2(b) show the amplitude [Fig.2(a)] and phase [Fig.2(b)] profiles of the FBG, whereas the corresponding power transmission (numerically-computed by the transfer matrix method) is depicted in Fig.2(c). Note that, according to the theoretical analysis, a strong and narrow resonance peak, at the detuning $E = E_0$, is clearly observable in the transmission spectrum [see the inset of Fig.2(c)], which is the signature of the surface state localized between the two grating regions at around $x = 0$. For parameter values $n_0 = 1.45$, $\Delta n = 1 \times 10^{-4}$, and $\lambda_B = 1560$ nm (as in Fig.1), the spatial $Z$ and temporal $T$ scales are given by $Z \simeq 5$ mm and $T \simeq 24$ ps, respectively, and hence in physical units the grating length is $L \simeq 25$ cm, the phase slips are separated by the distance $aZ \simeq 1$ cm, and the unit scale of (nonangular) frequency detuning $E$ from the reference Bragg frequency in Fig.2(c) is $1/(2\pi T) \simeq 6.6$ GHz.

4. Conclusions

In conclusion, in this work a photonic realization of the Dirac-Kronig-Penney model, describing the band structure of a periodic potential in the relativistic regime, as well as of relativistic surface Tamm states, has been proposed. Our photonic analogue is based on Bragg scattering of light waves in a uniform FBG with a periodic sequence of phase slips. Band structure and surface states of the relativistic lattice model can be simply observed from spectrally-resolved transmission measurements of the FBG. Design parameters of the grating structures, which are compatible with the current FBG writing technology [32], have been presented.

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