

Lindhard screening in graphene antidot lattices

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Regular perforations of a pristine graphene sheet, i.e., a formation of a graphene antidot lattice (GAL) [1], modify the electronic structure so that a gap may appear in the energy spectrum [2], thus possibly paving the way to nanoelectronic applications. A central concept in the theory of solids is screening, and in many instances an RPA-level theory is sufficient. In the case of graphene, several groups have addressed this issue, initially approximating the electronic spectrum by the linear Dirac cone (see, e.g., [3,4]), and, more recently, allowing for the full graphene dispersion [5]. Here, we report analogous results for GALs.

The calculations proceed in principle in the same way as discussed in [3-5], however in our case one has to resort to the numerically computed electronic dispersion relations, and one needs to evaluate the matrix elements using the (numerically) known Bloch eigenstates of the antidot lattice. Thus, we must evaluate

$$\chi_0^R(\mathbf{q}, \omega) = \frac{2}{(2\pi)^2} \sum_{nn'} \int_{1.BZ} d\mathbf{k} \left| \sum_{j=1}^M (c_{n\mathbf{k}}^j)^* c_{n'\mathbf{k}+\mathbf{q}}^j e^{-i\mathbf{q}\cdot\mathbf{d}_j} \right|^2 \frac{n_F(\epsilon_{n\mathbf{k}}) - n_F(\epsilon_{n'\mathbf{k}+\mathbf{q}})}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}+\mathbf{q}} + \omega + i\eta}$$

where the c-coefficients are obtained from the tight-binding wave function,

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \sum_{j=1}^M c_{n\mathbf{k}}^j \varphi(\mathbf{r} - \mathbf{R} - \mathbf{d}_j)$$

It is important to note that the j-sum runs over all the atoms in the unit cell of the antidot lattice (see Fig. 1, left), and that the energies are given by the antidot dispersion ([1], or Fig. 1, right). Thus, in the case of pristine graphene there are only two terms in the j-sum, while for antidot lattices there may be hundreds of terms, implying significant numerical work. Also, the convergence must be carefully tested. In practice, however, we have found that it is often possible to replace the matrix element by a wave-vector and band-index conserving Kronecker symbol, which simplifies the numerical work substantially. In the evaluation of the Brillouin-zone sums we used an improved triangle method [6]. We have benchmarked our numerical algorithm against Ref.[5], and find quantitative agreement for pristine graphene. The full details will be given elsewhere [7].

Figure 2 shows an example of the computed polarizabilities for two different azimuthal angles of the q -vector. Also shown are results for a simplified model, “gapped graphene”, where the dispersion is

$$\epsilon_{n\mathbf{k}} = n\sqrt{\Delta^2 + t^2 |\phi_{\mathbf{k}}|^2} \quad |\phi_{\mathbf{k}}| = |e^{i\mathbf{k}\cdot\boldsymbol{\delta}_1} + e^{i\mathbf{k}\cdot\boldsymbol{\delta}_2} + e^{i\mathbf{k}\cdot\boldsymbol{\delta}_3}|$$

Here, $n = \pm 1$, and δ_i are the nearest neighbors. The parameter Δ is chosen so that the antidot lattice gap is reproduced. We observe a qualitative agreement, however much of the fine structure is lost in the simple model. We have also computed the plasmon dispersion laws, and find an approximate square-root dependence on the wave-vector (as is the case for pristine graphene), however the dispersion is suppressed as compared to graphene. For plasmon dispersion laws the simple model and the full antidot calculation are in close agreement.

References

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Figures

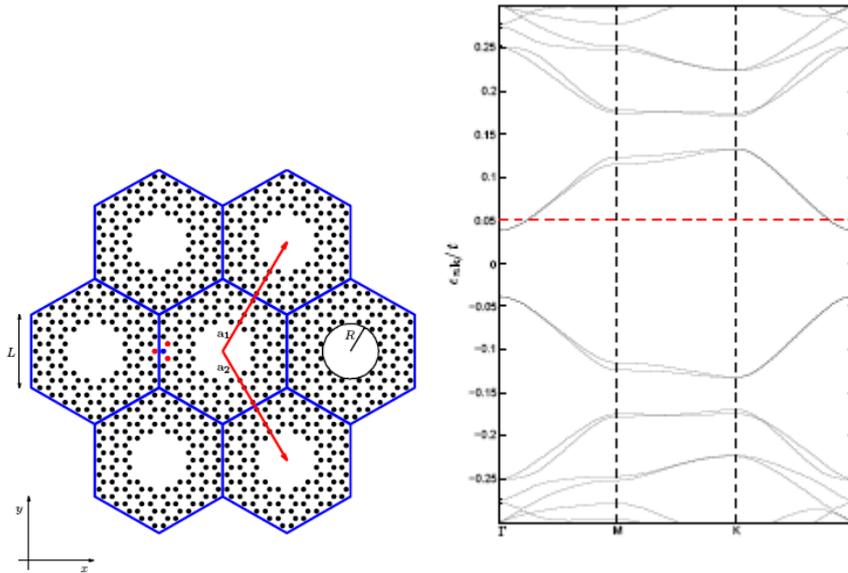


Figure 1. (Left) The geometry of the triangular graphene antidot lattice. The blue hexagons define the unit cell, R is the radius of the area from which carbon atoms have been removed, and the unit vectors $\mathbf{a}_{1,2}$ define the lattice symmetry. (Right) The band dispersion for a $\{12,3\}$ lattice, used in our calculations. The dashed line indicates value of the chemical potential, for which the polarizability calculations in Fig. 2 are carried out.

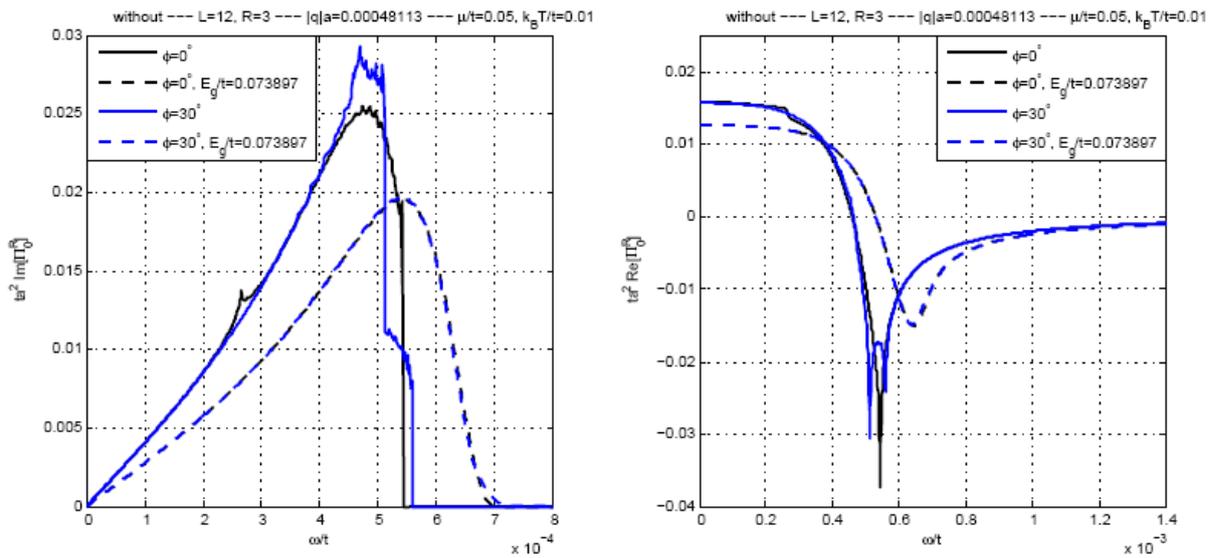


Figure 2. The imaginary (left panel) and the real (right panel) part of the polarization function, shown for two different azimuthal angles of the q -vector of length $qa = 0.00048223$, $kT/t = 0.01$, and $\mu/t = 0.05$. Continuous lines correspond to the full antidot model, while dashed lines correspond to “gapped graphene”.