A Letters Journal Exploring the Frontiers of Physics

August 2009

EPL, **87** (2009) 30002
doi: 10.1209/0295-5075/87/30002

www.epljournal.org

Holonomic quantum computation associated with a defect structure of conical graphene

K. Bakke, C. Furtado[(a)] and S. Sergeenkov

Departamento de Física, Universidade Federal da Paraíba - Caixa Postal 5008, 58051-970, João Pessoa, PB, Brazil

received 17 March 2009; accepted in final form 22 July 2009
published online 25 August 2009

PACS 03.67.Lx – Quantum computation architectures and implementations
PACS 73.22.-f – Electronic structure of nanoscale materials: clusters, nanoparticles, nanotubes, and nanocrystals

Abstract – A possibility of holonomic quantum computation based on the defect-mediated properties of graphite cones is discussed. Using a geometric description for the conical graphene, we demonstrate how one can construct the most important one-qubit quantum gates without invoking the adiabatic approximation. The control parameter which defines a particular qubit configuration is directly linked with the number of removed sectors in the graphene layer needed to create a particular conical configuration.

Introduction. – The idea of Holonomic Quantum Computation (HQC) is based on non-Abelian geometric phases [1], called holonomies [2,3]. The holonomies (the unitary transformations) have been proposed as quantum gates in many different implementations [4–13]. Recently, a feasible scheme for HQC realization in superconducting charge-phase qubits in a cavity has been suggested [14] which allows to implement a universal set of holonomic gates by modulating the corresponding experimentally controllable parameters.

Usually [5,6], in order to realize holonomic quantum gates, the adiabatic theorem needs to be taken into account. It means that the control parameters are chosen in the form adiabatically driven along the loops in the control manifold $\mathcal{M}$. These quantum gates are generated in the subspace C^N spanned on eigenvectors corresponding to the family of Hamiltonians $F=\{H(\lambda)=U(\lambda)H_0U^{\dagger}(\lambda);\lambda\in\mathcal{M}\}$, where $U(\lambda)$ is the unitary operator and λ is the control parameter [5,6].

The action of each quantum gate on one initial state $|\psi\rangle_{in}$ is described by the unitary operator U which brings it to a final state $|\psi\rangle_{out}=U|\psi\rangle_{in}$. This can be viewed in the following way [15]:

$$|\psi\rangle_{out}=e^{-iE_0t}\,\Gamma_A\,(C)\;|\psi\rangle_{in}, \tag{1}$$

where the first factor is the dynamical phase (which can be omitted if we redefine the energy levels by taking $E_0=0$). The second factor is the holonomy, $\Gamma_A(C)\in U(n)$ [3,5,6].

In this paper we follow the approach suggested by Aharonov and Anandan [16] based on calculation of the phase change of the wave function without adiabatic approximation. We shall consider all cyclic evolutions that can influence the phase change. As we shall show, the phase acquired by the wave function can be obtained via the holonomy directly, using the three-dimensional metric for the defect-mediated conical graphene. As a result, the holonomies associated with the conical graphene can be viewed as quantum logical gates for the most recognizable one-qubit configurations.

Recall that the phase change obtained by Aharonov and Anandan [16] is given by

$$\beta=\int_0^{\tau}\left\langle\tilde{\psi}\right|i\frac{\mathrm{d}}{\mathrm{d}t}\left|\tilde{\psi}\right\rangle\mathrm{d}t \tag{2}$$

with $|\tilde{\psi}\rangle=U|\psi\rangle$. Notice that in the above expression the phase β is independent of the Hamiltonian H for a given closed curve C.

The holonomy, Γ_A, is defined by the following expression:

$$\Gamma_A\,(C)=P\,\exp\!\left(\oint\Lambda_\mu\mathrm{d}x^\mu\right), \tag{3}$$

where P denotes the path ordering and Λ_μ is the gauge potential. In what follows, we propose how to realize one-qubit gates for a graphite cone using these holonomies. Notice that the connection of (3) comes from a similar relation to Aharonov-Anandan connection (2) where the projective space is the degenerate subspace of the Hamiltonian of the system.

[(a)] E-mail: furtado@fisica.ufpb.br

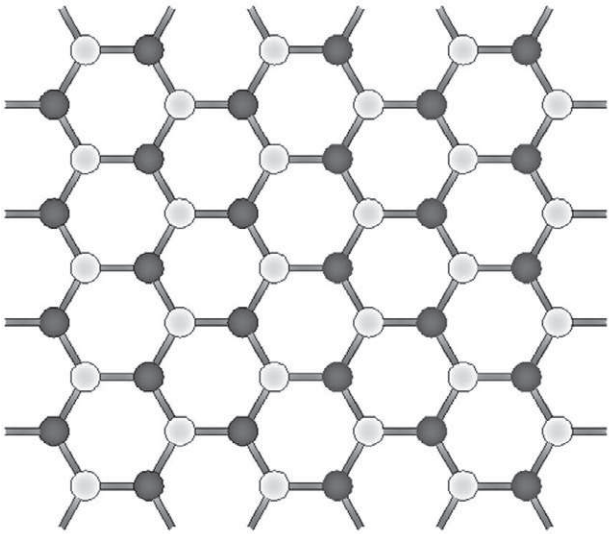

Fig. 1: Defect-free graphene lattice.

Topological defects in graphene. – The band of conduction of the graphene, which consists of a graphite layer, can be described by the tight-binding model. It is a two-dimensional material formed by an isolated layer of carbon atoms arranged in a honeycomb-like lattice (see fig. 1). In this context, the Fermi surface reduces to two **K**-points located in the Brillouin zone. In the low-energy limit, the graphene properties can be described by the free fermions theory [17] within a continuum model based on the Dirac equation [18,19]. Namely, in the absence of interactions (and in the above-mentioned limit), the Hamiltonian of the system reads

$$H_0 = -i\hbar v_f \left(\sigma^x \partial_x + \sigma^y \partial_y\right). \tag{4}$$

Here, σ^i are the Pauli spin matrices (acting on the A/B labels) and v_f is the Fermi velocity. The corresponding states of this system are labeled by the direction of the wave vector $\mathbf{K}$ and the index A or B for the sublattices. We represent these states as $|\mathbf{K}_\pm, A\rangle$ and $|\mathbf{K}_\pm, B\rangle$. Note that the Fermi level space is four-dimensional. So we can choose these states as a basis considering that $\mathbf{K}_- = -\mathbf{K}_+$ with the x axis being along $\mathbf{K}_+$. Thus, the above-introduced Hamiltonian describes transfer of an electron only from A sublattice to B sublattice and *vice versa*.

Recently, a number of papers [18–21] investigated the influence of topological defects in graphene layers on the transport properties of graphene. Topological defects in graphene can be conceptually generated by a "cut and glue" process, known in the literature as the Volterra process. If one cuts a $\pi/3$ sector and glues the opposite sides (as it is shown, *e.g.*, in [21,22]), one obtains two equations that can be interpreted in terms of the fluxes of fictitious gauge fields through the apex of the cone. One of them measures the angular deficit of the cones when a vector is transported in parallel around the apex and is generated by the variation of the local reference frame. The flux produced by this part acts only on A/B labels defined earlier and it reads [21,22]

$$\oint \omega_\mu \, \mathrm{d}x^\mu = -\frac{\pi}{6}\sigma^z, \tag{5}$$

while the second part, which is called the K spin flux and which mixes $\mathbf{K}_+$ and $\mathbf{K}_-$ components, gives

$$\oint A_\mu \, \mathrm{d}x^\mu = \frac{\pi}{2}\tau^y \tag{6}$$

It is important to note that τ^i are the Pauli matrices which act only on the $\mathbf{K}_\pm$ space.

By removing a $\pi/3$ sector of the lattice and gluing the edges we form a pentagon in the structure. In this way, the lattice acquires a conical geometry where the apex is characterized by the presence of a pentagon. In particular, this type of geometry has been studied in a gravity context where it is believed to be produced by cosmic strings [23] in the early universe. In condensed matter, the topological defect created by inserting or removing an angular sector is called disclination (this defect introduces curvature in the media [24]). In such a way, the presence of a pentagon (heptagon) introduces a locally positive (negative) curvature in the graphene layer [25,26]. To study the electronic properties due to the presence of a topological defect in graphene, it is natural to formulate the Dirac equation in curved space induced by this defect. The conical graphene leaves are described by the three-dimensional metric in the continuum approximation

$$\mathrm{d}s^2 = \mathrm{d}t^2 - \mathrm{d}\rho^2 - \alpha^2\rho^2\mathrm{d}\phi^2, \tag{7}$$

where α is the deficit or excess angle related to the angular sector λ (which is the sector that is removed or inserted to form the defect) as $\alpha = 1 \pm \lambda/2\pi$. We also can relate the deficit/excess angle to the number of sectors removed from the graphite monolayer in the following way:

$$\alpha = 1 - \frac{n_\Omega}{6}. \tag{8}$$

The values of α in the interval $0 < \alpha < 1$ ($1 < \alpha < \infty$) mean that we remove a sector from (insert a sector in) the leaf to form the defect. It is worth noting that eq. (7) also characterizes the geometry of a cosmic string in the two-dimensional space [27].

Let us now construct the holonomies associated with the two-dimensional metric of conical graphene. The corresponding holonomy is given by

$$U(C) = P\exp\left(-\oint \Gamma_\mu(x)\,\mathrm{d}x^\mu\right), \tag{9}$$

where $\Gamma_\mu(x)$ is the so-called spinorial connection. We can calculate the spinorial connection by defining a local reference frame at each point along the closed curve. The

local reference frame can be expressed via the tetrads as follows:

$$g_{\mu\nu}\left(x\right)=\eta_{ab}\,e_{\mu}^{a}\,e_{\nu}^{b}, \tag{10}$$

where the Greek indices run $\mu=t,\rho,z,\phi$ and Latin indices run $a=0,1,2,3$. In turn, the tetrads obey the following conditions:

$$e_{\mu}^{a}\,e_{b}^{\mu}=\delta_{b}^{a},\qquad e_{a}^{\mu}\,e_{\nu}^{a}=\delta_{\nu}^{\mu}. \tag{11}$$

To satisfy the above conditions, we can choose our tetrads as follows:

$$e_{\mu}^{a}=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\varphi & -\alpha\rho\sin\varphi\\ 0 & \sin\varphi & \alpha\rho\cos\varphi\end{pmatrix}. \tag{12}$$

The inverse tetrads read

$$e_{a}^{\mu}=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\varphi & \sin\varphi\\ 0 & -\frac{\sin\varphi}{\alpha\rho} & \frac{\cos\varphi}{\alpha\rho}\end{pmatrix}. \tag{13}$$

With the above-defined local reference frame, we can introduce the spinorial connection in the standard way [28]:

$$\Gamma_{\mu}\left(x\right)=\frac{i}{4}\omega_{\mu ab}\,\Sigma^{ab}=-\frac{1}{8}\omega_{\mu ab}\left[\gamma^{a},\gamma^{b}\right], \tag{14}$$

where the Dirac matrices γ^{a} are reduced in our case to the Pauli matrices, $\gamma^{a}=\sigma^{a}$. The term $\omega_{\mu b}^{a}$ is the one-form or spin connection which is obtained by the variation of the local reference frame along the curve, δe_{μ}^{a}. Namely

$$\omega_{\mu b}^{a}=-e_{\beta}^{a}\left(\partial_{\mu}e_{b}^{\beta}+\Gamma_{\mu\nu}^{\beta}\,e_{b}^{\nu}\right), \tag{15}$$

where $\Gamma_{\mu\nu}^{\alpha}$ are the Christoffel symbols.

Now we can obtain the expression for two non-zero spin connections for the metric $\omega_{\phi1}^{2}=-\omega_{\phi2}^{1}=1-\alpha$. The resulting spinorial connection reads

$$\Gamma_{\phi}=\frac{i}{2}\,\left(1-\alpha\right)\,\sigma^{3}. \tag{16}$$

The holonomy matrix, $U_1(C)$, that stands for parallel transport of a spinor along a path C around the cone is

$$\begin{aligned}U_{1}(\alpha)\;&=\;\cos\left[\left(1-\alpha\right)\pi\right]+i\sigma^{z}\sin\left[\left(1-\alpha\right)\pi\right]\\ &=\;\cos\left(\frac{n_{\Omega}}{6}\pi\right)+i\sigma^{z}\sin\left(\frac{n_{\Omega}}{6}\pi\right).\end{aligned} \tag{17}$$

This expression gives the quantum phase acquired by the wave function when it is parallel transported around the symmetry axis of the topological defect (see fig. 2). The expression (17) is sufficient to construct a one-qubit gate without specification of the taken path.

The second holonomy matrix associated with the graphene was earlier considered by Lammert and Crespi [20,21]. They assumed that the gauge transformation on the K spin part is a rotation about the 2-axis. This transformation takes into account the exchange between A and B sublattices when the $\pi/3$ sector is removed and the opposite sides are glued together. The final expression for this holonomy matrix reads [20,21]

$$U_{2}\left(n_{\Omega}\right)=T_{l-m}\,\left(\cos\left(\frac{n_{\Omega}}{2}\pi\right)-i\,\tau^{y}\,\sin\left(\frac{n_{\Omega}}{2}\pi\right)\right). \tag{18}$$

Here T_{l-m} corresponds to the translation of the lattice vector (l,m) acting on Bloch states (which depends only on $n-m$ (mod3)) while the Pauli matrix τ^{y}, in the expression (18), acts on the $\mathbf{K}$ part of the spinor component. The term T_{l-m} gives us two different expressions for the quantum flux in the $\mathbf{K}$ spin part, corresponding to either $l=m$ or $l\neq m$. Let us rewrite the above expressions in terms of the control parameter α. We have

$$U_{2}(\alpha)=\cos(3\pi(1-\alpha))-i\tau^{y}\sin(3\pi(1-\alpha)) \tag{19}$$

for $l=m$ and

$$U_{2}(\alpha)=e^{-i\frac{\pi}{6}\sigma^{3}}\left[\cos\left(3\pi\left(1-\alpha\right)\right)-i\tau^{y}\sin(3\pi(1-\alpha))\right] \tag{20}$$

for $l\neq m$, respectively.

Graphene quantum gates. – We suggest to realize one-qubit quantum gates based on graphene cones through the appropriate choice of the control parameter α within the range $0<\alpha<1$. This can be done by removing a number of sectors in the graphene layer. For example, if we want to construct a quantum gate using the holonomy $U_1(\alpha)$, we need a configuration with the holonomy $U_2(\alpha)$ given by (19) or (20) be equal to the identity matrix. On the other hand, if we want to construct a quantum gate using the holonomy $U_2(\alpha)$, we need to impose the condition $U_1(\alpha)=1$. We can obtain the first configuration by taking the value of α that gives an even number of removed sectors in the construction of the graphene cone between two graphene slices without defects. The second configuration is obtained by the application of the so-called multicones [27] where we take two cones: one that has the flux (5) and the other with the opposite flux. The first flux is given by a cone that was made by removed sectors, while the second flux is created by the excess of sectors between two graphene slices without defects.

However, in order to realize the holonomic quantum computation in graphene, first of all we need to establish the logical space. Since the Fermi level space is four-dimensional, we can introduce the following two-component logical states:

$$\begin{aligned}\left|0_{L}\right\rangle&=\left|\mathbf{K}_{+},A/B\right\rangle,\\ \left|1_{L}\right\rangle&=\left|\mathbf{K}_{-},A/B\right\rangle,\end{aligned} \tag{21}$$

assuming that the σ^{i} matrices act on the A/B sublattices of the logical states as $I\otimes\sigma^{i}$ (with I being the 2×2 identity matrix) providing a phase shift according to the electron transfer between the A and B sublattices, while the τ^{i} matrices act on the $\mathbf{K}$-spin part of the logical states as $\tau^{i}\otimes I$ providing the mixing between the $\mathbf{K}_{+}$ and $\mathbf{K}_{-}$

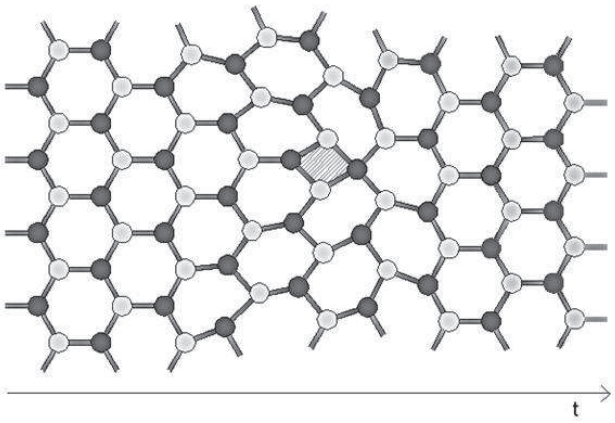

Fig. 2: Phase-shift gate $\mathcal{Q}_2$, given by expression (23), constructed with a cone of graphene with two removed $\pi/3$ sectors (shown in gray). We can see how the presence of defect distorts the lattice of the graphene. The arrow indicates the direction of motion of the electron when it passes around the topological defect.

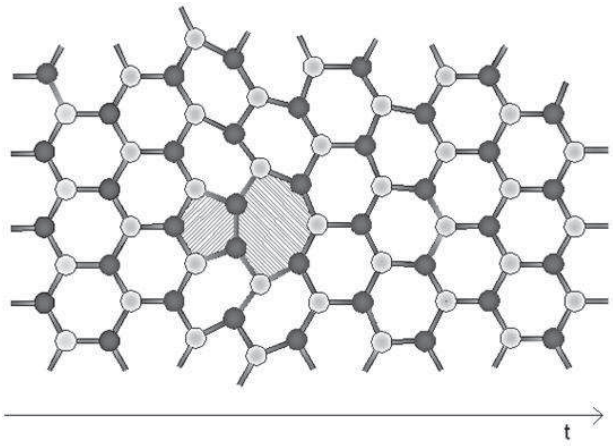

Fig. 3: The swap and phase quantum gate: one cone constructed with one sector removed and other cone with one sector inserted. The net result is identical to the behavior of multicones where the fluxes of the cones cancel each other. The arrow indicates the direction of the motion of an electron which passes around the multicone.

Fermi points. Since σ^i and τ^i related logical subspaces do not interfere with each other, no information leakage is expected in the qubits suggested here.

The first case where we build a one-qubit quantum gate corresponds to the choice of the control parameter $\alpha = 1/3$ with $l = m$. In this case we obtain $U_2(1/3) = 1$ and the associated one-qubit quantum gate is given by

$$\mathcal{Q}_1 = U_1\left(1/3\right) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\frac{4\pi}{3}} \end{pmatrix}. \tag{22}$$

Likewise, if we choose $\alpha = 2/3$ with $l = m$, we obtain

$$\mathcal{Q}_2 = U_1\left(2/3\right) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\frac{2\pi}{3}} \end{pmatrix}, \tag{23}$$

which is another one-qubit phase-shift gate, up to a global phase. Notice that this quantum gate does not change the Fermi points, but it provides a phase shift in the logical states (21) depending on the transfer of one electron between the sublattices A and B.

Observe that the phase gate $\mathcal{Q}_1$ requires that $n_\Omega = 4$ sector of the graphene layer be removed before the cone is constructed, while $\mathcal{Q}_2$ phase gate realization requires removal of $n_\Omega = 2$ sector. Figure 2 shows the graphene layer with a conical defect (disclination) corresponding to removal of two $\pi/3$ sectors.

The second case is the choice of the control parameter $\alpha = 5/6$ with $l = m$. Now we want to use two cones of graphene with opposite fluxes between two graphene slices. As was pointed out in [27], the behavior of these cones is identical to the behavior of multicones when we have $n_\Omega^{eff} = \sum_{i=1}^{m} n_\Omega^i$ for the number of removed sectors. The formation of this topological defect in the graphene layer is depicted in fig. 3, where we have a dipole of conical defects forming a dislocation (pentagon-heptagon pair) [26]. In this case, the associated one-qubit quantum gate is given by (using the notation of [29])

$$\mathcal{Q}_S = U_2\left(5/6\right) = e^{-i\frac{\pi}{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{24}$$

It represents swap and phase quantum gate that acts on both logical states (21) by changing the $\mathbf{K}_\pm$ Fermi points and providing a phase shift.

Hence, the swap and phase gate can be realized if we construct the cone after the removal of $n_\Omega^{eff} = 1$ sectors from graphene layer (up to a global phase factor of $\pi/2$). If we choose $\alpha = 1/2$, we obtain the same quantum gate but with $n_\Omega^{eff} = 3$ removed sectors. Likewise, if we choose $\alpha = 1/6$, the corresponding quantum gate is obtained with $n_\Omega^{eff} = 5$ removed sectors (up to a global phase factor of $-\pi/2$).

The third case is related to situations when $l \neq m$. Let us take $\alpha = 1/3$ as an example. The quantum gate associated with this choice is given by

$$\mathcal{Q}_z = e^{-i\frac{\pi}{6}\sigma^3} U_1\left(1/3\right) = e^{i\frac{\pi}{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{25}$$

and represents an analog of the Z-Pauli gate [29], up to a global phase factor. Notice that this quantum gate acts on the logical basis (21) which depends on the transfer of one electron between the sublattices A and B, but it does not change the Fermi points.

This quantum gate can be built with one cone of graphene between two slices of graphene without defects where $n_\Omega = 4$ sectors were removed (up to a global phase factor of $\pi/2$). As expected, if we take $\alpha = 2/3$, we obtain the same quantum gate but with $n_\Omega = 2$ removed sectors in the cone. This quantum gate is identical to the phase gate $\mathcal{Q}_2$ shown in fig. 2.

Conclusion. – We have suggested a possibility to realize one-qubit gates for a holonomic quantum computer associated with defect-mediated properties of conical graphene. The feasibility and implementation of the construction suggested here is based on the realistic possibility to incorporate topological defects (disclinations and dislocations) into the graphene structure in a controllable way [30,31] allowing to modify the geometric properties of the layers needed to create specific quantum gates. For each cone or multicones in the graphene layer, there is a specific quantum phase acquired by the wave function of moving particles which encircles the topological defect. This quantum phase is equivalent to the Aharonov-Anandan quantum phase [16] and provides the realization of the elementary one-qubit quantum gates without using the adiabatic approximation for the implementation of the holonomic quantum computation [2,3]. The control space $\mathcal{M}$ becomes the structure of the topological defect inserted in the graphene monolayer (which is, in this case, a disclination represented by the control parameter α). More precisely, the control parameters governing the qubit operations have been linked with the number of removed sectors n_Ω in the graphene monolayer needed to create a specific conical configuration. In particular, we have shown that a graphite cone with $n_\Omega = 4$ removed sectors is equivalent to a phase-shift gate. By combining different defect structures in graphene layers, we managed to construct the so-called Z-Pauli and swap and phase quatum gates. However, to obtain a universal set of quantum gates in this approach, we need to construct a two-qubit gates. We hope to report on this possibility in a future paper.

* * *

This work was partially supported by PRONEX/ FAPESQ-PB, FINEP, CNPq, CAPES and CAPES/ PROCAD.

REFERENCES

[1] Wilczek F. and Zee A., *Phys. Rev. Lett.*, **52** (1984) 2111.

[2] Zanardi P. and Rasetti M., *Phys. Lett. A*, **264** (1999) 94.

[3] Pachos J., Zanardi P. and Rasetti M., *Phys. Rev. A*, **61** (2000) 010305R.

[4] Unanyan R. G., Shore B. W. and Bergmann K., *Phys. Rev. A*, **59** (1999) 2910.

[5] Pachos J. and Chountasis S., *Phys. Rev. A*, **62** (2000) 052318.

[6] Pachos J., *Phys. Rev. A*, **66** (2002) 042318.

[7] Faoro L., Siewert J. and Fazio R., *Phys. Rev. Lett.*, **90** (2003) 028301.

[8] Li Y., Zhang P., Zanardi P. and Sun C. P., *Phys. Rev. A*, **70** (2004) 032330.

[9] Cholascinski M., *Phys. Rev. B*, **69** (2004) 134516.

[10] Fuentes-Guridi I., Girelli F. and Livine E., *Phys. Rev. Lett.*, **94** (2005) 020503.

[11] Zhang P., Wang Z. D., Sun J. D. and Sun C. P., *Phys. Rev. A*, **71** (2005) 042301.

[12] Florio G., Facchi P., Fazio R., Giovannetti V. and Pascazio S., *Phys. Rev. A*, **73** (2006) 022327.

[13] Zhang X. D., Zhang Q. and Wang Z. D., *Phys. Rev. A*, **74** (2006) 034302.

[14] Zhi-Bo Feng and Xin-Ding Zhang, *Phys. Lett. A*, **372** (2008) 1589.

[15] Lloyd S., *Phys. Rev. Lett.*, **75** (1995) 346.

[16] Aharonov Y. and Anandan J., *Phys. Rev. Lett.*, **58** (1987) 1593.

[17] Di Vincenzo D. P. and Mele E. J., *Phys. Rev. B*, **29** (1984) 1685.

[18] Gonzales J., Guinea F. and Vozmediano M. A. H., *Phys. Rev. Lett.*, **69** (1992) 172.

[19] Gonzales J., Guinea F. and Vozmediano M. A. H., *Nucl. Phys. B*, **406** (1993) 771.

[20] Lammert P. E. and Crespi V. H., *Phys. Rev. Lett.*, **85** (2000) 5190.

[21] Lammert P. E. and Crespi V. H., *Phys. Rev. B*, **69** (2004) 035406.

[22] Pachos J. K. and Stone M., *Int. J. Mod. Phys. B*, **21** (2007) 5113.

[23] Vilenkin A., *Phys. Rep.*, **121** (1985) 263.

[24] Nelson D. R., *Defects and Geometry in Condensed Matter Physics* (Cambridge University Press) 1982.

[25] Cortijo A. and Vozmediano M. A. H., *EPL*, **77** (2007) 47002.

[26] Cortijo A. and Vozmediano M. A. H., *Nucl. Phys. B*, **763** (2007) 293.

[27] Furtado C., Moraes F. and Carvalho A. M. de M., *Phys. Lett. A*, **372** (2008) 5368.

[28] Nakahara M., *Geometry, Topology and Physics* (Institute of Physics Publishing, Bristol) 1998.

[29] Nielsen M. A. and Chuang I. L., *Quantum Computation and Quantum Information* (Cambridge University Press) 2000.

[30] Ewels C. P., Heggie M. I. and Briddon P. R., *Chem. Phys. Lett.*, **351** (2002) 178.

[31] Capio A., Bonilla L. L., de Juan F. and Vozmediano M. A. H., *New J. Phys.*, **10** (2008) 053021.