THE INFLUENCE OF THE DISCRETIZED RASHBA SPIN-ORBIT INTERACTION ON THE HARPER MODEL

O. BORCHIN and E. PAPP
Department of Theoretical Physics, Faculty of Physics
West University of Timisoara, Bul. Vasile Parvan nr.4, RO-300223
Timisoara, Romania
E-mail: ovidiuborchin@yahoo.com
E-mail: erhardt_papp_2005@yahoo.com

Abstract

The movement of the electrons under the simultaneous influence of a scalar periodic potential and of a uniform transversal magnetic field is described by the well-known second order discrete Harper equation. This equation originates from a two-dimensional energy dispersion law under the minimal substitution. Here one deals with the Harper model under the additional influence of the discretized spin orbit interaction. Converting the spin-orbit interaction in terms of discrete derivatives opens the way for analytical and numerical studies. One finds coupled equations for the spin dependent wave functions, which leads to an appreciable alteration of the nested energy subbands characterizing the self-similar structure of the usual Harper spectrum. To this aim the transfer matrix method has been applied to selected spin-up and spin-down wavefunctions. Accordingly, very manifestations of spinfiltering and of spin correlations are accounted for. Our energy-bands calculations show that the splitting effect implemented by such wavefunctions is appreciable.

Keywords: Harper equation, Rashba spin-orbit coupling, recursive energy bands

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1 INTRODUCTION

Two-dimensional systems of electrons submitted to the simultaneous influences of the periodic potential and of a homogeneous external magnetic field
have received great interest \cite{1,2} in the last four decades. Such studies led to the celebrated Harper equation \cite{1}:

\[ \psi_{n+1} + \psi_{n-1} + 2\Delta \cos(2\pi \frac{\phi}{\phi_0} n + k_2a)\psi_n = E_s \psi_n \]  

(1)

which has been extensively investigated. This equation originates from the influence of the minimal substitution on the energy dispersion law. Here \( E_s = 2E/E_0 \) denotes the dimensionless energy, which comes from a single band tight binding description with nearest neighbor hopping.

Further, \( \Delta \) denotes the anisotropy parameter, while \( \beta = \phi/\phi_0 \) stands for a commensurability parameter expressing the number of flux quanta per unit cell. The magnetic flux and the flux quantum are denoted by \( \phi = Ba^2 \) and \( \phi_0 = h/e \) respectively, while \( k_2a \) stands for the Brillouin phase.

Equation (1), is a second order discrete equation which has been studied numerically in terms of the transfer matrix method by Hofstadter \cite{3}. It has been found that the spectrum is characterized by a nested band structure i.e. by the so called Hofstadter-butterfly. Besides experimental relevance \cite{4}, the Harper-equation provides ideas for useful applications concerning electrons on lattices under the influence of a transversal magnetic fields \((0,0,B)\) \cite{5}.

On the other hand, it has been demonstrated that the influence of the spin-orbit interaction (SOI) \cite{6,7} produce sensible effects \cite{8}. Such results open the way of controlling the electron’s spin under the influence of an external electric field or of a gate voltage, too \cite{9}.

In order to investigate the influence of the Rashba-SOI (RSOI) on the Harper model, we shall supplement the Harper Hamiltonian with the discretized version of the Rashba energy term:

\[ H_{so} = \frac{\Lambda}{\hbar} (\sigma_x p_y - \sigma_y p_x) \]  

(2)

where \( \Lambda \) is the Rashba coupling parameter, \( \sigma_x \) and \( \sigma_y \) are the Pauli matrices, while \( p_x \) and \( p_y \) stand for momentum operators, as usual.

This later discretization has its own interest as it provides the possibility to account for the influence of an underlying electric field in a rather consistent manner. This differs, of course, from the magneto-electric Harper equation discussed before \cite{10,11,12}. In this paper one deals with the numerical energy-bands realization of the superposition of (1) and (2), now by accounting for selected wave functions. Such solutions concern spin-up and spin-down wave functions, respectively, but inter-related ones will also be considered.

The paper is organized as follows. The discretized RSOI model as well as the derivation of the coupled equations are presented in section II. Numerical investigations of the coupled equations are done in section III by resorting to some selected wave functions. First one accounts solely for the influence of
the spin-up and spin-down wave functions, respectively, which is reminiscent to spin-filtered systems. Next, one deals with inter-related spin-up and spin-down wave functions. The conclusions are presented in section IV.

2 DERIVATION OF COUPLED EQUATIONS

In order to implement the discretized version of RSOI into the Harper model, we have to resort to the modified interaction Hamiltonian

$$\tilde{H}_{so} = c\Lambda \begin{pmatrix} 0 & \partial_1 - i\partial_2 + eBx/h \\ -\partial_1 - i\partial_2 + eBx/h & 0 \end{pmatrix}$$

(3)

where $e > 0$, $\partial_1 = \partial/\partial x$ and $\partial_2 = \partial/\partial y$. For this purpose one proceeds by applying the minimal substitution to (2), by using the Landau-gauge for which the vector potential is given by $(0, Bx, 0)$.

Next, one resorts to the factorization

$$\psi(x, y) = \exp(ik_2y) \begin{pmatrix} \psi^\uparrow(x) \\ \psi^\downarrow(x) \end{pmatrix}$$

(4)

where $\psi^\uparrow(x)$ and $\psi^\downarrow(x)$ stands for spin-up and spin-down wave functions, respectively. This leads to the RSO-Hamiltonian

$$\tilde{H}_{so} = c\Lambda \begin{pmatrix} 0 & D_1^{(+)} \\ D_1^{(-)} & 0 \end{pmatrix}$$

(5)

where

$$D_1^{(\pm)} = \pm\partial_1 + k_2 + \frac{e}{\hbar}Bx.$$  

(6)

On the other hand, the Harper-equation is generated by the energy dispersion law

$$E_{disp}(k_1, k_2) = E_0(\cos k_1a + \Delta \cos k_2a)$$

(7)

under the influence of the Peierls substitution. This results in the substitution rules $k_1 \rightarrow -i\partial_1$ and $k_2 \rightarrow -i\partial_2 + eBx/h$. These rules are responsible for the onset of the Harper-Hamiltonian such as given by

$$\tilde{H}_{Har} = E_0 \left[ 2 \cosh(a\partial_1) + 2\Delta \cos \left( \frac{aeBx}{\hbar} + k_2 \right) \right].$$

(8)

One would than obtain the second-order discrete equation

$$\frac{2}{E_0} \tilde{H}_{Har}\psi_{\uparrow,\downarrow}(x) = \psi_{\uparrow,\downarrow}(x + a) + \psi_{\uparrow,\downarrow}(x - a) + 2\Delta \cos \left( \frac{ae}{\hbar}Bx + k_2a \right) \psi_{\uparrow,\downarrow}(x)$$

(9)
which reproduces equation (1) in terms of the space-discretization $x = na$, where $n$ is an arbitrary integer. What then remains is to establish the discretized version of equation (5), by proceeding via

$$\partial_1 f(x) = \delta_1 f(x) + \mathcal{O}(a^2)$$

where $\delta_1$ stands for discrete derivative. It is understood that

$$\delta_1 f(x) = \frac{1}{a} \sinh(a \partial_1) f(x) = \frac{1}{2a} (f(x + a) - f(x - a)) .$$

Accordingly, $\partial_1$ and $\delta_1$ become identical to first $a$-order. This shows that the discretization one looks for, is provided by the modified substitution rule

$$D_1^{(\pm)} \to \pm \delta_1 + k_2 + 2\pi n \frac{1}{a} \phi_0 \phi \phi_0$$

which stands for the discrete counterpart of equation (6). The eigenvalue equation characterizing the total Hamiltonian is then given by

$$H_{\text{tot}} \psi_\uparrow, \downarrow(x) = (\tilde{H}_{\text{Har}} + \tilde{H}_{\text{so}}) \psi_\uparrow, \downarrow(x) = E \psi_\uparrow, \downarrow(x)$$

where $E$ denotes the total energy and where $\tilde{H}_{\text{so}}$ stands for the discretized $\text{RSO}$-Hamiltonian. This results in the coupled equations

$$E_s \varphi_\uparrow(n) = \varphi_\uparrow(n + 1) + \varphi_\uparrow(n - 1) + 2\Delta \cos(2\pi \beta n + k_2 a) \varphi_\uparrow(n) +$$

$$+ \frac{\Gamma}{2a} [\varphi_\downarrow(n + 1) - \varphi_\downarrow(n - 1)] + \varphi_\downarrow(n) \frac{\Gamma}{a} (k_2 a + 2\pi \beta n)$$

with

$$E_s \varphi_\downarrow(n) = \varphi_\downarrow(n + 1) + \varphi_\downarrow(n - 1) + 2\Delta \cos(2\pi \beta n + k_2 a) \varphi_\downarrow(n) +$$

$$+ \frac{\Gamma}{2a} [-\varphi_\uparrow(n + 1) + \varphi_\uparrow(n - 1)] + \varphi_\uparrow(n) \frac{\Gamma}{a} (k_2 a + 2\pi \beta n)$$

where $\Gamma = -2\Delta/E_0$ contains the Rashba coupling parameter. In order to highlight the meaning of the coupled equations, we shall resort, this time, to some quickly tractable simplifications.

3 NUMERICAL INVESTIGATIONS

At this point we have to realize that $E_0$ can be established in terms of the effective mass $m^*$ of the electron as $E_0 = -\hbar^2/m^*a^2$. Using $m^* = 0.067m_e$ and
\( a = 10 \text{nm} \) \[13\] then gives \( E_0 \simeq 11.37 \text{meV} \). In addition one has \( \Lambda \simeq 5 \times 10^{-11} \text{eVm} \) \[14, 15\]. A first simplification is to assume that spin-down wave functions are zero \( \varphi \downarrow(n) = 0 \), which can be viewed as relying on spin filter devices \[16\] or spin separation processes \[17\].

This Ansatz leads to a \( s = 1 \) spin-selection and \( \theta_2 = k_2 a \), as

\[
\varphi_\uparrow(n + 1) + \varphi_\uparrow(n - 1) = -2\Delta \cos(2\pi \beta n + \theta_2) + E_s \varphi_\uparrow(n) \tag{16}
\]

with

\[
\varphi_\uparrow(n + 1) - \varphi_\uparrow(n - 1) = 2(2\pi \beta n + \theta_2) \varphi_\uparrow(n) \tag{17}
\]

which proceed irrespective of \( \Gamma \). Under such conditions we obtain

\[
\varphi_\uparrow(n + 1) = \varphi_\uparrow(n) \left[ \frac{E_s}{2} - \Delta \cos(2\pi \beta n + \theta_2) + (2\pi \beta n + \theta_2) \right] \tag{18}
\]

with \( \varphi_\uparrow(n - 1) = \varphi_\uparrow(n) \left[ \frac{E_s}{2} - \Delta \cos(2\pi \beta n + \theta_2) - (2\pi \beta n + \theta_2) \right] \tag{19} \)

so that

\[
\frac{\varphi_\uparrow(n + 1)}{\varphi_\uparrow(n)} = \frac{E_s - 2\Delta \cos(2\pi \beta n + \theta_2) - 2(2\pi \beta n + \theta_2)}{2} \tag{20}
\]

and

\[
\frac{\varphi_\uparrow(n)}{\varphi_\uparrow(n + 1)} = \frac{2}{E_s - 2\Delta \cos(2\pi \beta n + \theta_2) + 2(2\pi \beta n + \theta_2)} \cdot \tag{21}
\]

Applying the standard transfer matrix method, one obtains

\[
\begin{pmatrix} \varphi_\uparrow(1) \\ \varphi_\uparrow(2) \end{pmatrix} = T_1 \begin{pmatrix} \varphi_\uparrow(0) \\ \varphi_\uparrow(1) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \varphi_\uparrow(2) \\ \varphi_\uparrow(3) \end{pmatrix} = T_2 T_1 \begin{pmatrix} \varphi_\uparrow(0) \\ \varphi_\uparrow(1) \end{pmatrix} \tag{22}
\]

which can be generalized via

\[
\begin{pmatrix} \varphi_\uparrow(n) \\ \varphi_\uparrow(n + 1) \end{pmatrix} = T_{n-1} \cdots T_2 T_1 \begin{pmatrix} \varphi_\uparrow(0) \\ \varphi_\uparrow(1) \end{pmatrix}. \tag{23}
\]

This amounts to consider

\[
\begin{pmatrix} \varphi_\uparrow(n) \\ \varphi_\uparrow(n + 1) \end{pmatrix} = T_n \begin{pmatrix} \varphi_\uparrow(n - 1) \\ \varphi_\uparrow(n) \end{pmatrix} \tag{24}
\]

where

\[
T_n = \begin{pmatrix} \frac{1}{2\Delta \cos(2\pi \beta n + \theta_2) + (2\pi \beta n + \theta_2)} & 0 \\ 0 & \frac{E_s - 2\Delta \cos(2\pi \beta n + 2\pi \beta n + \theta_2) - 2(2\pi \beta n + 2\pi \beta n + \theta_2)}{2} \end{pmatrix} \tag{25}
\]
supposing that
\[ |Tr(T_n)| = |2\Delta \cos(2\pi \beta n + \theta_2)| \leq 2\Delta . \]  \hspace{1cm} (26)

Note that \( \Delta = 1 \) case, which will be assumed hereafter, represents the critical point of a metal-insulator transition. We are now in position to perform numerical studies in accord with (24)-(25). One realizes that this time, the usual symmetries of the Harper-spectrum like such as the exact energy reflection symmetry \( E \to -E \) and the \( \beta \)-symmetry, i.e. the symmetry under \( \beta = 1/2 \to \beta = 1 - 1/u \) \((u = 1, 2, 3, 4, \ldots)\), cease to be fulfilled.

The understanding is that by virtue of the \( s = 1 \)-selection one deals with a different experimental situation. The flux dependence of the energy bands when \( s = 1 \) (i.e. \( \gamma = 0 \)) is displayed in Fig.1, as illustrated by the bands located in the upper half plane. However, we can also select \( \varphi_\uparrow = 0 \) (instead of \( \varphi_\downarrow = 0 \)), in which case one deals with \( s = -1 \) (instead of \( s = 1 \)).

\[ \text{Fig.1} \hspace{0.5cm} \text{The flux dependence of energy bands for } s = 1 \text{ (upper half plane) and } s = -1 \text{ (lower half plane).} \]

This time the energy-bands get located inside the lower half plane.

One remarks that bands become increasingly dispersed as the magnetix flux increases. This means that \( \beta \)-symmetry is completely lost. When the flux approaches unity, the bands become equidistant, in accord with the behavior of Landau levels. Such patterns can be gathered together as
\[ 2 \frac{E}{E_0} = sF_\pm(\beta, k) \]  \hspace{1cm} (27)
in which \( s = 1 \) or \( s = -1 \), respectively. In addition there is \( F_\pm(k) > 0 \) and
\[ F_+(\beta, k) \approx F_-(\beta, k) \]  \hspace{1cm} (28)
which is responsible for energy reflection symmetry. The next approximation is to consider inter-related spin-up and spin-down wave functions say \( \varphi_\downarrow(n) = \gamma \varphi_\uparrow(n) \), where \( \gamma \) is a real parameter.

One would then obtain

\[
\begin{align*}
 [E_s - 2\Delta \cos(2\pi \beta n + k_2 a) - 2\gamma \Gamma^*(k_2 a + 2\pi \beta n)]\varphi_\uparrow(n) = \\
= (1 + \gamma \Gamma^*)\varphi_\uparrow(n + 1) + (1 - \gamma \Gamma^*)\varphi_\uparrow(n - 1)
\end{align*}
\]

(29)

with

\[
\begin{align*}
 [E_s \gamma - 2\gamma \Delta \cos(2\pi \beta n + k_2 a) - 2\Gamma^*(k_2 a + 2\pi \beta n)]\varphi_\uparrow(n) =
\end{align*}
\]

Fig. 2 The flux dependence of energy bands for subunitary values of the \( \gamma \)-parameter, like \( \gamma = \pm 1/4, \pm 1/2, \pm 17/20 \) and \( \gamma \pm 1 \).
\[
(\gamma - \Gamma^*)\varphi_\uparrow(n + 1) + (\gamma + \Gamma^*)\varphi_\uparrow(n - 1)
\]

by virtue of (14) and (15), respectively.

Fig. 3 The flux dependence of energy bands for values of supraunitary modulus of the \(\gamma\)-parameter, like \(\gamma = \pm 1.05, \pm 1.2, \pm 2\) and \(\gamma = \pm 99\).

These later equations lead in turn to

\[
\frac{\varphi_\uparrow(n - 1)}{\varphi_\uparrow(n)} = \frac{(\gamma - \Gamma^*)E_1(n) - (1 + \gamma \Gamma^*)E_2(n)}{(\gamma - \Gamma^*)(1 - \gamma \Gamma^*) - (1 + \gamma \Gamma^*)(\gamma + \Gamma^*)}
\]  

and

\[
\frac{\varphi_\uparrow(n)}{\varphi_\uparrow(n + 1)} = \frac{(\gamma + \Gamma^*)(1 + \gamma \Gamma^*) - (1 - \gamma \Gamma^*)(\gamma - \Gamma^*)}{(\gamma + \Gamma^*)E_1(n) - (1 - \gamma \Gamma^*)E_2(n)}
\]
where $\Gamma^* = \Gamma/2a$ so that $\Gamma^* \simeq 7.043 \cdot 10^{-20}$ is vanishingly small. In addition
\begin{equation}
E_1(n) = E_s - 2\Delta \cos(2\pi \beta n + k_2 a) - 2\gamma \Gamma^*(k_2 a + 2\pi \beta n)
\end{equation}
and
\begin{equation}
E_2(n) = E_s \gamma - 2\gamma \Delta \cos(2\pi \beta n + k_2 a) - 2\Gamma^*(k_2 a + 2\pi \beta n)
\end{equation}
denotes the energies from (31) and (32). Using again the method of the transfer matrix, one finds energy-band realization which are rather sensitive to $\gamma$. In addition we have to remark that by now $E_s = 2E/E_0$ is an even function of $\gamma$. When $|\gamma| < 1$, the energy bands exhibit dispersions decreasing with $|\gamma|$, as shown in Fig.2 for $\gamma = \pm 1/4, \pm 1/2, \pm 17/20$ and $\gamma = \pm 1$. We have to remark that in this latter case energy dispersion effect get inhibited, now by preserving both energy reflection and $\beta$-symmetries. We have also to remark that the plots displayed in Fig.2 for $\gamma = \pm 1$ reflect, within a reasonable approximation, the onset of a two level configuration, say
\begin{equation}
2 \frac{E}{E_0} \simeq \pm 2.36
\end{equation}
proceeding irrespective of the magnetic flux. Such configurations are of a special interest for applications in the field of optoelectronics [18, 19]. Next we found that supraunitary values of the $\gamma$ parameter lead to an asymmetric location in the flux dependence of energy bands, as shown in Fig.3 for $\gamma = \pm 1.05, \pm 1.2, \pm 2$ and $\gamma \pm 99$. One sees that in the later two cases the energies exhibit positive values, only.

4 CONCLUSION

In this paper we have investigated both theoretically and numerically the competition effects between the Harper model and the discretized RSOI.

Coupled equations for the spin dependent wave functions have been established in some particular cases. Unlike the Harper spectrum, which, is characterized by exact symmetries mentioned before, the presence of the RSOI leads to dispersion effects in the flux dependence of the energy bands, excepting the $\gamma = \pm 1$ plots in Fig.2.

Using the transfer matrix technique, we found that the RSOI produces dispersive effects in the energy dependence on the magnetic flux. Such effects get visualized by a sensible alteration of the rather symmetrical nested energy sub-bands characterizing the self-similar structure of the usual Harper spectrum. We then have to realize that, excepting of course the special $\gamma = \pm 1$ case mentioned above, both energy-reflection and $\beta$-symmetries are lost. Our
first but restrictive approximation is to account only for the influence of spin-
down and spin-up wave functions, respectively. The modified energy bands
established in this manner are displayed in Fig. 1.

Our next approximation is to account for inter-related spin-up and spin-
down wave functions. Now we found that energy bands exhibit again visible
modifications, as shown in Fig. 2 and Fig. 3.

In other words we found that supplementing the Harper-Hamiltonian
with the discretized RSOI leads to significant modifications of energy bands,
which serves to a better understanding of the electronic structure. This opens
the way to further applications concerning the influence of the spin-orbit effect,
with a special emphasis of two-level realizations mentioned above which are of
interest in the field of optoelectronics. More general wave functions can also
be considered, but such goals go beyond the immediate scope of this paper.

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