Dot-bound and Dispersive States in Graphene Quantum Dot Superlattices

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Abstract

We use numerically exact Chebyshev expansion and kernel polynomial methods to study transport through circular gate-defined graphene quantum dots in the framework of a tight-binding honeycomb lattice model. Our focus lies on the regime where individual modes of the electrostatically defined dot dominate the charge carrier dynamics. In particular, we monitor the scattering of an injected Dirac electron wave packet for a single quantum dot, electron confinement in the dot, and the propagation of an electronic excitation along a linear array of dots. Moreover we consider a square lattice configuration of dots and calculate local density of states and the momentum resolved photoemission spectrum. Again we find clear evidence for a series of quasibound states at the dots. We further investigate the interplay of the superlattice structure with dot-localized modes on the electron energy dispersion. Effects of disordered dot lattices are discussed too.

Model & Computational scheme

- tight-binding Hamiltonian

$$H = \sum_i V_i c_i^\dagger c_i - t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$$

on-site potential $V_i = V \sum_{(n,m)} \Theta(R - |\vec{r}_i - \vec{r}_{(n,m)}|)$

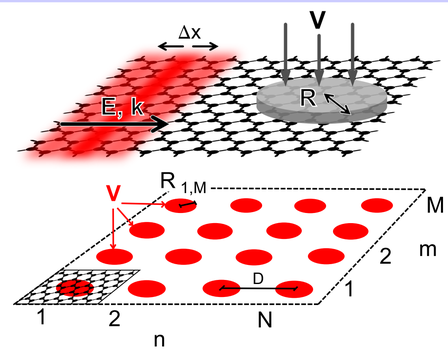
- wave packet propagation $|\psi(\tau)\rangle = U(\tau, \tau_0)|\psi(\tau_0)\rangle$
- expansion in Chebyshev polynomials of first kind $T_l(x)$

$$U(\Delta\tau) = e^{\frac{-ib\Delta\tau}{\hbar}} \left[c_0 \left(\frac{d\Delta}{\hbar} \right) + 2 \sum_{l=1}^{M} c_l \left(\frac{d\Delta\tau}{\hbar} \right) T_l(\tilde{H}) \right]$$

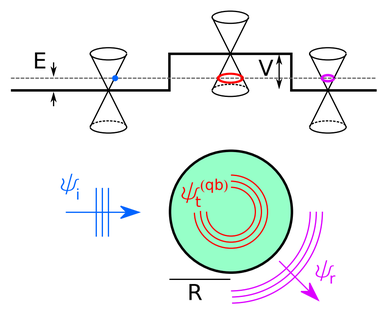
$c_l(d\Delta\tau/\hbar) = (-i)^l J_l(d\Delta\tau/\hbar)$, J_l Bessel function,
$\tilde{H} = (H - b)/d$ rescaled Hamiltonian

- particle density $n_i(\tau) = |\langle i|U(\tau, \tau_0)|\psi(\tau_0)\rangle|^2$
- current density $\vec{j}_i(\tau) = |\langle i|(-\vec{J}/e)U(\tau, \tau_0)|\psi(\tau_0)\rangle|^2$

current operator $\vec{J} = -(ite/\hbar) \sum (\vec{r}_j - \vec{r}_i)(c_i^\dagger c_j - c_j^\dagger c_i)$

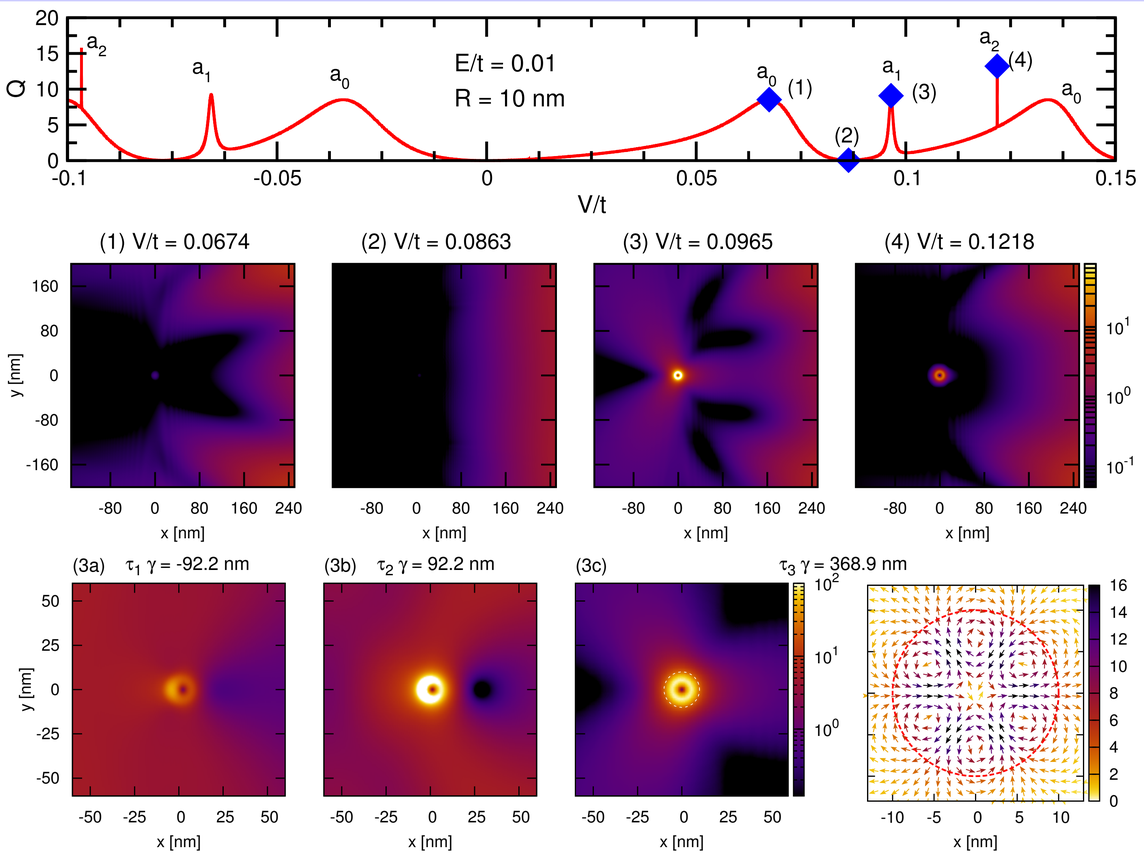


Schematic representation of the scattering geometry. Upper panel: An electron wave packet of energy E, momentum k and width Δx propagates in a broad graphene sheet. It impinges on a circular, electrostatically defined dot with radius R and applied potential V. Lower panel: Graphene quantum dots arranged in a square superlattice with lattice constant D.



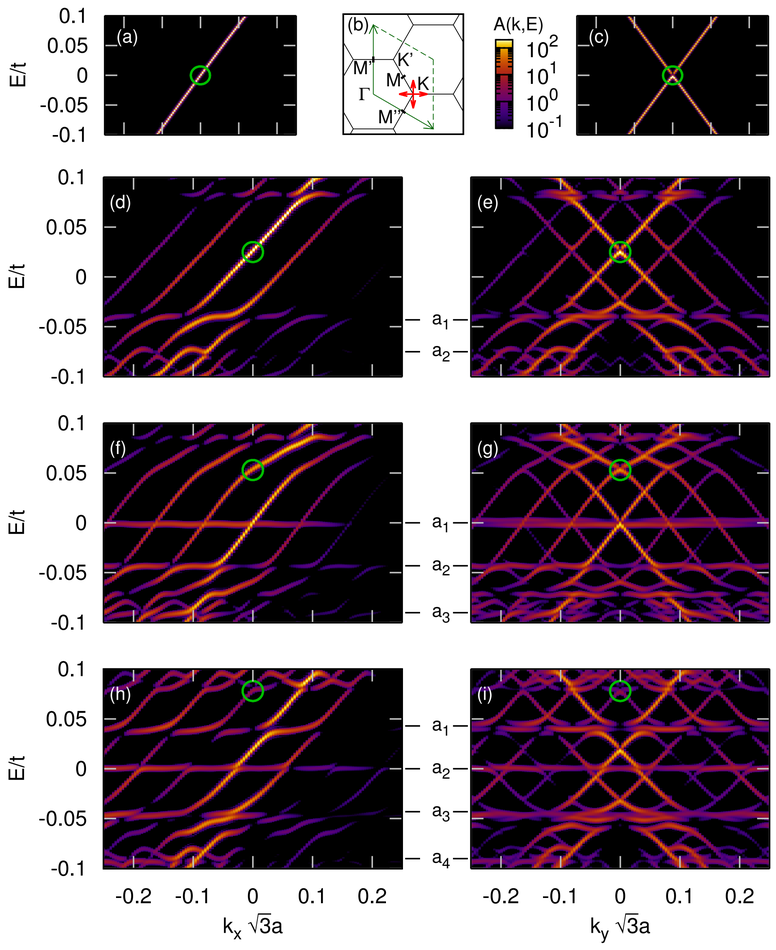
Dirac electron scattering at a single dot. For $E < V$, the incident (ψ_i) and reflected (ψ_r) electron waves reside in the conduction band, while the transmitted (ψ_t) wave inside the dot corresponds to a state in the valence band.

Scattering by a single gate-defined quantum dot



Scattering and particle confinement by a gate-defined circular quantum dot. The scattering efficiency Q (defined as scattering cross section divided by the geometric cross section) for plane-wave scattering in the Dirac approximation (top) shows resonances when specific modes a_m are excited. Below we show density snapshots obtained numerically for the tight-binding model for the scattering of a wave packet with $\Delta x = 148$ nm after passing through the dot. The lower panels show three time steps during the scattering process at the a_1 resonance [marker (3)]. Here we also show the current field exhibiting six vortices. The circumference of the quantum dot is indicated by the dashed circle.

Spectral properties of a quantum dot superlattice

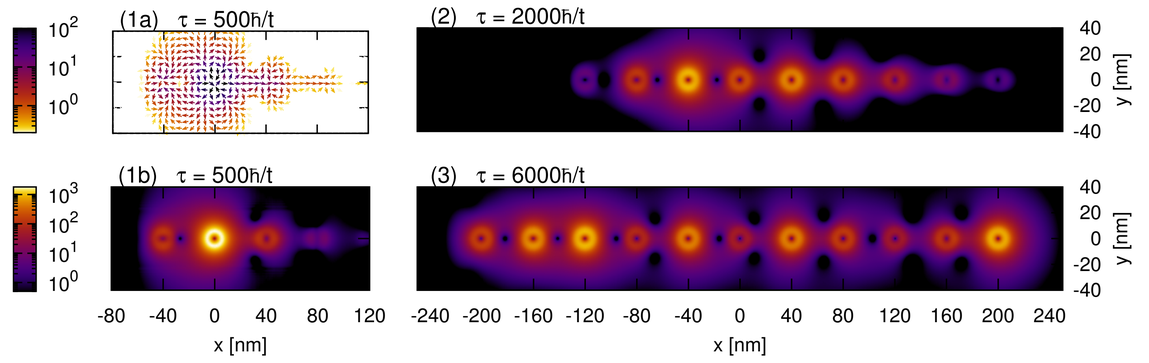


Single-particle spectral function for a 20x20 dot superlattice with R = 4.775 nm and D = 19.1 nm along the $\overline{\Gamma K}$ direction (horizontal; left-hand panels) and parallel to the $\overline{\Gamma M'}$ direction (vertical, right-hand panels) through the Dirac K point, as indicated in the upper central figure (b).

Panels (a) and (c) give $A(\vec{k}, E)$ for a finite sample of pristine graphene. In (d) and (e) $V/t = 0.107$ (mode a_0 falls on $E = 0$), in (f) and (g) $V/t = 0.171$ (mode a_1 on E = 0), and in (h) and (i) $V/t = 0.229$ (mode a_2 on $E = 0$). The green marker (circle) traces the energy shift of the nodal point for pristine graphene when V is increased. In view of transfer of spectral weight to other nodal points it should, however, no longer be identified as the genuine Dirac point. Within the KPM 8192 moments were used.

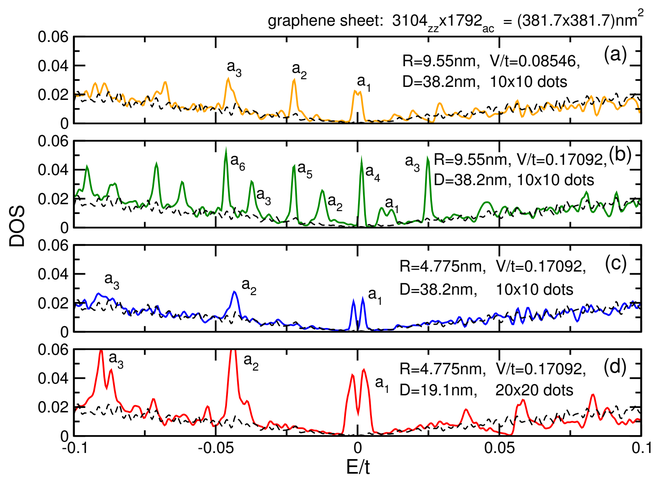
[1] R. L. Heinisch, F. X. Bronold, and H. Fehske, Phy. Rev. B **87**, 155409 (2013).
[2] A. Pieper, R. L. Heinisch and H. Fehske, Europhys. Lett. **104**, 47010 (2013).
[3] A. Pieper, R. L. Heinisch, G. Wellein and H. Fehske, Phy. Rev. B **89**, 165121 (2014).

Transport through a linear array of dots

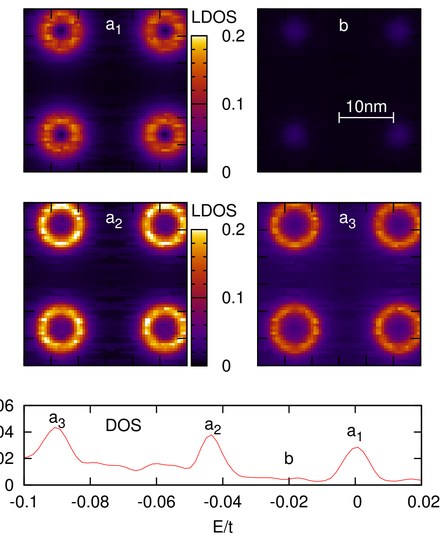


Propagation of an electronic excitation along a linear chain of dots. The eleven dots are aligned on a graphene sheet with $N_z \times N_a = 12000 \times 4000$ sites corresponding to (1476×852) nm^2. The parameters are $R = 10$ nm, $D = 40$ nm and $V/t = 0.081615$. At time $\tau = 0$ the a_1 mode (energy $E = 0$) is excited at the central dot. The left panels show the current field (top) and the density profile (bottom) after $\tau = 500\hbar/t$. The right panels give two density snapshots at later times.

Localized modes in a square array of dots

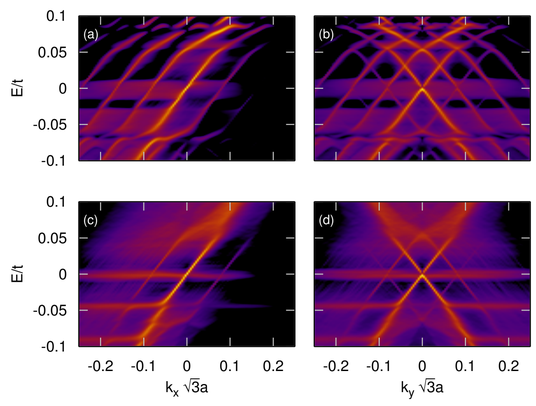


Density of states of the dot superlattice in dependence on R, D, and V. Peaks related to quasibound dot modes are designated by a_m. Dot parameter $\eta = VR/v_F$ is the same in panels (a), (c), and (d) – a_1 is pinned to $E = 0$. The DOS for the case $V_i = 0\ \forall i$ is included (dashed lines). The DOS is calculated by the KPM using 16384 Chebyshev moments.



Intensity plots for the local DOS in the central part of a larger (square) dot superlattice. Parameters are same as in the left figure panel (d); since only 4096 Chebyshev moments were used the a_m band splittings are not resolved.

Disorder effects



Spectral function near the Dirac K point for a disordered 20x20 dot superlattice. Parameters are $R = 4.775$ nm, $D = 19.1$ nm and $V/t = 0.171$ nm, i.e., the a_0 mode falls on $E = 0$. Panels (a) and (b) give $A(\vec{k}, E)$ with random $R_{(n,m)}/R \in [0.9, 1.1]$. Panels (c) and (d) show $A(\vec{k}, E)$ if the dots were displaced from their regular superlattice sites by $r_{(n,m)}/R \in [0, 0.4]$ in random direction.

Conclusions

- Employing analytical and exact numerical techniques we have studied the electronic properties of graphene with circular gate-defined quantum dots.
- Tracing the time evolution of wave packet scattering on a free-standing dot we find temporary particle trapping at the dot when normal modes become resonant. Signatures of dot-bound states also appear in the optical conductivity. Tuning the chemical potential transitions between these states can be selected.
- Following the propagation of an excitation along a linear chain of dots we can identify an effective inter-dot hopping on a reduced time scale.
- For graphene quantum dot superlattices with only one sharp localized mode at the charge neutrality point a dispersionless dot band emerges while the conical energy dispersion is preserved and pinned to $E = 0$. For other choices of the dot potential the group velocity at the Dirac cone is significantly renormalized.
- In disordered superlattices, quasi-bound dot states still exist but their coherence is lost; near the Dirac model points dispersive graphene states are rather inert against the disorder induced by random R or D .

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