Computation of resonances in locally perturbed periodic quantum systems

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Abstract

We introduce a new numerical method to compute resonances induced by localized defects in crystals. This method solves an integral equation in the defect zone to compute analytic continuations of resolvents. Such an approach enables one to express the resonance in terms of a localized, compact-supported function. The kernel of the integral equation is the Green function of the undefective region, which is extended by a complex deformation of the Brillouin zone, thereby generalizing in reciprocal space the concept of complex coordinate transformations.

Keywords: Resonances, Green function, defect in a solid, complex scaling.

1 Introduction

We consider a one-body (possibly mean-field) Hamiltonian H, describing for instance a molecule or a defect in a solid. The motivation and the expected applications come from mean-field models such as time-dependent density functional theory (TDDFT). Knowledge of the resolvent $R(z)$ of the Hamiltonian close to the real axis is of interest to calculate the density of states, or for time-dependent response properties for instance. When the Hamiltonian is a small perturbation of a reference Hamiltonian that has both bound and continuous states at the same energy E , the coupling between these states typically results in a bump of R at E. This corresponds to a resonance, which can be formally defined as a pole in the analytic continuation of the resolvent of the system from the upper complex plane into the lower, through the essential spectrum of H. This extension of the resolvent makes sense only if we consider $R(z)$ applied on localized functions, which we will always do.

However, the truncation of H to a finite region of space will discretize the energy spectrum, not allowing for this extension. This is related to qualitative differences in wave propagation described by the full and truncated Hamiltonians. Quantities on the real axis can be obtained by approximating $R(\omega)$ by $R(\omega + i\eta)$ for some finite artificial dissipation $\eta > 0$, but it does not allow to reach the resonances below the real axis.

We propose a method to express the continuation of resolvent on and below the real spectrum for Hamiltonians of the form $H = H_0 + V$, where H_0 is periodic on an infinite domain, and V is localized.

2 Method

We reformulate the problem as an integral equation posed in the region of the defect, similar to the Lippman-Schwinger method used in scattering problems. It allows to write the resolvent as $R(z) = R_0(z)(1 - VR_0(z))^{-1}$. VR_0 being localized, the essential of the work consists in computing R_0, the resolvent of the periodic part H_0 of the Hamiltonian, possibly extended the lower complex plane of energies z. Resonances can then be found with a Newton method applied to the determinant of $1 - VR_0(z)$.

The resolvent for a crystal Hamiltonian can be expressed as an integral on k over the Brillouin zone, which we deform using a multi-dimensional generalization of the Cauchy integral formula. We choose the deformation function $\mathbf{k}_i : \mathbf{k} \mapsto \mathbf{k} + i\mathbf{k}_i(\mathbf{k})$ so that the singularities of the integrand get pushed down into the lower complex plane for z, extending the domain of validity of the integral formula below the essential spectrum. An analogy can be drawn with the complex scaling method, which is a deformation in the real space rather than the reciprocal space.

This new method is based on ideas that have been used for theoretical studies [1–3] and recently been used as a numerical method in 1D

scattering problems [4]. The resulting scheme only requires unit cell computations.

3 Resolvent for a graphene lattice

We apply our method on a graphene tight-binding model (discrete Schrödinger operator). We will first compute the resolvent of the unperturbed Hamiltonian H_0 and extend it below the real axis.

The Bloch-Floquet transform of H_0 is a 2×2 complex matrix $H_{\mathbf{k}}$. We plot Figure 1 the eigenvalues $\varepsilon_{n\mathbf{k}}$ of this matrix over the Brillouin zone $\mathcal{B}$.

At a given energy z, the points $\mathbf{k}$ of the Brillouin zone at which the $\varepsilon_{n\mathbf{k}}$ are equal to z will cause a singularity, since the integral is:

$$R_0(\mathbf{R}, \mathbf{R}'; z) = \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')} \sum_{n=1}^{N} \frac{|u_{n\mathbf{k}}\rangle\langle u_{n\mathbf{k}}|}{z - \varepsilon_{n\mathbf{k}}} d\mathbf{k}.$$

Using a generalization of the Cauchy integral theorem, we deform the integration path by adding an imaginary part $i\mathbf{k}_i(\mathbf{k})$ to $\mathbf{k}$ around those points. Choosing $\mathbf{k}_i$ in the opposite direction to the gradient of the eigenvalue, we ensure that points z at which the integrand of the resolvent is singular are pushed downwards the real axis at first order. The deformation $\mathbf{k}_i$ over the Brillouin zone is shown Figure 1.

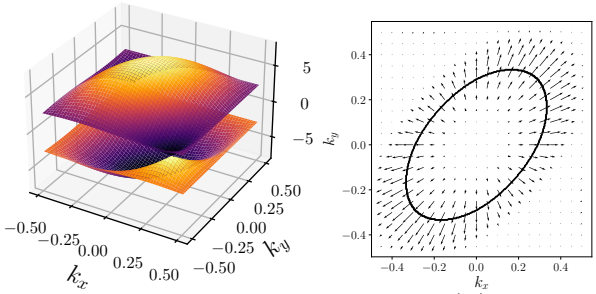

Figure 1: Dispersion relation $\varepsilon(\mathbf{k})$ of the graphene, and example of deformation $\mathbf{k}_i$ at $z = 2$ over the renormalized Brillouin zone.

This provides an extension of R_0 below the real axis as shown Figure 2.

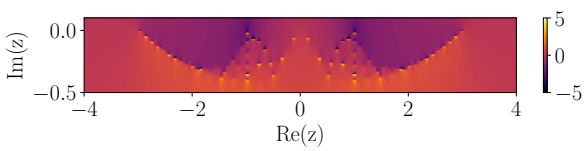

Figure 2: Imaginary part of the trace per unit cell of the resolvent. The integral is approximated by a Riemann sum of $N = 13$ terms.

4 Perturbation of the lattice with an adatom

We now add a single adatom on the lattice, linked to one site of the lattice with hopping constant ϵ, and with an energy E. We use the R_0 computed as above to look for the zeros of the determinant of $(1 - VR_0(z))$ (see Figure 3) with a Newton descent. These zeros are resonances of the system. We show Figure 4 the resonant state of the system $\psi = R_0(z_{\text{res}})\phi$, where ϕ is the localized state associated to the eigenvalue 0 for $(1 - VR_0(z_{\text{res}}))$.

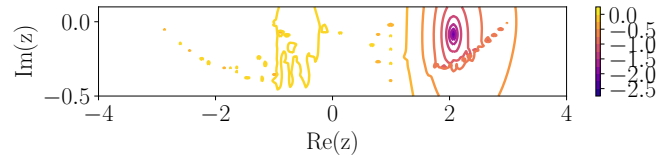

Figure 3: Log10 modulus of the smallest singular value of $I - VR_0$. One pole appears at $2.1 - 8.6e^{-2}i$.

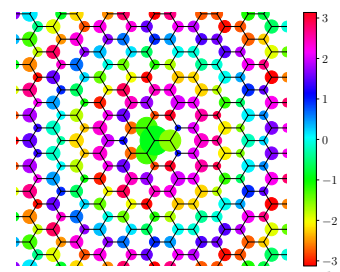

Figure 4: Resonant state associated to the resonance $2.1 - 8.6e^{-2}i$. The size of the dots is proportional to the modulus of the state, the color represents the phase.

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