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# Thermal entanglement between $\pi$-electrons in silicene and photons; occurrence of phase transitions

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ABSTRACT

In this article, the thermal entanglement between $\pi$-electronic states in a monolayer silicene sheet and a single mode quantized electromagnetic field is investigated. We assume that the system is in thermal equilibrium with the environment at a temperature $T$, so that the whole system is described by the Boltzmann distribution. Using the states of total Hamiltonian, the thermal density matrix and, consequently, its partially transposed one is computed, giving rise to the determination of negativity. Our analytical calculations, along with representative figures, show that the system is separable at zero temperature, exhibits a maximum, at a specific temperature, and asymptotically vanishes. Along these lines we also report the effects of electron–photon coupling, as well as the silicene buckling, on the entanglement. Specifically, we demonstrate that the maximal value of entanglement is larger for stronger electron–photon coupling, while it decreases for larger buckling effect. Moreover, we show that the gap in the total energy spectrum remains intact for any value of the buckling parameter. There is, however, one state whose energy changes sign, at a specific buckling, indicating a change of phase.



## 1. Introduction

Quantum entangled states have been recognized as the milestone of quantum information processing, especially, quantum teleportation, quantum computation, quantum cryptography [1–6]. In this respect, it is desirable that the states participating in the entanglement should naturally posses long relaxation time and length [7,8], to preserve the information placed on it. As a result, one seeks an entity, with limited number of states, which fulfills such requirements. Moreover, for practical purposes in quantum information processing, it is essential to explore entanglement in solid materials [9,10]. To this end, the electronic states in nanostructures, particularly, honeycomb materials, have been proposed as most suitable for the generation and, in turn, characterization of entanglement [11–14]. Meanwhile, it is also of advantage that the stored information be transferred with highest possible speed. Motivated by these facts, the composite system of $\pi$-electrons in graphene or silicene *and* single-mode photons has attracted immense interest [15–17]. In the present article, therefore, we report an extensive investigation of entanglement between the $\pi$-electronic states in *silicene* and photons. The novel idea of our investigation is the fact that the whole system is assumed to be at thermal equilibrium with a heat reservoir, so that the electronic, as well as photonic, states occur according to the Boltzmann distribution.

The technical process of synthesizing silicene, a honeycomb monolayer of silicon atoms, has by now been well established and advanced that research on the properties of silicene has become the subject of enormous reports [18–20]. Even though most of the delicate features (such as long relaxation time and length [7,8], to name a few) of graphene, a honeycomb monolayer of carbon atoms, may be straight forwardly transferred to silicene, they drastically differ in one aspect. In silicene, as opposed to graphene, the so-called "$A$" and "$B$" sublattices are shifted relative to each other, giving rise to the buckling effect [21,22]. A profound consequence of the buckling effect is the fact that it breaks the space inversion symmetry and, as a result, a quantum mechanical change of phase may be anticipated [23–25]. Recalling the fact that the buckling effect can be externally controlled, one also expects that the degree of entanglement between $\pi$-electronic and photonic states can also be externally controlled. Moreover, there exists an intrinsic spin-orbit coupling, much larger than that in graphene [26], which manifests itself in the intrinsic generation of quantum spin Hall effect [27]. Since the spin-orbit coupling involves the sublattices operators, it also affect the energy band structure, consequently, the behavior of entanglement. In what follows, therefore, we con-

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sider the interaction of a single mode, plane-polarized quantized electromagnetic field with $\pi$-electrons in silicene and report the properties of photon–electron *thermal* entanglement, in which the states involved obey the Boltzmann distribution.

To accomplish our goal, we first present the governing Hamiltonian and discuss the commuting Casimir operator that we introduced in [28]. The Hamiltonian, expressed in the bases of the latter, is then block-diagonal and thus the total energy eigenvalues, from which the thermal density operator is constructed, are calculated straightforwardly. An illustration of the energy spectrum versus the buckling parameter reveals that, in spite of the interaction with photons, there exists an energy state which changes sign at some value of the buckling parameter, giving rise to a quantum phase transition [23–25]. Furthermore, we employ the concept of negativity to determine the temperature-dependent degree of entanglement between the $\pi$-electrons and photons. To this end, a partial transposition of the thermal density matrix is made and the negative eigenvalues of the result are calculated. Consequently, we demonstrate that the system is separable at absolute zero temperature, but reaches a maximal entanglement and asymptotically becomes separable again as the temperature rises. A noteworthy point in the behavior of negativity is that for low buckling parameter and at extremely low temperature, a minute change in the latter results a rapid increase in the entanglement, confirming the quantum phase change.

This article is organized as follows. In the next section, after presenting the system Hamiltonian, we employ the bases of the Casimir operator introduced in [28] to calculate and discuss the states of the system. Section 3 is devoted to the construction of the thermal density operator from the Boltzmann distribution, followed by the manner of partial transposing it. The procedure of calculating the negative eigenvalues of the partially transposed density matrix along with a discussion of negativity are also the subject of this section. In Sec. 4 we explicitly compute the negativity for the system in hand, illustrating its behavior versus temperature and (or) the buckling parameter (electron–photon coupling). The more important findings of our report are highlighted in the concluding section.

## 2. The model

The present section is devoted to a brief review of the system's total Hamiltonian and its diagonalization. In the following section the eigenvalues and eigenstates so obtained shall be employed to construct the thermal density operator. The total Hamiltonian of $\pi$-electrons in a silicene sheet, interacting with a single mode, plane-polarized quantized electromagnetic field of frequency $\omega$, reads [29,30],

$$H = \alpha\tau(\sigma_+ a + \sigma_- a^\dagger) + (\lambda_{SO}\tau\, s_z - \Delta_z)\sigma_z + \hbar\omega\, a^\dagger a. \tag{1}$$

In writing Eq. (1) it is assumed that the silicene sheet defines the $x$–$y$ plane while the vector potential (quantized) is taken as, $\vec{A} = \sqrt{\frac{\hbar}{2\varepsilon_0 V\omega}}(a + a^\dagger)\hat{x}$, with $a^\dagger$ ($a$) being the photonic creation (annihilation) operator. The fact that free $\pi$-electrons behave as Dirac particles propagating at Fermi speed, $v_f$ ($\simeq 5\times 10^5 \frac{m}{s}$ in silicene [29]) is implicit in Eq. (1). Moreover, the operators in Eq. (1) are pseudospin, $\vec{\sigma}$ (acting upon the sublattice states, $|A(B)\rangle$ with the ladder operators $\sigma_\pm = |A(B)\rangle\langle B(A)|$), spin, $\vec{s}$ (acting upon the spin states $|+(-)\rangle$ with the ladder operators $s_\pm = |+(-)\rangle\langle -(+)|$), and valley, $\vec{\tau}$ (acting upon the valley states $|K'(K)\rangle$ with the ladder operators $\tau_\pm = |K'(K)\rangle\langle K(K')|$). The first term in Eq. (1) describes the electron–photon interaction with a strength, $\alpha = e v_f \sqrt{\frac{\hbar}{2\varepsilon_0 V\omega}}$ ($e$ and $V$ denote the electronic charge and electromagnetic field quantization volume, respectively) while the second term, frequently known as the mass term, consists of spin-orbit coupling at different valley sites with a strength of $\lambda_{SO}$ ($= 3.9$ to $7.9$ meV [31]) and the buckling effect through $\Delta_z$. As is well known the latter, with a direct influence on electron–photon entanglement, may be externally varied from vanishingly small values up to $2\lambda_{SO}$ [31]. It is also in order to mention the fact that Eq. (1) is valid only at the Dirac points and under the rotating-wave approximation. The combined Hilbert space is thus swept by the basis, $|A(B)\rangle \otimes |n\rangle \otimes |K(K')\rangle \otimes |\pm\rangle \doteq |A(B), n, K(K'), \pm\rangle$, where $n$ defines the photonic Fock states. The matrix representation of the Hamiltonian of Eq. (1) in these bases is evidently of infinite dimensions, but reducible. The Hamiltonian may be reduced by noting that the operators,

$$\hat{N}_e = a^\dagger a + \sigma_+\sigma_- + s_+ s_- + \tau_+\tau_- \tag{2}$$

and,

$$\hat{N}_{s\tau} = s_+ s_- + \tau_+\tau_-, \tag{3}$$

commute with each other and the total Hamiltonian, so that they form the constants of motion. Physically, $\hat{N}_e$ with eigenvalue $N_e$ gives the total excitations in the system while $\hat{N}_{s\tau}$ with eigenvalues $N_{s\tau}$ indicate the sum of spin and valley excitations. To this end, we have assigned the values one (zero) to sublattice $|A\rangle$ ($|B\rangle$), spin up (down) state and valley state $|K'\rangle$ ($|K\rangle$). The Hamiltonian is block diagonal with respect to the eigenvalues ($= N_e$) of $\hat{N}_e$ which then limits the valley and spin states appearing in each block. The eigenvalues of $\hat{N}_{s\tau}$ are clearly $N_{s\tau} = 0, 1$ and $2$ with the condition that $N_{s\tau} \leq N_e$. The first block corresponds to $N_e = 0$ is $1\times 1$ with one basis $|B, 0, K, -\rangle$, while for $N_e = 1$ it is $4\times 4$ with four bases, $|B(A), 1(0), K, -\rangle$ and $|B, 0, K(K'), +(-)\rangle$. This block consists of two $2\times 2$ subblocks corresponding to the eigenvalues, $N_{s\tau} = 0, 1$. The next block corresponds to $N_e = 2$ and is a $7\times 7$ matrix with the bases, $|B(A), 2(1), K, -\rangle$, $|B(A), 1(0), K, +\rangle$, $|B(A), 1(0), K', -\rangle$ and $|B, 0, K', +\rangle$. This block consists of one $1\times 1$ and three $2\times 2$ subblocks. For total excitations larger than 2, the blocks are all $8\times 8$, comprising of four $2\times 2$ subblocks, formed by the bases, $|B, n, K, -\rangle$, $|A, n-1, K, -\rangle$, $|B, n-1, K, +\rangle$, $|A, n-2, K, +\rangle$, $|B, n-1, K', -\rangle$, $|A, n-2, K', -\rangle$, $|B, n-2, K', +\rangle$ and $|A, n-3, K', +\rangle$. The band structure of the system is obtained by diagonalizing of a number of $2\times 2$ matrices and two diagonal elements related to the two $1\times 1$ blocks. The number of total excitations characterizes the number of $2\times 2$ matrices.

Despite the fact that we have obtained analytical expressions for the eigenvalues and eigenstates of the total Hamiltonian, for brevity we avoid stating the results here. The corresponding identity operator reads,

$$\sum_{N_e=0}^{2}\sum_{i=1}^{3N_e+1} |\psi_{N_e,i}\rangle\langle\psi_{N_e,i}| + \sum_{N_e=3}^{\infty}\sum_{i=1}^{8} |\psi_{N_e,i}\rangle\langle\psi_{N_e,i}| = 1, \tag{4}$$

where $|\psi_{N_e,i}\rangle$ are the eigenvectors of the total Hamiltonian and each block is labeled by the subscript $i$. In the following section we utilize the eigenstates and the eigenvalues of the total Hamiltonian of Eq. (1), expressed as the identity in Eq. (4), to calculate the thermal density operator and consequently the negativity.

## 3. Thermal density operator; the negativity

The mixed state of a system in equilibrium with a heat reservoir at a temperature T is given by the thermal density operator,

$$\rho = \frac{-\beta H}{Z}, \tag{5}$$

where $Z = \sum_{N_e=0}^{2}\sum_{i=1}^{3N_e+1} e^{-\beta E_{N_e,i}} + \sum_{N_e=3}^{\infty}\sum_{i=1}^{8} e^{-\beta E_{N_e,i}}$ is the partition function and $\beta^{-1} = K_B T$, with $K_B$ the Boltzmann constant, is the thermal energy. Using the identity of Eq. (4), the thermal density operator becomes,