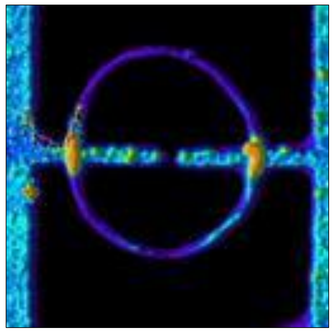

Quantum transport on carbon nanotori in nanodevices and metamaterials – from effective models to non-equilibrium Green's function methods

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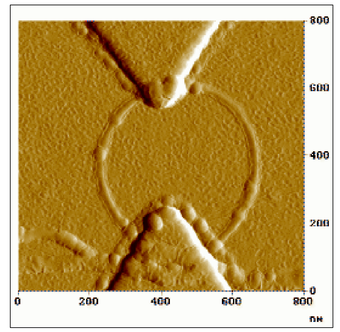
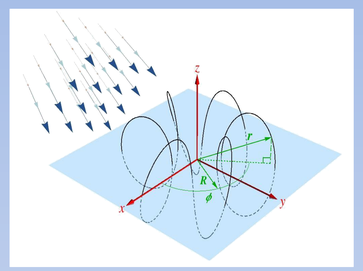


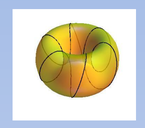
Abstract

Graphene-based allotropes such as toroidal carbon nanotubes hold the promise of completely new nanodevice and metamaterials applications. Due to the compactification of the honeycomb lattice to a toroidal manifold, additional modular symmetries are predicted to drastically reduce the number of spectrally distinct ring geometries and thus transport properties. In addition to persistent current and Aharonov-Bohm effects, new electromagnetic moments such as the toroidal moment will be generated by the ring currents. In a metamaterial of nanorings, a significant enhancement of these quantum signatures may be expected due to coherence of the individual electromagnetic responses resulting in unique electronic and optical material characteristics. First, in an effective model, the Hamiltonian for a single charge constrained to motion near a toroidal helix is developed. The resulting three-dimensional Schrödinger equation is reduced to an effective one-dimensional formula inclusive of curvature effects in form of two resulting effective curvature potentials. The effective model also elucidates how a surface current may be driven by a properly polarized incoming electromagnetic wave front to generate a specific multipole response. Alternatively, density-of-states, transmission function and source drain current between two metallic leads are calculated in a tightbinding model for armchair and zigzag carbon nanotori using a recursive non-equilibrium Green's function method for realistic system sizes of 10,000 atoms and more. An object-oriented C++ code was developed using sparse matrix software libraries such as PETSc for large-scale parallel inversion of the effective Hamiltonian between metallic leads. The code may be expanded to incorporate additional effects such as electron-phonon coupling, exciton transport, or electron-plasmon coupling in second- or third-nearest-neighbor type calculations.

Quantum transport on a nanohelix – effective model

Recently, it was suggested that quantum methods be employed in an effort towards understanding toroidal moments induced by currents supported on nanoscale metaparticles and the interactions of those moments with time-dependent electromagnetic fields. Because of the theoretical and practical interest in toroidal moments, a toroidal helix (TH) of adjustable *eccentricity* has been chosen here to investigate the role of quantum effects. Being closed, a TH can support current carrying solutions allowing for the existence of *a toroidal moment*. Furthermore, the TH has the advantage of having sufficient symmetry to allow for a clean reduction of the full Hamiltonian to a one dimensional effective Hamiltonian.





Sketch of nanohelix with external magnetic flux.

Here, a constant magnetic field (on the order of 1 Tesla) with arbitrary orientation is applied to the helix to study the induced toroidal moments as a function of field strength, orientation, and coil eccentricity. The introduction of the field requires accounting for its effect in the one dimensional reduced model. It is not enough to simply evaluate the value of the vector potential for a given field on the points of the wire. Self-consistency with the well known procedure by which *curvature potentials* arise from dimensional reduction requires a careful accounting of the coil curvature-field coupling.

Parameterization of nanohelix and B-field:

$$\vec{r}(\phi) = [R + a\cos(\omega\phi)]\hat{\rho} + b\cos(\omega\phi)\hat{\mathbf{k}}$$

$$\vec{B} = B_\rho\hat{\rho}_M + B_z\hat{\mathbf{k}}$$

Specifically, there exits a prescription that allows for degrees of freedom extraneous to the particle's 'motion' on a manifold to be shuttled into effective curvature potentials in the Schrödinger equation.

3-dim wave Hamiltonian:

$$H_w^3 = -\frac{\hbar^2}{2m_e}\left[\frac{1}{f(\phi)^2}\frac{\partial^2}{\partial\phi^2} - \frac{f'(\phi)}{f(\phi)^3}\frac{\partial}{\partial\phi} - \kappa(\phi)\frac{\partial}{\partial q_N} + \frac{\partial^2}{\partial q_N^2} + \frac{\partial^2}{\partial q_B^2}\right. \\ \left. + 2i\frac{e}{\hbar}\left(\frac{1}{f(\phi)}A_T\frac{\partial}{\partial\phi} + A_N\frac{\partial}{\partial q_N} + A_B\frac{\partial}{\partial q_B}\right) - \frac{e^2}{\hbar^2}A^2 + V_e(q_N) + V_e(q_B)\right]$$

Effective 1-dim Hamiltonian

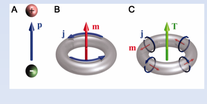
$$H_w^1 = \frac{1}{2m_e}\left[-\hbar^2\left(\frac{1}{f(\phi)^2}\frac{\partial^2}{\partial\phi^2} - \frac{f'(\phi)}{f(\phi)^3}\frac{\partial}{\partial\phi} + \frac{1}{4}\kappa(\phi)^2\right)\right. \\ \left. - 2ie\hbar\left(\frac{1}{f(\phi)}A_T(\phi)\frac{\partial}{\partial\phi} + \frac{1}{2}\kappa(\phi)A_N(\phi)\right) + e^2A(\phi)^2\right]$$

Basis set expansion to solve effective 1-dim Schrödinger equation:

$$\chi_n^{(pa)}(\phi) = \frac{\exp[ip\phi]}{f(\phi)^{1/2}}\sum_n C_n^{pa}\exp[in\omega\phi]$$

Toroidal moment:

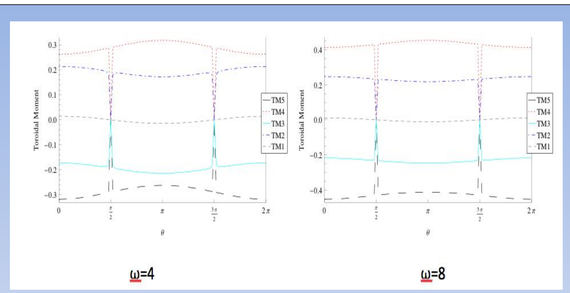
$$\vec{T}_M^{pa} = \frac{1}{10}\int_0^{2\pi}\left[\left(\vec{j}^{pa}(\phi)\cdot\vec{r}(\phi)\right)\vec{r}(\phi) - 2r^2\vec{j}^{pa}(\phi)\right]f(\phi)d\phi$$



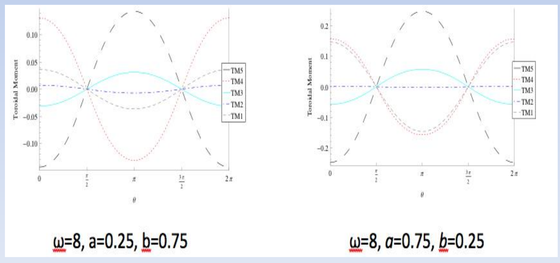
T. Kaelberer at al., *Science 10, 1510-1512 (2010).*

Toroidal moment eigenvalues TM1…5 for nanohelix currents with polar angle θdependence: a. circular, b. elliptical helix cross section (a,b: major/minor axis; ω : winding number).

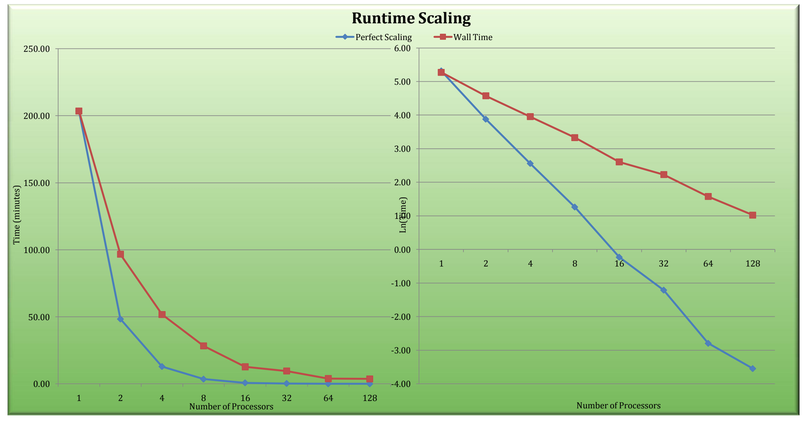
a.



b.

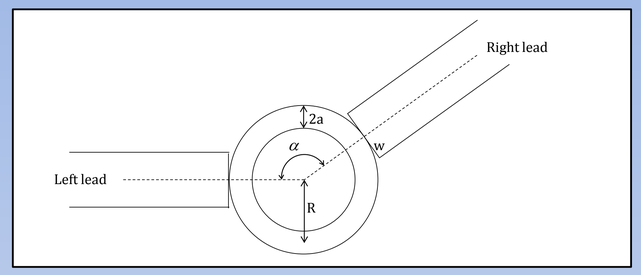


Scaling behavior of tightbinding nanotorus simulations.



Device geometry for nanotorus simulation

Electronic transport characteristics in a mesoscopic device configuration are calculated for variable source-drain voltage bias with a fast *tight-binding* algorithm using a *non-equilibrium recursive Green's function method (NEGF)*. The basic geometry of the device is shown below with the carbon nanotorus centered and adjustable metallic lead attachments to the sides.



Device setup with toroidal carbon nanotube and metallic leads.

Tight-binding approximation and NEGF method used in the simulation

Hamiltonian of the device region (time-independent):

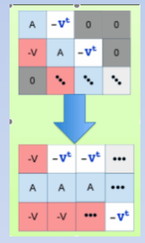
Definition of Green's function: $H'G_d = \left[E - H - \Sigma_L - \Sigma_R \pm i\eta\right]G_d = I$

The non-equilibrium Green's function can then be used to find the transmission function and source drain current.

Density of states: $D(E) = G_d\{\Gamma_L + \Gamma_R\}G_d^\dagger$

Transmission function: $T(E) = \mathrm{Trace}\left[\Gamma_L G_d \Gamma_R G_d^\dagger\right]$

The source drain current: $I = \frac{2e}{\hbar}\int_{-\infty}^{\infty} dE\; T(E)\left[f_0(E-\mu_1) - f_0(E-\mu_2)\right]$



Structuring the simulation

A run for device configuration comprises at least 8000 *N x N* matrix inversions. Naturally, this meant adapting the simulation to make use of various HPC resources such as *NSF XSEDE, Florida State University's* and *University of Miami's High-Performance Computing Centers (HPC)*. For maximum flexibility of the code to other device geometries, sparse matrix inversions were performed with the Portable, Extensible Toolkit for Scientific Computation (PETSc) coupled with a Multifrontal Massively Sparse Direct Solver (MUMPS) available as matrix libraries at Argonne National Lab. PETSC provides a generalized framework where the number of processors used can be determined at runtime.

Acknowledgements

Funding for this project was provided in parts (AB, LD) by the NSF Office of Cyber Infrastructure through the Blue Waters Undergraduate Petascale Education Program (UPEP). AB, LD and MJ would also like to thank the staff at the Texas Advanced Computing Center (TACC) and the Florida State University and the University of Miami HPC Centers as part of the *Sunshine State Education and Research Computing Alliance (SSERCA)* for available computing resources and helpful discussions.