# Julia Library for QFT in Graphene

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What sets graphene apart from many other intensively studied materials is the relative simplicity of its lattice structure. The honeycomb lattice composed of fairly small atoms whose electronic properties are dominated by $p_z$ orbitals makes a minimal tight-binding description with the nearest-neighbor hopping sufficient for computing a variety of experimentally observable quantities. The fact that such a simple model can retain so much of the experimentally relevant realism makes graphene an excellent platform for investigating basic scientific phenomena, in addition to its tremendous potential for technological applications.

Although most of the analytical work on graphene is performed using the continuum Dirac equation, the tight-binding formalism allows one to preserve the discrete nature of the lattice when introducing defects, vacancies, or other kinds of external perturbations. To study vacancies or defects using the tight-binding approach, one defines a sufficiently large system, where the features of interest are far from the edge. Next, one can diagonalize the Hamiltonian to extract the desired quantities. The need to avoid edge effects restricts the minimum system size, increasing the computational cost. A possible alternative is to use the field-theoretic approach within the tight-binding formalism, removing the finite-size artifacts.

Recently, several works have used quantum field theory and the full tight-binding Hamiltonian to study the effects of defects and vacancies in graphene.[1-3] Unfortunately, the code used in these numerical calculations is either not readily available or not easily adaptable by other research groups. Consequently, the scientific community members have to either perform a lot of redundant work or forego the approach altogether. This unnecessary overhead impedes scientific progress, with researchers spending time debugging the code instead of focusing on physics. Therefore, we propose a curated and tested extendable library[4] to perform field-theoretic calculation in graphene, written in the fast Julia language.[5] The library can grow continuously as new features are added by researchers, allowing the community to take advantage of earlier work.

## REFERENCES

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2. K. Noori, H. Biswas, S. Y. Quek, and A. Rodin, Phys. Rev. B **101**, 115421 (2020)
3. K. Noori, S. Y. Quek, and A. Rodin, Phys. Rev. B **102**, 195416 (2020)
4. https://github.com/rodin-physics/GrapheneQFT.jl
5. J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah, SIAM Rev. **59**, 65 (2017)

## FIGURES

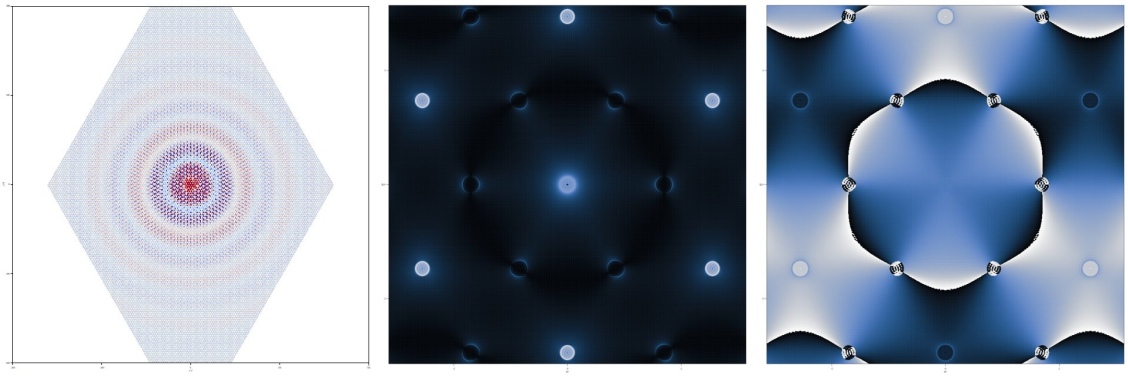

**Figure 1:** Figures generated by the code. (Left) Real-space spectral function for a single Nitrogen impurity in graphene for energy 0.4eV above the Dirac point. Note the Friedel oscillations. (Middle) Magnitude of the Fourier transform of the real-space data demonstrating the intra- and inter-valley scattering. (Right) Phase of the Fourier transform.