Influence of the spin-orbit interaction in the impurity-band states of n-doped semiconductors

Guido A. Intronati,1,2 Pablo I. Tamborenea,1,2 Dietmar Weinmann,2 and Rodolfo A. Jalabert2

1Departamento de Física and IFIBA, FCEN, Universidad de Buenos Aires, Ciudad Universitaria, Pab. I, C1428EHA Ciudad de Buenos Aires, Argentina
2Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, CNRS-UdS, 23 rue du Loess, BP 43, 67034 Strasbourg Cedex 2, France

We study numerically the effects of the Rashba spin-orbit interaction on the model of electrons in n-doped semiconductors of Matsubara and Toyozawa (MT). We focus on the analysis of the density of states (DOS) and the inverse participation ratio (IPR) of the spin-orbit perturbed states in the MT set of energy eigenstates in order to characterize the eigenstates with respect to their extended or localized nature. The finite sizes that we are able to consider necessitate an enhancement of the spin-orbit coupling strength in order to obtain a meaningful perturbation. The IPR and DOS are then studied as a function of the enhancement parameter.

PACS numbers: 72.25.Rb, 71.70.Ej, 71.30.+h, 71.55.Eq

The metal-insulator transition (MIT) is one of the paradigms of Condensed Matter Physics and new features constantly appear according to the physical properties under study, the specific system or the emerging experimental techniques. The richness of the physics around the MIT stems from the fact that it is a quantum phase transition where disorder and Coulomb interactions coexist and compete in the determination of the ground state. In the case of the n-doped semiconductors, the MIT appears at doping densities where the Fermi level is in the impurity band. This observation allows a description taking into account only the electronic states built from the hydrogenic ground state of the dopant. The Fermi level is then studied as a function of the enhancement parameter.

The recently developed field of spintronics is contributing to the MIT again into the focus of the condensed matter community. A key concept for possible applications of spintronics is the spin relaxation time, that is, the typical time in which the electron spin loses its initially prepared direction. Interestingly, the maximum spin relaxation times in n-doped semiconductors have been observed for impurity densities close to that of the MIT. This intriguing physics is not completely understood at present, and various mechanisms of spin relaxation have been thought to be active at the MIT region. At the level of models, the generalization of the Anderson model in order to include some spin-orbit coupling has been provided by Ando. While this model is very useful to study the progressive breaking of the spin symmetry, its connection with experimentally relevant systems requires the estimation of coupling parameters which are not obtainable from first principles. This situation has lead us to reconsider the MT model of impurity sites randomly placed in order to incorporate in it the spin-orbit interaction. The various spin-orbit couplings (intrinsic and extrinsic) can be included and lead to effective Hamiltonians which depend on fundamental material constants, rather than on adjustable parameters.

In this paper we first consider the MT model in order to characterize the regions of extended and localized states, analyzing the limitations of the model and the conditions of applicability. We then include one of the sources of spin-orbit coupling, the Rashba interaction to study how the previous picture evolves under increasing values of the coupling strength. This work is a necessary step towards the understanding of spin dynamics in the generalized models that will allow us to extract the spin relaxation times close to the MIT.

We start by considering the MT Hamiltonian

\[ \mathcal{H}_0 = \sum_{m\neq m',\sigma} t^{\sigma\sigma}_{m'm} c^\dagger_{m'\sigma} c_{m\sigma}, \]

(1)

where \( c^\dagger_{m'\sigma} (c_{m\sigma}) \) represents the creation (annihilation) operator for the ground state of the impurity at site \( m' \) (\( m \)) with spin projection \( \sigma \) in the \( z \)-direction. The spin degree of freedom is irrelevant for the MT model, but it will become crucial later. The hopping matrix element is

\[ t^{\sigma\sigma}_{m'm} = \langle \phi_{m'} | V_{m'm} | \phi_m \rangle = -V_0 \left( 1 + \frac{R_{m'm}}{a} \right) \exp \left( -\frac{R_{m'm}}{a} \right), \]

(2)

where \( \phi_r (r) = \phi (|r - R_p|) \), with \( \phi (r) = 1/(\pi a^3)^{1/2} \times \exp (-r/a) \), and \( a \) is the effective Bohr radius. The Coulombic potential produced by the impurity placed at \( R_p \) is \( V_{p}(r) = -V_0(a/|r - R_p|) \), where \( V_0 = e^2/\varepsilon a \) and \( \varepsilon \)
stands for the static dielectric constant of the semiconductor.

In order to characterize the electronic eigenstates in the impurity band from the point of view of their extended or localized nature, we solve numerically the eigenvalue problem defined by the Hamiltonian \( \mathbf{H} \) for given configurations in which \( N \) impurities are randomly placed in a three-dimensional volume. Performing the impurity average we obtain (Fig. 1) the density of states (DOS) and the inverse participation ratio (IPR) for three densities on the metallic side of the transition. The impurity band develops around the \( E = 0 \) level of the isolated impurity in an asymmetric fashion: the DOS exhibits a long low-energy tail while the high-energy part is bounded by \( E = 1 \) (in units of \( V_0 \)). We verify that the width of the impurity band increases with the doping density.

The highest-energy states correspond to electronic wave functions localized on small clusters of impurities. This clustering is known to happen in realistic systems due to the lack of hard-core repulsion between impurities on the scale of a \( \alpha \).

Before continuing with the analysis of the numerical results obtained from the MT model, we discuss some technical features of the model and the difficulties that we face in trying to improve upon it. Firstly, we notice that the chosen basis set is not orthogonal. In principle, we can deal with this issue by writing a generalized eigenvalue problem which includes the matrix of orbital overlaps. This procedure results in unphysical high-energy states (with \( E \gg 1 \)) that necessitate the inclusion of hydrogenic states beyond the 1s orbital in order to be described properly. However, care must be taken since enlarging the basis set leads to the problem of overcompleteness. Fortunately, for the properties we are interested in, the effects arising from non-orthogonality are known to be small for moderate doping densities, and that is why we will not consider them in the numerical work, thus staying within the original MT model. Finally, another drawback of the MT model is that the high-energy edge of the impurity band overlaps with the conductance band, which starts at \( V_0/2 \) (the effective Rydberg) and is not included in the MT description. As seen in Fig. 1 the DOS beyond \( V_0/2 \) is always very small, and therefore we can ignore the effects that the hybridization of the bands would yield in a more complete model.

The IPR measures the degree of extension of the electronic wave function. Large values of the IPR denote in general extended states while low values are associated with localized states. In particular, an homogeneously distributed wave function would have an \( \text{IPR}/N = 1 \), while a localized state would exhibit a vanishing \( \text{IPR}/N \) upon increasing values of \( N \). In our study of spin relaxation it is important to know whether the states near the Fermi energy are in the region of extended or localized states.

The determination of the mobility edges from the size scaling of Fig. 1 is not straightforward. This difficulty arises from the heavily structured DOS of the MT model. At low energy the small values of the DOS translates into a poor statistics for feasible sizes. In the high-energy part of the impurity band the separation between the curves corresponding to different values of \( N \) is masked by the small values of the \( \text{IPR}/N \).

For the highest density (top panel) the IPR\( /N \) exhibits a relatively flat region at intermediate energies, which is approximately independent of \( N \) for the two largest system sizes. The lower mobility edge can be located roughly at \( E \sim 3.5 \), where the latter curves separate. For lower impurity densities (lower panels) the previous analysis becomes increasingly demanding in terms of system sizes. We see that the flat region of IPR\( /N \) shrinks from which we can conclude that the lower mobility edge is shifting towards higher values of \( E \).

The study of spin relaxation in doped semiconductors with densities close to the that of the MIT calls for a generalization of the previously discussed MT model that incorporate spin-orbit coupling. Such an extension was done in Ref. [13], where a spin-flip term

\[
\mathcal{H}_1 = \sum_{m\neq m',\sigma} t_{m\sigma}^{m'\sigma} c_{m\sigma}^\dagger c_{m'\sigma} \tag{3}
\]

was added to \( \mathcal{H}_0 (\tilde{\sigma} = -\sigma) \). Similarly to the spin-
conserving case, we have
\[ t_{m\sigma'}^m = \sum_{p \neq m} (\tilde{\psi}_m^\sigma|V_p|\tilde{\psi}_m^\sigma). \] (4)

The wave function \( \tilde{\psi}_{m\sigma} \) is a spin-mixed conduction-band state with an envelope part \( \phi_m(r) \) and a lattice-periodic part which has a small spin admixture. In Ref. [15], the expression of the matrix elements of Eq. (4) within an 8-band Kane model were obtained. Since the two-center integrals \( p = m, m' \) were shown to vanish, the spin-flip hopping amplitude is given by the sum of three-center integrals with \( p \neq m, m' \). The three-center integrals cannot be analytically solved in general. In Ref. [15] we provided approximate analytical expressions of \( t_{m\sigma'}^m \) which allowed us to estimate the spin relaxation times. On the other hand, in this work we take the route of the numerical evaluation of the three-center integrals.

Spin-orbit coupling is known to favor the delocalization of disordered systems in two dimensions. In what follows we repeat the previous analysis, done for the MT model, for the spin-orbit generalized model in this case, for increasing values of the spin-orbit coupling \( R_e \) (the subindex \( r \) stands for Rashba).

For the realistic values of the spin-orbit coupling strength \( (R_e = 1) \) considered in Ref. [13], the spin-admixtures perturbation energies are, even for largest system sizes that we can treat numerically, orders of magnitude smaller than the MT level spacing. In Fig. 2 we show the spectral decomposition of a MT eigenstate with \( \sigma = 1 \) in the basis of spin-admixed eigenstates of \( H_0 + H_1 \). Only for enhanced values of \( R_e \) do we obtain significant projections into the two spin-admixed subspaces.

The study of larger values of \( R_e \) then appears not only as a useful tool for analyzing the progressive inclusion of spin-orbit effects, but also as a need for numerical simulations of the spin dynamics.

In Fig. 3 we present the DOS and IPR/\( N \) of the extended model for the three densities previously treated and various values of the spin-orbit coupling strength \( R_e \). The DOS does not noticeably change with \( R_e \), and that is why we only present the \( R_e = 1 \) case. The spin-orbit coupling results in the increase of the IPR/\( N \) as a function of \( R_e \) in the region of extended states. This effect is more prominent for the larger density. The low-energy sector that has localized states in the MT model exhibits IPR/\( N \) curves approximately independent of \( N \), which is a signature of the delocalization tendency.

In Fig. 4 we perform a finite-size scaling of the IPR/\( N \) for a given density above the MIT critical density and one value of the spin-orbit coupling enhancement factor, \( R_e = 50 \).

In conclusion, we revisited the problem of the characterization of the eigenstates of the Matsubara-Toyozawa model from the point of view of their localization, and performed a similar analysis in an extended model proposed recently which includes the structural inversion asymmetry spin-orbit mechanism. Analyzing the effect of spin-orbit coupling of various strengths is necessary in order to address the study of the spin dynamics in the impurity band of doped semiconductors. We found that while the density of states is not considerably modified by the spin-orbit interaction, the nature of the states is noticeably affected by it showing a tendency to the delocalization.

We acknowledge the financial support of the Collège Doctoral Européen of the Université de Strasbourg and of UBACYT through grant number X495.

[1] Conduction in non-crystalline materials, by Sir Nevill Mott (Oxford Science Publications, Clarendon Press, Oxford, 1987).
[2] The Mott Metal Insulator Transition: Models and Methods, by Forian Gebhard (Springer, Berlin, 2010).
FIG. 3. Density of states (DOS, solid line and right scale) and inverse participation ratio (IPR, dashed lines and left scale) for three different densities on the metallic side of the metal-insulator transition. Dashed lines with increasing thickness are for $R_e = 50$, 150 and 250, respectively. The vertical lines indicate the Fermi energy.

FIG. 4. Density of states (DOS, thick line and right scale) and inverse participation ratio (IPR, left scale) for a density on the metallic side of the metal-insulator transition, three different system sizes, and a fixed spin-orbit enhancement factor of $R_e = 50$. The solid, dashed and dotted curves of IPR/N are for $N = 2744, 3375$ and 4096, respectively, and the vertical line indicates the Fermi energy.

[3] Electronic properties of doped semiconductors, by B. I. Shklovskii and A. L. Efros, (Springer Verlag, New York, Tokyo, 1984).
[4] T. Matsubara and Y. Toyozawa, Prog. Theoret. Phys. 26, 739 (1961).
[5] B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56, 1469 (1993).
[6] B. Kramer, A. MacKinnon, T. Ohtsuki, and K. Slevin, Int. J. Mod. Phys. 24, 1841 (2010).
[7] V. Zarifi and T. G. Castner, Phys. Rev. B 36, 6198 (1987).
[8] J. M. Kikkawa and D. D. Awschalom, Phys. Rev. Lett. 80, 4313 (1998).
[9] I. Dzhioev, K. V. Kavokin, V. L. Korenev, M. V. Lazarev, B. Y. Meltser, M. N. Stepanova, B. P. Zakharchenya, D. Gammon, and D. S. Katzer, Phys. Rev. B 66, 245204 (2002).
[10] L. Schreiber, M. Heidkamp, T. Rohleder, B. Beschoten, and G. Güntherodt, arXiv:0706.1884v1.
[11] M. Römer, H. Bernien, G. Müller, D. Schuh, J. Hübner, and M. Oestreich, Phys. Rev. B 81, 075216 (2010).
[12] B. I. Shklovskii, Phys. Rev. B 73, 193201 (2006).
[13] K. V. Kavokin, Phys. Rev. B 64, 075305 (2001).
[14] W.O. Putikka and R. Joynt, Phys. Rev. B 70, 113201 (2004).
[15] P. I. Tamborenea, D. Weinmann, and R. A. Jalabert, Phys. Rev. B 76, 085209 (2007).
[16] T. Ando, Phys. Rev. B 40, 5325 (1989).
[17] Y. Asada, K. Slevin, and T. Ohtsuki, Phys. Rev. Lett. 89, 256601 (2002).
[18] G. A. Thomas, M. Capizzi, F. DeRosa, R. N. Bhatt, and T. M. Rice, Phys. Rev. B 23, 5472 (1981).
[19] N. Majlis and E. Anda, J. Phys. C: Solid State Phys. 11, 1607 (1978).
[20] W. Y. Ching and D. L. Huber, Phys. Rev. B 26, 5596 (1982).