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Electronic structure and the minimum conductance of a graphene layer on SiO₂ from density functional methods

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Abstract

The effect of the SiO₂ substrate on a graphene film is investigated using realistic but computationally convenient energy-optimized models of the substrate supporting a layer of graphene. The electronic bands are calculated using density functional methods for several model substrates. This provides an estimate of the substrate charge effects on the behaviour of the bands near E_F , as well as the local variation of the Fermi energy of the graphene sheet. A model of a wavy graphene layer positioned on the substrate is used to help understand the nature of the minimum conductance of graphene.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Ideal graphene is a two-dimensional (2D) sheet of carbon atoms arranged on a honeycomb lattice. Given the already rich physics of graphene, a tremendous effort is being focused on its basic physics as well as its technological applications [1–3]. These include applications based on carbon nanotubes [4, 5], or structures based on graphene itself [6, 7]. Unlike carbon nanotubes (CNTs) which may be semiconducting or metallic, pure graphene is a 2D zero-gap material having electron and hole mobilities similar to those of CNTs [7]. The honeycomb structure with two C atoms per unit cell has two degenerate Fermi points at the \mathbf{K} and \mathbf{K}' points of the hexagonal Brillouin zone. The conduction and valence bands touch at the Fermi points, with linear energy dispersion, implying a zero-mass Dirac–Weyl (DW) spectrum for very low excitation energies. This leads to new physics which is strikingly different to that of typical 2D electron systems. Thus an unusual quantum Hall effect, and also a π phase shift in the de Haas–Shubnikov oscillations have experimentally confirmed the Dirac–Weyl spectrum. The existence of a ‘minimum conductivity (MC)’ has also been claimed, although it is not clear if this is a ‘universal’ MC, or a sample dependent quantity [2, 3]. The density of states in the DW

spectrum falls to zero at the Fermi energy, and hence the conductance should drop to zero as the gate voltage $V_g \rightarrow 0$. Instead, the conductance reaches a saturation value σ_m for small gate voltages $V_g < v_m$, with $v_m \sim 0.5$ eV. Although this may appear to contradict the behaviour expected from the DW-like effective Hamiltonian defined near the \mathbf{K} points of the idealized 2D lattice, the neglected features of the real graphene sheet need to be considered when we consider the $V_g \rightarrow 0$ limit. The graphene sheets are not perfect 2D systems, but are supported on a SiO_2 surface. These are locally crystalline or amorphous structures containing charged atoms, and their theoretical structural description is quite complex [8–10], and as yet incomplete. The charged sites on these substrates may have an effect [11, 12] on the DW spectrum that becomes crucial as $V_g \rightarrow 0$. Many authors have examined the effect of simple models of charged centres using Thomas–Fermi screenings models, Boltzmann or Kubo–Greenwood conductivity theories [13–15]. While these methods exploit simple theoretical methods, they ignore the microscopic details of the graphene layer and the SiO_2 substrate. However, it is important to develop atomistic models of the graphene–substrate which go beyond linearly screened structureless scattering models. Hence we study atomistic models of graphene on SiO_2 substrates *via* first-principles calculations.

Even if we assume that the graphene sheet does not interact strongly with the substrate (due to, say, adsorbed atmospheric N_2 layers in between the graphene and the SiO_2), or if the graphene film is considered suspended in space [16], the assumption of an ideally flat graphene sheet is clearly untenable. Ideal 2D layers (which are not part of a 3D structure) are expected to be unstable for a variety of theoretical reasons [17, 18]. Even a 3D solid at non-zero temperatures acquires vacancies and lattice defects to gain entropy and minimize its free energy. Hence some authors [19, 20] have considered that graphene is a disordered system with a distribution of vacancies. One may consider that the effect of the vacancies may be used to blunt the behaviour near the ideal \mathbf{K} points. Our calculations [21, 26] for vacancies in graphene show that the energy costs of breaking the σ bonding network are too great to allow any significant vacancy formation. In fact, the demonstration by Meyer *et al* [16] that graphene sheets are intrinsically wavy provides a key to the properties of free-standing or SiO_2 -supported graphene. Here we note that pyrolytically prepared graphene on SiC is multi-layered and protects the active graphene layer from the effects of the substrate [22].

In section 2 we present band calculations for a graphene sheet positioned on model SiO_2 surfaces. One type of model of the substrate surface is full of dangling bonds, while the other is saturated; but both surfaces have charged centres. These calculations show that E_F is modified by the variations in substrate structure. These calculations are reviewed in the context of a wavy graphene sheet as it brings in the statistical fluctuations of the position of the sheet in the z direction. The relative orientation of the C atoms with respect to O and Si in the SiO layer will differ spatially. The resulting *relative fluctuations* in E_F are mainly due to the top SiO layer and hence the well known complex problems of modelling SiO structures can be largely sidestepped. These results are used to provide a simple understanding of the minimum conductance of graphene.

2. Density functional calculations of graphene/substrate systems

Simple tight-binding methods (TBM) or the even more restricted Dirac–Weyl model could be successfully exploited within a limited energy window for pure graphene. The two sublattices of the bipartite graphene lattice become inequivalent if vacancies are introduced. Vacancies rupture the σ bonding network and involve energies such that elementary models become unreliable. In a previous paper [21] we presented calculations for vacancies in graphene (at concentrations of $\sim 3\%$ and above) and showed that the DW model does not even hold for

such systems. Thence we concluded that graphene films used in quantum Hall studies must be very high quality flakes free of vacancies. The experimental results of Mayer *et al* [16] are in agreement with this conclusion. Hence an understanding of other possible effects on the electronic structure is needed. One possibility is the effect of the electrostatic field of charged sites present in the SiO₂ surface. The quasi-cristobalite-like SiO₂ is a complex structure where bond angles, bond lengths etc, can take a variety of values [10]. In earlier times, such systems were presented using ‘random tetrahedral networks’ and other phenomenological models, or simply ignored in electron-gas-like models. Even today, the silica/vacuum interface is not definitively known [8–10] and hence the full simulation of the silica/graphene interface is outside the scope of this study. Similarly, the inclusion of van der Waals interactions [23] etc, are a higher level of refinement well outside the scope of this study, and perhaps not relevant since our main objective is to determine the *local relative variation in the Fermi energy of the system*, as explained below.

We consider simpler atomistic models which exploit the bonding versatility of SiO₂ and retain the essential physics. We construct a stable SiO ring structure which provides a model substrate with charged oxygen and Si centres. Unlike in simulations with Si slabs, this SiO₂ system needs *no* passivating H atoms. In fact, by attaching H atoms we can introduce dangling bonds which form dispersive bands near the Fermi energy. The existence of SiO ring structures with three oxygens, or four fold and six fold rings in various silica surfaces is well known [8, 9]. However, after decades of research, the real structures of typical silica surfaces are still a matter of debate. This too makes us focus on well defined energy-optimized *theorist’s models* as the basis of our study.

Thus we consider a *stable* 2D Si–O ring structure which satisfies the lattice vectors of the honeycomb structure (see figures 1, 2). The Si–O bond length in bulk SiO₂ is ~ 1.6 – 1.7 Å and the bond angles are optimal at 106°, although smaller and bigger angles from 96° to 126° are seen near Si/SiO₂ surfaces [10]. A wider range is found in fused silica simulations [9] which are, however, not yet able to reproduce the experimental ring distributions. Thus there is considerable freedom with respect to bond angles and lengths. In the structures developed here, bond lengths ranging from ~ 1.43 to 1.75 Å are found (on total-energy minimization) as stable structures. The longer bond length is accommodated by SiO₂ layers which are puckered. The relative distribution of the Fermi energy on changing the structure of the surface layer is largely insensitive to the deeper SiO layers, and here we use models containing just one SiO layer.

The structure with valencies $Z = 4$, and 2 (and two lone pairs) for Si and O is similar to a charge-transfer N–N system where $Z = 3$. The N–N system has no charge centres, where as the Si–O system has positive charges on Si and negative charges on O. It turns out that there are several possible structures which are at their energy minima. They are useful as models for the interaction of the graphene sheet with a SiO₂ substrate. We have studied the following cases, depicted in figure 1. (i) The substrate is represented by a single stable sheet of SiO rings where the Si and O atoms sit (in the z direction) underneath the C atoms, with the carbon hexagons *aligned* with the Si–O rings; this will be called the ‘aligned ring structure’ (ARS). (ii) The Si atoms are under the C atoms and close to the graphene plane, while the O are below the centre of the carbon hexagons and further away; this structure will be called the ‘staggered oxygen structure’ (SOS). (iii) The O atoms are under the C atoms and close to the graphene plane, while the Si are below the centre of the carbon hexagons and further away from the graphene plane; this is a ‘staggered Si structure’ (SSiS). (iv) The Si–O rings are fully staggered from the carbon hexagons; i.e., a staggered ring structure (SRS). (v) The ARS with H atoms attached to the Si atoms and optimized. (vi) H atoms attached to the Si in the SSiS structure and optimized to give a stable structure. Unlike the SOS and SSiS structures, the SRS system treats

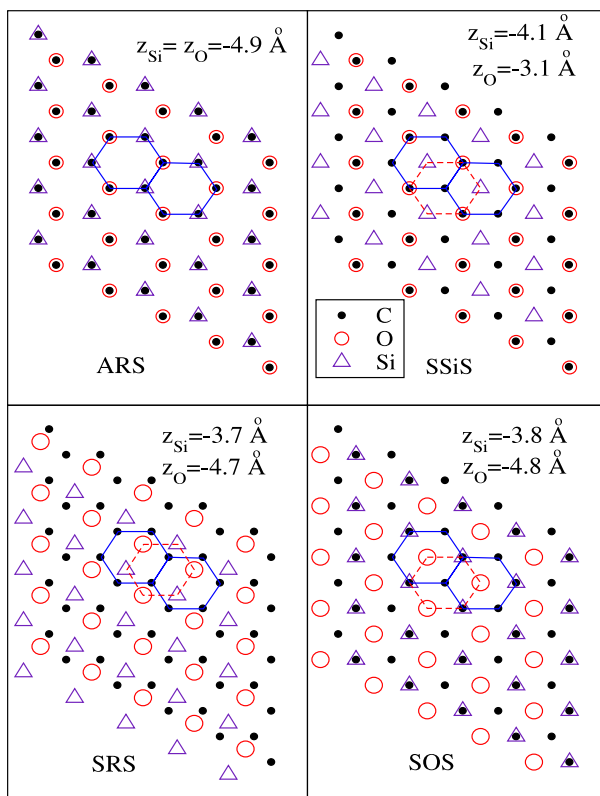


Figure 1. The top view of the C, Si, and O atoms for the structures ARS, OSS, SiSS and SRS, as described in the text. The O and Si atoms are below ($-ve z$) the graphene ($x-y$) plane. The z distances are indicated in each panel. In H-containing structures, the H atoms are directly underneath the Si atoms.

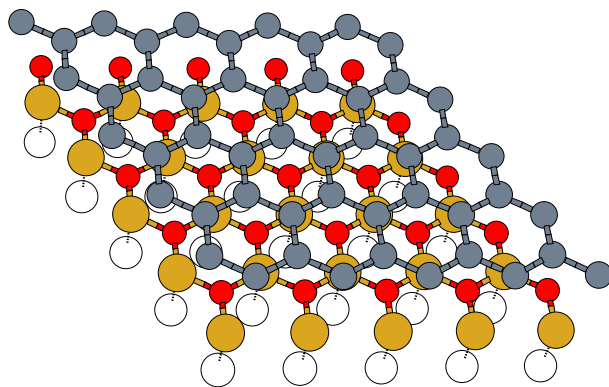


Figure 2. Three-dimensional view of the structure ARS with H atoms attached to Si, and where the SiO hexagon is aligned underneath the carbon hexagons.

the bipartite sublattices equivalently. The SRS structure is metastable, and relaxes to SOS or SSiS if annealed using molecular dynamics.

We have used the Vienna *ab initio* simulation package (VASP) [25] which implements a density functional periodic plane-wave basis solution where the ionic coordinates are also equilibrated to negligibly small Hellmann–Feynman forces. The projected augmented wave (PAW) pseudopotentials [25] have been used for the carbon potential. This C pseudopotential has already been used with confidence in several graphene-type calculations (e.g., [21, 24]). The usual precautions with respect to k point convergence, size of the simulation cell, the extent of the plane-wave basis etc, have been taken [21] to ensure convergence. Thus, having found a stable SiO hexagon which obeyed the lattice periodicity of the graphene system, we were able to use two C atoms, one O and one Si atom per simulation cell in the x – y plane with periodic boundary conditions. The SiO rings are in a plane approximately 3–5 Å, below the graphene plane, and their locations as well as the locations of the C atoms were optimized, with one of the C atoms held fixed. The lattice parameter itself was optimized, and this effect was found to be negligible. The z direction cell dimension was 14.8 Å, i.e., the equivalent of six graphene unit cells. This z distance was sufficient to ensure that the graphene–SiO system was isolated from its periodic repetitions in the z direction. An $8 \times 8 \times 6$ Monkhorst–Pack k mesh including the Γ point (i.e., an unshifted grid) was used and checked to give good convergence. An energy cut-off of ~ 494.63 eV was used for the plane-wave basis, together with a Ceperley–Alder exchange correlation functional (as parametrized by Perdew and Zunger), implemented via the VASP package.

2.1. Band structure in the presence of the substrate

In figure 3, we show the band structure of several graphene–SiO systems (projected on the graphene Brillouin zone) along the $\mathbf{K} \rightarrow \Gamma \rightarrow \mathbf{M} \rightarrow \mathbf{K}$ symmetry directions. The bands for the structures identified in figure 1 as SSiS, ARS, SOS and SRS, and *without* any H atom attachments, are shown in the figure. The pure graphene bands are also shown (as continuous lines) in panel (a). It is clear that the fully aligned flat SiO structure is not an acceptable model for the graphene substrate. The other three models largely preserve the linear dispersion in the $\mathbf{K}\Gamma$ direction. However, the behaviour near the \mathbf{K} point, towards the \mathbf{M} direction is affected by the intrusion of a flat band. The bands shown in panels (a), (c) and (d) also have a small (~ 0.15 eV) energy gap which cannot be seen on the scale of the plots. However, as we discuss below, the Fermi energy itself moves by about ± 0.6 eV from structure to structure and hence this band gap splitting is not significant in a real substrate where many local orientations (of the SSiS, SOS, SRS types) could occur.

In figure 4 we show the bands of the SSiS system with an H atom attached to the Si atoms. This introduces an additional band criss-crossing the Fermi energy (E_F is set to zero in the figure), and marked as a dashed line with circles. This criss-crossing is contrary to experiment. Hence the H atom system is not an acceptable model for graphene on a SiO substrate. Even the more satisfactory models, i.e., SSiS, SOS and SRS shown in figure 3 show that the graphene layer interacts with the substrate in a significant manner.

If we consider a graphene sheet lying on a substrate the charge structure near different parts of the graphene in different regions will differ. The different staggered structures represent local configurations which would occur in different parts of a substrate/graphene system. The change in the E_F in going from one part of the substrate where one structure (e.g., the staggered oxygen structure) prevails, to another where another structure (e.g., the staggered Si structure) prevails locally, would be a measure of the local fluctuations of the graphene bands and the position of E_F , caused by the substrate. The calculations for the Si–O systems shown here, as well as other similar systems not discussed here, give us an E_F variation $|\Delta E_F|$. Moving the graphene film from $z \sim 3$ Å to $z \sim 5$ Å changes E_F insignificantly, although there are

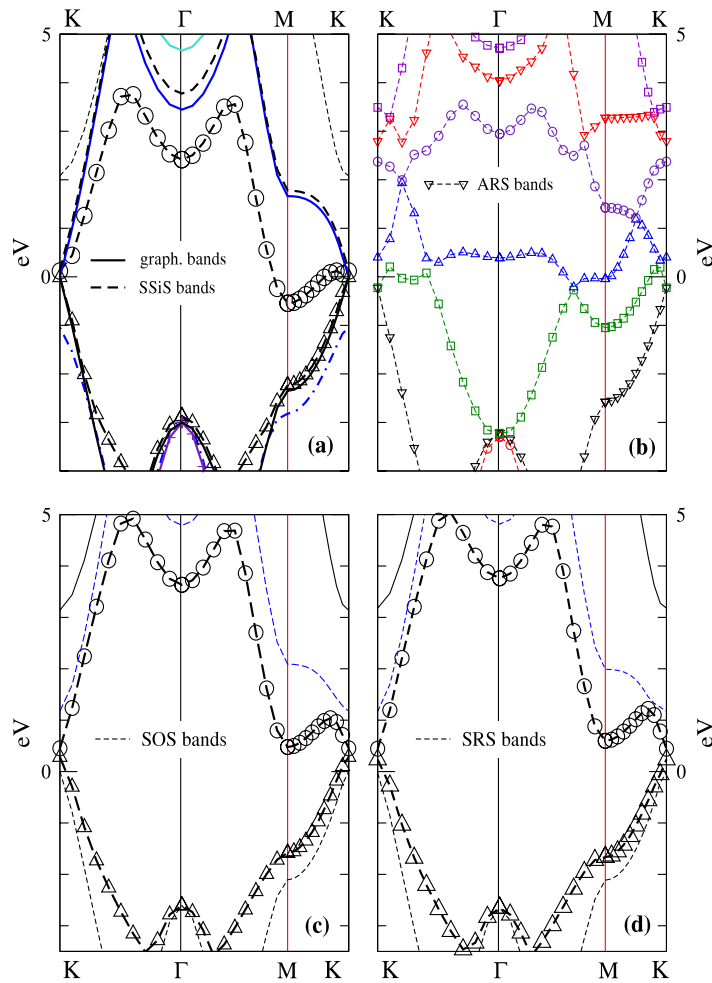


Figure 3. Kohn–Sham energy bands along the $\mathbf{K}\ \Gamma\ \mathbf{M}\ \mathbf{K}$ directions of the graphene Brillouin zone, inclusive of substrate effects. (a) The thick lines are from pure graphene. Dashed lines with or without data points are for graphene on a SiO substrate with the O atoms under a C atom. The Si atoms are staggered to the centre of the C hexagons (SSiS). (b) The flat Si–O rings are aligned directly under the C hexagons (ARS) and the corresponding bands are shown. In panel (c) The Si atoms are under a C atom, and the O atoms are staggered to the centre (SOS), and the resulting bands are shown. The bands in panel (d) are very similar to those in (c), and is the case where the whole SiO ring is staggered with respect to the C hexagon (SRS). E_F is set to zero in all panels.

changes in the band structure. Changing the alignment of the C hexagons from the Si–O hexagons produces a change of ± 0.6 eV in E_F . These calculations suggest that, when the Si–O substrate modifies the graphene bands without disrupting the DW behaviour, it could still lead to a spatially varying Fermi energy $E_F(\vec{r})$, with a variation of about $|\Delta E_F| \sim 0.6$ eV. We also note that the equilibrium separation between a large graphene sheet and the substrate would vary with the *local* substrate structure. Thus, in effect, the graphene sheet would not be flat but determined by the structural features of the substrate and the resultant interactions. It should also be noted that a sheet of graphene simply ‘put’ on a substrate does not necessarily assume the lowest energy conformation, unless an annealing process is performed. Instead,

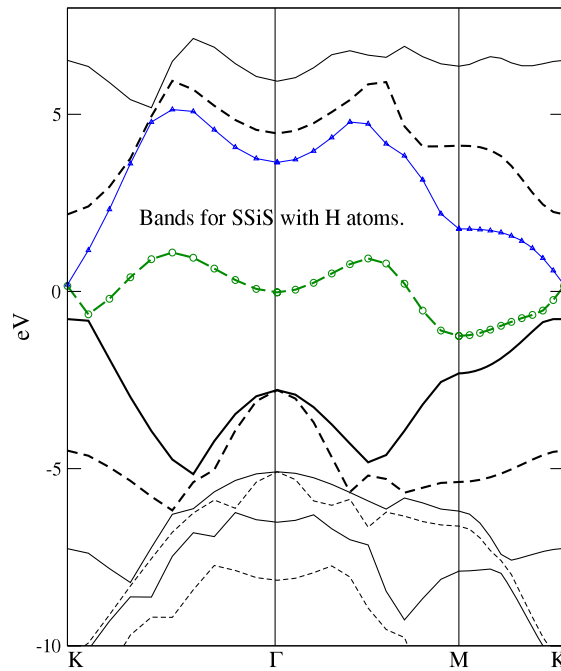


Figure 4. Kohn-Sham energy bands along the $\mathbf{K}\ \Gamma\ \mathbf{M}\ \mathbf{K}$ directions of the graphene Brillouin zone, with graphene on a SSiS substrate where the Si atoms carry H atoms. The dashed line with circles as data points is a new band arising from the H atoms. E_F is set to zero.

the film would have a number of ‘touch points’ where it would approach the substrate to some near-optimal distance (3–5 Å). These ‘touch points’ would hold the film on the substrate, while the rest of the film could be at other distances. The optimal distance Z_g of 3–5 Å is that obtained from the total energy at zero temperature (and not from a free energy, at the ambient temperature) for the SiO substrates considered here. The *average* distances of up to 8 Å, or similar values, quoted in experimental studies could easily occur in different samples, and are of the same magnitude as Z_g .

These arguments assume that the various possible arrangements of graphene and substrate can be used to model the local variations leading to an element of ‘disorder’ in graphene.

Our calculations, unlike linear response or Thomas Fermi models, take account of the structural features of graphene, the essential features of the Si–O substrate, as well as the non-linear response, bound state structure and bond length modifications, via the self-consistent Kohn–Sham calculations used here. However, just as the Si/SiO₂ interface structure of field-effect transistors required many decades of study [9, 10], the graphene/SiO₂ interface would also require more microscopic calculations.

3. Discussion

In this section we discuss the implications of our first-principles calculations. A single sheet of graphene gently placed on a SiO₂ substrate or suspended in space is driven to deviations from perfect flatness as a consequence of well known thermodynamic constraints [16–18]. Our calculations also showed that the local variations in the equilibrium distance (Z_g) would occur at different ‘touch points’ of the graphene sheet, where different local substrate configurations would occur. These would also have locally different values of the Fermi energy E_F . Hence a

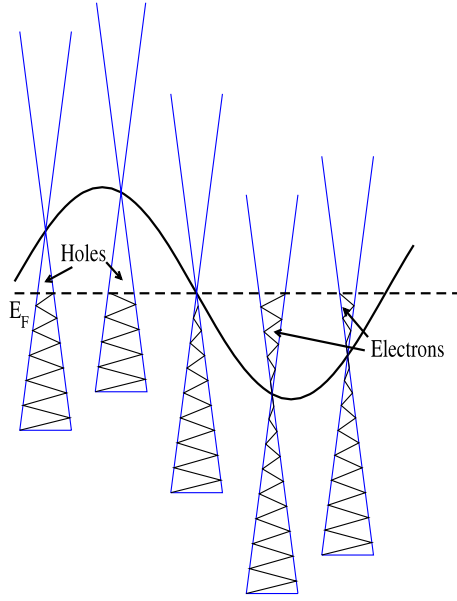


Figure 5. Position dependent Dirac–Weyl energy-dispersion cones arising from a single Fourier component of a wavy graphene sheet (shown as a thick black curve), and the resultant pockets of electrons and holes. These are defined by the common electrochemical potential of the system.

form of the wavy graphene sheet (WGS) model of Mayers *et al* [16], quenched somewhat by the electrostatic potential of the substrate, is consistent with our results for the graphene sheet sitting on a SiO₂ substrate.

The DW effective Hamiltonian remains valid in the neighbourhood of k_F which is at the \mathbf{K} points. The low energy DW excitations are actually associated with a high k Fourier component (near k_F) of the system. The Dirac–Weyl model, i.e., the (linear dispersion) is valid within an energy range of about 2.7 eV of the Fermi energy, and near wavevectors $k \sim K_F$. The elastic energies associated with the waviness affect the small k regime near $k \rightarrow 0$. However, the waviness affects the distance between the substrate and the graphene layer. If L_z is taken as a measure of the z direction undulation for a typical distance L_{xy} in the plane, then experiments suggest that the waviness involves a 1:10 to 1:50 ratio [16] in $L_z:L_{xy}$. A value for L_{xy} is not available within our simulations. But if L_z is taken as the fluctuation in Z_g , then L_{xy} would be 20–100 Å.

We found that the E_F for the various graphene/SiO substrate configurations differed by ~ 0.6 eV. Equivalently, the energy cones at \mathbf{K} , \mathbf{K}' may be thought of as ‘bobbing up and down’ in different regions of the graphene sheet. This means that there would be small puddles of electrons and holes even when the gate voltage is zero (see figure 5). Those calculations assumed the existence of lattice periodicity in each model, with the graphene sheet located at an optimized value Z_g (3–5 Å), depending on the substrate configuration. The configuration of the substrate presented to the graphene sheet (i.e., whether it is SSiS, SOS, or SRS) will differ more or less randomly, at different ‘touch points’. Thus the \mathbf{K} -point energy at each touch point will differ, with a variation of about ~ 0.6 eV. A statistical averaging over an ensemble of such models can be carried out, inclusive of charge–charge correlations, using methods well known in astrophysics [27], plasma physics [28], and as in recent discussions of random charge centres acting on graphene [12].

We note that there are several effects arising from the ‘waviness’ associated with the substrate–graphene interaction presented here. Thus:

- (i) Breakdown of the lattice periodicity a and the zone-edge periodicity $2\pi/a$.
- (ii) The modification of the energy at the zone edge and specifically at \mathbf{K} when E_F becomes space dependent, creating small pockets of electrons and holes even for zero gate voltage.
- (iii) Replacement of the ideally 2D charge density $n(z) = \delta(z)$ by a distribution *confined* within the range of variation of z imposed by the waviness of the graphene sheet, i.e., we have a quasi-2D electron layer of thickness L_z .

Given similar methods of preparation and similar conditions of observation, the L_z/L_{xy} parameter and the resultant carrier density would be approximately ‘universal’ in the sense that it would lie within a limited range of possible values.

We explore the consequences of the L_z motion available to the electron [30]. Its allowed energy states would be quantized with a spectrum of discrete energies $\epsilon_n(l_z)$. The lowest of these would correspond to the $n = 1$ state of some effective minimum value of the z direction parameter. A number of such states would be occupied, depending on V_g . Once V_g falls below v_m , one may assume that only the lowest of these states, i.e., $n = 1$ would be occupied. In each Dirac cone, the in-plane energy $\epsilon(k) = \pm v_F k$ will combine with the $\epsilon_n(l_z)$ energy of the z motion. Thus we see that this system can indeed reduce to just a single conduction channel (lowest energy channel). A single channel has a conductance of e^2/h , i.e., the quantum of conductance [29]. However, each such channel in graphene has a spin and valley degeneracy (unless an external field is present) taking the spin and pseudospin degeneracy into account. Thus a minimum conductance of $4(e^2/h)$ would be expected for these systems. That is, although the value of the threshold v_m would *not* be universal, the conductance will have a minimal universal value corresponding to the occupation of the lowest z quantized state. The above argument is independent of the actual values of L_z, L_{xy} , as long as L_z is small enough to establish z quantization. This picture may also be approached from the mobility-edge conductance model of disordered semiconductors [31], although perhaps less transparently.

4. Conclusion

In this study we have shown that simple models of the silicon dioxide substrate can be constructed and used to give some insight into the spatial fluctuation in E_F due to the substrate/graphene interaction. These models show that if the substrate is free of dangling bonds, a graphene layer positioned at about 3–5 Å away from the substrate preserves its DW bands. However, the energy at the \mathbf{K} point acquires a spatial variation. The atomically thin 2D layer effectively acquires a z extension, and the z confined states in this quasi-2D system provide the quantization necessary to define a minimum conductance of $\sim 4e^2/h$. This behaviour is *different* from what is expected of ideal graphene where the conductance should go to zero when the gate voltage goes to zero.

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