Detection of helical edge states in a square shaped HgTe quantum dots

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***Abstract*— We investigate electronic properties of square HgTe quantum dots. The semi-empirical tight binding model in $sp^3d^5s^*$ basis of orbitals is used for calculations. The hopping links were limited to the first nearest neighbors and spin-orbit coupling is included in the model. We demonstrate appearance of topologically protected edge states in the energy gap of square HgTe quantum dot. The results provide the basis for future calculations of optical and transport properties of edge states in HgTe quantum dots.**

***Index Terms*—HgTe, square quantum dots, edge states, topological insulators.**

I. Introduction

In the last few years, topological insulators (TI) have been intensively studied because of their potential application in spintronic and quantum computing [1-5]. Two-dimensional (2-D) TI's, which are also known as quantum spin Hall insulators, are a new kind of materials with specific features. They have an energy gap in the bulk and robust, topological (spin-polarized) and gapless states protected by the time reversal symmetry.

The existence of such exotic states was first proposed in graphene [6], where the main drawback is the lack of the band gap. It was expected that the spin-orbit interaction will open an energy gap in the bulk and cause the emergence of states inside the gap. These states should be located at the edges of a nanostructure. However, it was found that the spin-orbit interaction in graphene is too small to be able to induce the appearance of energy gap in the experiments [7].

On the other hand, in 2006, Bernevig, Hughes and Zhang were theoretically predicted the existence of the edge states in the CdTe/HgTe/CdTe quantum wells [8]. By adjusting the thickness of the well, bands become inverted, thus the quantum phase transition occurs. The critical thickness of HgTe layer when the edge states appear equal d_c=6.3 nm is predicted, which was confirmed later in the experiments [9].

Another example of experimentally confirmed TI's are quantum wells with type II band alignment, such as the InAs/GaSb/AlSb devices [10]. These systems also have *s-p* inversion between the conduction and valence bands. However, hybridization of energy gap is much weaker than in CdTe/HgTe/CdTe heterostructures, which is explained by the fact that the valence and conduction bands in the InAs/GaSb/AlSb systems are spatially separated.

In the last few years three-dimensional (3D) TI's are brought to the focus of theoretical and experimental work. These materials represent generalization of the quantum spin Hall effect in three dimensions [11]. Examples of 3D materials in which surface states have been experimentally observed are Bi_xSb_{1-x} [12] and Bi_2Se_3 [13]. Similar behavior is predicted for a number of alloys made of heavy elements, for which the spin–orbit coupling is strong.

In this paper we use the semi-empirical tight-binding (TB) model in search of helical edge states in HgTe quantum dots. This method is characterized by overlap integral parameterization found from a fit from fundamental *ab initio* calculations. The alignment between the results of the two methods is good. Therefore, results are more realistic than the one found using effective k·p models [14].

Quantum dots are structures in which the carriers are confined in all three spatial directions. Varying parameters and techniques for fabrication, different shapes of quantum dots can be obtained. Here we study square shaped quantum dots. Furthermore, the electronic structure of a quantum dot is determined by the shape and composition. Therefore, we can setup desirable performance of nanoelectronic device that is suitable for the target application.

An adjustment of energy gap can lead to inversion of the conduction and the valence bands. For HgTe the valence band has an *s*-like character and possesses Γ_6 symmetry, while the conduction band has a *p*-like character and Γ_8 symmetry. In the inversion process, the energy gap is closed, and after it is reopened the quantum phase transition occurs [8]. In this new quantum state, HgTe quantum dot has a finite energy gap in the bulk and helical edge states that are robust to any imperfections in the sample [15].

This paper is organized into four sections. The next section provides theoretical bases of the TB method with the emphasis on the process of parameterization. The third chapter presents the main results obtained from the TB method, such as the energy spectrum and the densities of certain bulk and edge states in the square HgTe quantum dot. In the last chapter certain conclusions were made.

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II. THE METHOD

One of the most widely used method for solving the problem of electron localization in a semiconductor with periodic potential is based on the TB method. The roots of the method can be found in [16]. The eigenstates are constructed from the linear combination of atomic orbitals belonging to the atoms which form crystal structure. The coefficients found from the expansion are the weights of the plane waves exp(**k**·**R**), where vector **R** represents the position of atom in a lattice [17]. Rigorous use of the TB method involves calculation of a large number of overlap integrals between different atomic orbitals that makes it more complex than commonly used effective models. On the other hand, there are numerous advantages of this method. One of them is that it provides solutions not only around points of high symmetry, but it is possible to obtain the solution at any point in the Brillouin zone [17].

The TB method is useful for a number of cases where the quantum effects are considerable, and where the size of the system makes *ab initio* methods impractical for application [18]. It is more demanding, but much more accurate, than widely used effective methods. However, when comparing to more comprehensive *ab initio* methods it is less accurate but also extremely less demanding. Therefore, it can be more than an order of amplitude faster than *ab initio* methods, especially for systems built of a large number of atoms, where essentially *ab initio* method is not applicable.

The electrons in atoms are generally localized around the core and the probability of leaving atoms is exceptionally small. However, when two atoms get closer, the orbits of two electrons of different atoms may overlap in space, which means that there is a finite probability of electron transition from one atom to another. In this case, the energy of an isolated atom splits into two energies: one that is above and the other which is below energy of isolated atom. This can be generalized to a situation with large number of atoms that is occurring in the semiconductor crystal: electrons move from one atom to the other in the energy bands.

Within the TB method, we first introduce the atomic orbitals $\varphi_n(\mathbf{r})$ which are solutions of Hamiltonian $H_A(\mathbf{r})$ for isolated atom. In a system which consists of a large number of atoms, an overlapping of orbitals occurs. If the electrons are tightly bounded, the overlap is small. The Hamiltonian for the new system can be rewritten in the following form:

$$H = \sum_n H_A(\mathbf{r} - \mathbf{R}_n) + \Delta V(\mathbf{r}), \tag{1}$$

where atomic potential correction $\Delta V(\mathbf{r})$ has small value in the TB approximation.

A wave function $\psi_n(\mathbf{r})$, which is the solution of the Hamiltonian $H(\mathbf{r})$, is found as a linear combination of atomic orbitals $\varphi_n(\mathbf{r})$

$$\psi_m(\mathbf{r}) = \sum_n c_m(\mathbf{R}_n) \cdot \varphi_m(\mathbf{r} - \mathbf{R}_n). \tag{2}$$

Based on the translational invariance of the system and the Bloch theorem, it is easy to show that

$$\psi_m(\mathbf{r}) \approx \frac{1}{\sqrt{N}} \cdot \sum_n e^{i\cdot\mathbf{k}\cdot\mathbf{R}_n} \cdot \varphi_m(\mathbf{r} - \mathbf{R}_n). \tag{3}$$

Here $c_n(0) \approx 1/\sqrt{N}$, with N denoting the number of atomic sites. By using the function defined in equation (3), energy of the m-th state could be determined as

$$\begin{aligned} \varepsilon_m &= \int \psi^*(\mathbf{r}) \cdot H \cdot \psi(\mathbf{r}) \cdot d^3 r \\ &= E_m - \frac{B_m + \sum_n \sum_l e^{i\cdot\mathbf{k}\cdot\mathbf{R}_n} \cdot C_{m,l}(\mathbf{R}_n)}{1 + \sum_n \sum_l e^{i\cdot\mathbf{k}\cdot\mathbf{R}_n} \cdot A_{m,l}(\mathbf{R}_n)}, \end{aligned} \tag{4}$$

where E_m is the energy of the m-th atomic level, while B_m, $A_{m,l}$ and $C_{m,l}$ are matrix elements integrals of the TB method.

The element

$$A_{m,l} = \int \varphi_m^*(\mathbf{r}) \cdot \varphi_l(\mathbf{r} - \mathbf{R}_n) \cdot d^3 r, \tag{5}$$

is the overlap integral between corresponding orbitals of the adjacent atoms.

The atomic energy shift due to the potential on neighboring atoms is

$$B_{m,l} = \int \varphi_m^*(\mathbf{r}) \cdot \Delta V(\mathbf{r}) \cdot \varphi_m(\mathbf{r}) \cdot d^3 r, \tag{6}$$

These two matrix elements usually have small values, whereas the most significant matrix element of the TB method represents the bond energy

$$C_{m,l} = \int \varphi_m^*(\mathbf{r}) \cdot \Delta V(\mathbf{r}) \cdot \varphi_l(\mathbf{r} - \mathbf{R}_n) \cdot d^3 r, \tag{7}$$

and is usually called "the two center integral".

The matrix elements between orbitals in the TB method are generally limited to the first, second or third nearest-neighbor interactions [19]. In this paper we use $sp^3d^5s^*$ basis set, while the hopping terms are restricted to the first nearest neighbors.

The TB parameters for HgTe crystal are given in Table 1 [19]. Terms denoted by capital E represents the on-site matrix elements, while the V terms define the hopping matrix elements as it is explained in [17]. Subscripts s, p and d denote type of an orbital. Due to the T_d symmetry of HgTe crystal, d-type orbitals used for description of the conduction band (xy,yz,zx) and (x^2-y^2,$3z^2$-r^2) are different. Values of parameters are given for temperature 0 K. Parameters at finite temperature are obtained by linear interpolation.

TABLE I
TB PARAMETERS FOR HGTE CRYSTAL IN ORTHOGONAL BASIS $SP^3D^5S^*$ [19]. VALUES ARE GIVEN FOR TEMPERATURE OF 0 K, AND THE LATTICE PARAMETER IS 6.453 Å.

TB Parameters for HgTe (eV)			
E_s	−10.04016	E_s	−1.502103
E_p	1.580003	E_p	5.929255
$E_{d_{xy}}$	10.139959	$E_{d_{xy}}$	15.108978
$E_{d_{x^2-y^2}}$	13.145395	$E_{d_{x^2-y^2}}$	15.431086
E_{s^*}	12.611213	E_{s^*}	14.801158
Δ	0.375000	Δ	0.465000
$V_{ss\sigma}$	−0.904384	$V_{s^*s^*\sigma}$	−1.570513
$V_{ss^*\sigma}$	0.357261	$V_{ss^*\sigma}$	−0.242580
$V_{sp\sigma}$	1.085069	$V_{sp\sigma}$	2.014492
$V_{s^*p\sigma}$	1.175059	$V_{s^*p\sigma}$	1.405375
$V_{sd\sigma}$	−0.525896	$V_{sd\sigma}$	−1.067102
$V_{s^*d\sigma}$	0.485896	$V_{s^*d\sigma}$	0.696627
$V_{pp\sigma}$	3.166827	$V_{pp\pi}$	−0.945694
$V_{pd\sigma}$	−1.789915	$V_{pd\sigma}$	−0.653612
$V_{pd\pi}$	1.406422	$V_{pd\pi}$	1.657517
$V_{dd\sigma}$	−0.529629	$V_{dd\pi}$	2.424709
$V_{dd\delta}$	−1.064207	/	/

III. MAIN RESULTS

Geometry of HgTe quantum dot is shown in the Fig. 1. HgTe material has a zinc blende crystalline structure. It is easy to see that Hg and Te atoms are forming two interpenetrating face centered cubic crystal lattices, that are shifted by a quarter of the main diagonal along it. The unit cell of the crystal is characterized by tetraedal coordination where each atom of one type is surrounded by four atoms of second type, positioned as the vertex of a regular tetrahedron. For systems with a tetraedal coordination average number of valence electrons per atom is four, and a bond configuration is suitable for the case of two electrons per bond, which contributes to a strong covalent bond character that has been determined for such materials. The removing of central atom in a tetraedal coordination, leads to the breaking of covalent bonds, which corresponds to the situation of four unbound electrons. Surface atoms in the TB contribute to the formation of dangling bonds which typically can cause occurrence of edge states within the energy gap of the material.

In this paper we studied HgTe quantum dots. The dot is composed of 100 unit cells arranged inplane forming a square array. The lattice parameter is 6.453 Å, thus the size of square structure considered here is 6.453nm × 6.453 nm. Due to finite dimensions of the structure in the lateral plane, some edge atoms are connected with less than two neighbouring atoms. These are so called dangling atoms. They contribute to the edge states that are not in the focus of our intrest, so we removed them from the dot.

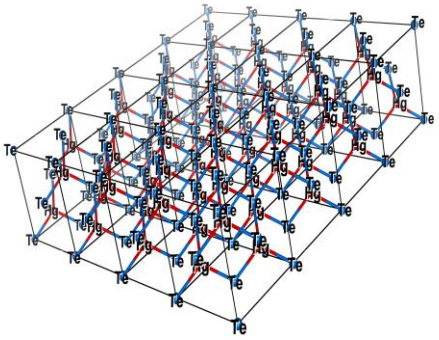

Fig. 1. Schematic view of a square shaped HgTe quantum dot. Due to better visibility we show 4×4 quantum dot that is smaller than analyzed.

The eigen-energies of square quantum dot considered here is shown in the Fig. 2. Each state represents one orbital from selected basis. Quantum dots are systems in which carriers are confined in all three spatial directions and because there is no *k*-space to be filled with electrons, all possible states exist as a discrete energy in Fig. 2. The zoom of eigenenergies in vicinity of the Γ point is shown on the insert in Fig. 2.

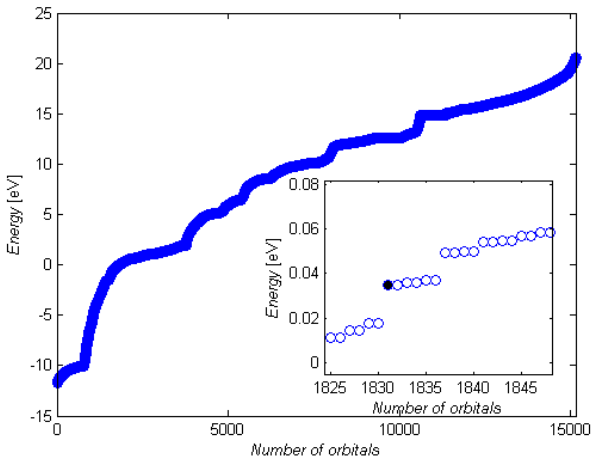

Fig. 2. Eigen-energies of square HgTe quantum dot with a total number of 100 unit cells. The insert in Fig. 2 shows eigenenergies around the Γ point.

We also want to visualize localization in a particulare energy state. Therefore, we plot real space probability as in Figs. 3 and 4. Here, the position of each atom in the figure is represented by blue circle. The probability is represented by a filled circle whose radius corresponds to amplitude of the probability density for finding the electron at a given atomic site. An example of the probability distribution for bulk and edge state are shown in Fig. 3 and Fig. 4, respectively. Both figures shown the distribution projected in the (x-y) plane, that is satisfying for thin sheets.

Fig. 3 show the probability distribution of finding an

electron in a low energy state at the top of the valence band. We note that distribution is elongated along the diagonal of the square quantum dot, that is due to anisotropy.

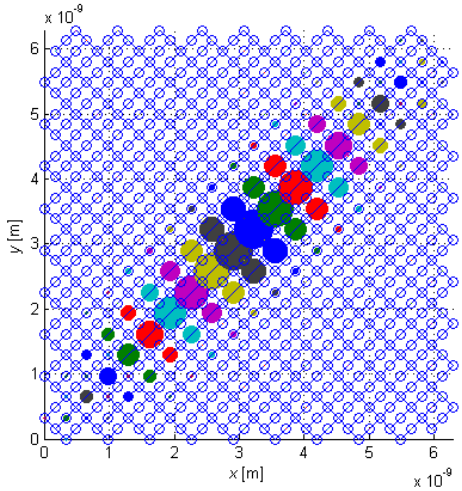

Fig. 3. The probability distribution for the state at the top of the valence band in HgTe square quantum dot.

The probability distribution for the edge state is displayed in Fig. 4. This state is closest to the state at the top of the valence band (marked by colored circle in the insert of Fig. 2). It is evident that this state is mostly localized near the square vertex point and along two edges that crosses creating the vertex. We found one more state with the same energy and localization. These two states show a distinct helical property, which means that they have opposite spin-polarization at the given edge. This is in accordance with Kramer's theorem which states that for every energy eigenstate of a time-reversal symmetric system with half-integer total spin, there is at least one more eigenstate with the same energy.

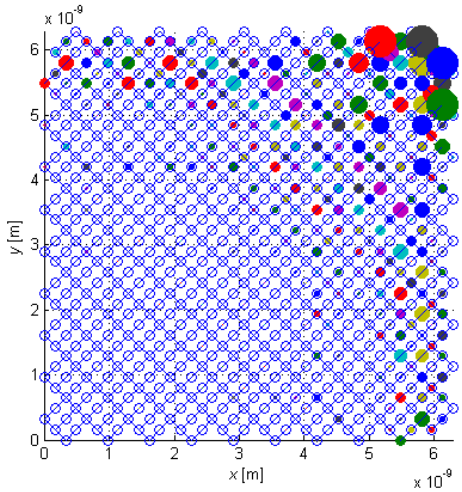

Fig. 4. The probability distribution for electron in the edge state in HgTe square quantum dot.

We found that the edge states are almost entirely composed of *p* orbitals. Their localization is mainly on the Te atoms that are positioned around the half of dots thickness. We may also note that the upper right vertex is wider than the other three. Due to this leack of symmetry, simmilar edge states that are localized in the lower left vertex have higher eigenenergies.

IV. Conclusion

We study the exotic quantum states in square shaped quantum dot. The dot is made from HgTe crystal that has inverted band structure. We show that topological edge states exist in this nanostructure. These states are mainly composed of Te *p* orbitals. The functionality of devices based on HgTe quantum dots may be controlled by applying external fields. Therefore, important aspect such as influence of an electric and magnetic fields in tuning electronic properties of these quantum dots will be part of our future work.

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References

[1] H. Zhu, C. A. Richter, E. Zhao, J. E. Bonevich, W. A. Kimes, H. J. Jang, H. Yuan, H. Li, A. Arab, O. Kirillov, J. E. Maslar, D. E. Ioannou and Q. Li, "Topological Insulator Bi_2Se_3 Nanowire High Performance Field-Effect Transistors", *Sci. Rep.*, vol. *3*, no. *1757*, pp. *1-5*. Apr., 2013.

[2] M. Ezawa, "Quantized conductance and field-effect topological quantum transistor in silicene nanoribbons", *App. Phys. Lett.*, vol. *102*, no. *172103*, pp. *1-5*. Apr., 2013.

[3] S. Cho, N. P. Butch, J. Paglione, and M. S. Fuhrer, "Insulating Behavior in Ultrathin Bismuth Selenide Field Effect Transistors", *Nano. Lett.*, vol. *11*, pp. *1925-1927*. Apr., 2011.

[4] F. Xiu, L. He, Y. Wang, L. Cheng, L. T. Chang, M. Lang, G. Huang, X. Kou, Y. Zhou, X. Jiang, Z. Chen, J. Zou, A. Shailos and K. L. Wang, "Manipulating surface states in topological nanoribbons", *Nat. Lett.*, vol. *6*, pp. *216-221*. Apr., 2011.

[5] J. Liu, T. H. Hsieh, P. Wei, W. Duan, J. Moodera and L. Fu, "Spin-filtered edge states with an electrically tunable gap in a two-dimensional topological crystalline insulator", *Nat. Mat.*, vol. *13*, no. *2*, pp. *178-183*. Feb., 2014.

[6] C.L. Kane and E.J. Mele, "Quantum Spin Hall Effect in Graphene", *Phys. Rev. Lett*, vol. *95*, no. *226801*, pp. *1-4*, Nov., 2005.

[7] Z. Wang, D. K. Ki, H. Chen, H. Berger, A. MacDonald, A. F. Morpurgo, "Strong interface-induced spin–orbit interaction in graphene on WS_2", *Nat. Commun*, vol. *6*, pp. *8339/1-7*, Sep., 2015.

[8] B.A. Bernevig, T.L. Hughes, S.C. Zhang, "Quantum spin Hall effect and topological phase transition in HgTe quantum wells", *Sci.*, vol. *314*, no. *5806*, pp.*1757-1761*, Dec., 2006.

[9] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X. L. Qi, S. C. Zhang, "Quantum spin hall insulator state in HgTe quantum wells", *Sci.*, vol. *318*, no. *5851*, pp. *766-770*, Nov., 2007.

[10] M. Graf and P. Vogl, "Quantum Spin Hall Effect in Inverted Type-II Semiconductors", *Phys. Rev. Lett.*, vol. *100*, no. *23*, pp. *236601/1-4*, Jun., 2008.

[11] L. Fu, and C. L. Kane, "Topological insulators with inversion symmetry", *Phys. Rev. B*, vol. *76*, no. *4*, pp. *045302/1-17*, Jul., 2007.

[12] D. Hsieh, L. Qian, Y. X. Wray, Y. S. Hor, R. J. Cava, and M. Z. Hasan, "A topological Dirac insulator in a quantum spin Hall phase", *Nature*, vol. *452*, pp. *970-974*, Apr., 2008.

[13] Y. Xia., D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava, and M. Z. Hasan, "Observation of a large-gap topological-insulator class with a single Dirac cone on the surface" *Nat. Phys.*, vol. *5*, no. *6*, pp. *398-402*, 2009.

[14] O. Marquardt, D. Mourad, S. Schulz, T. Hickel, G. Czycholl, and J. Neugebauer, "A comparison of atomistic and continuum theoretical approaches to determine electronic properties of GaN/AlN quantum dots", *Phys. Rev. B* vol. *78*, no. *23*, pp. *235302/1-9*, Dec., 2008.

[15] W. Beugeling, E. Kalesaki, C. Delerue, Y.-M. Niquet, D. Vanmaekelbergh and C. Morais Smith, "Topological states in multi-

orbital HgTe honeycomb lattices", *Nat. Commun*, vol. *6,* no. *6316*, pp. *1-7*, 2015.

[16] F. Bloch, "Uber die Quantenmechanik der Elektronen in Kristallgittern", *Z. Physik*, vol. *52*, no. *555*, pp. *555-600*, Aug., 1928.

[17] J. C. Slater and G. F. Koster, "Simplified LCAO Method for the Periodic Potential Problem", *Phys. Rev*, vol. *94*, no. *6*, pp. *1498-1524*. Jun., 1954.

[18] C. M. Goringe, D. R. Bowler and E Hernández, "Tight-binding modelling of materials", *Rep. Prog. Phys.*, vol. *60*, pp. *1447-1512*. Apr., 1997.

[19] G. Allan and C. Delerue, "Tight-binding calculations of the optical properties of HgTe nanocrystals", *Phys. Rev. B.*, vol. *86,* no. *16*, pp. *165437/1-6*., Oct., 2012.