LevelSetIntegrate

This code is written by Phum (Gene) Siriviboon.

Problem Statement

Calculate the integration of the form

$$I = \int_V dx \frac{p(x)}{q(x) + i0^+}.$$

Assuming that the singularity on the integrand only emerges due to zeros of $q(x)$

Introduction

using an identity $\frac{1}{x+i0^+} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$, we can see that

$$\operatorname{Re} I = \mathcal{P}\int_V dx\, \frac{p(x)}{q(x)},$$

$$\operatorname{Im} I = -\pi \int_V dx\, \delta(q(x))p(x).$$

which can also be rewitten as

$$\operatorname{Re} I = \mathcal{P}\int \frac{dc}{c} \int_{q(x(t))=c} dx(t)\, \frac{p(x(t))}{|\nabla q(x(t))|},$$

$$\operatorname{Im} I = -\pi \int_{q(x(t))=0} dx(t)\, \frac{p(x(t))}{|\nabla q(x(t))|}.$$

We can see that for both the real and imaginary part, the integrand is concentrated near $q(x) = 0$ which would result in major contribution of the integral. Here, we propose the following scheme.

Initial mesh subsampling [Getting Level set]

Here we outline the algorithm for the initial mesh subsampling

1. Initiate a mesh e.g. $2 \times N \times N$ triangular grid
2. Calculate $q(x)$ for every vertices of the meshes
3. Label every triangles with subsample tags
4. Iterate through the faces with following

- For triangle xyz calculate $q_x = q(x), q_y = q(y), q_z = q(z)$
- If three of the function are zero label the face with subsample tag
- If two of q_i are zero or $q_i q_j < 0$, tag the triangle with singularity tag and test the following
  - consider edge i, j: find midpoint k if $|q_k - (q_i + q_j)/2| > l_{ij}\varepsilon$ where l_{ij} are the distance between i andj, label the triangle with subsample tag
- Else, remove the subsample tags

5. Subsample on all the triangles with the subsample tag.
6. Repeat 3 and 4 for n times or until run out of subsampled tag

Integration

Imaginary Part

1. For each triangle, find zero using k-step newton-raphson method and return edge(s) ij
2. Approximate $|\nabla q(x)|$ with finite difference method and linear interpolation
3. Integrate $p(x)/|\nabla q(x)|$ along ij using adaptive trapeziod rule

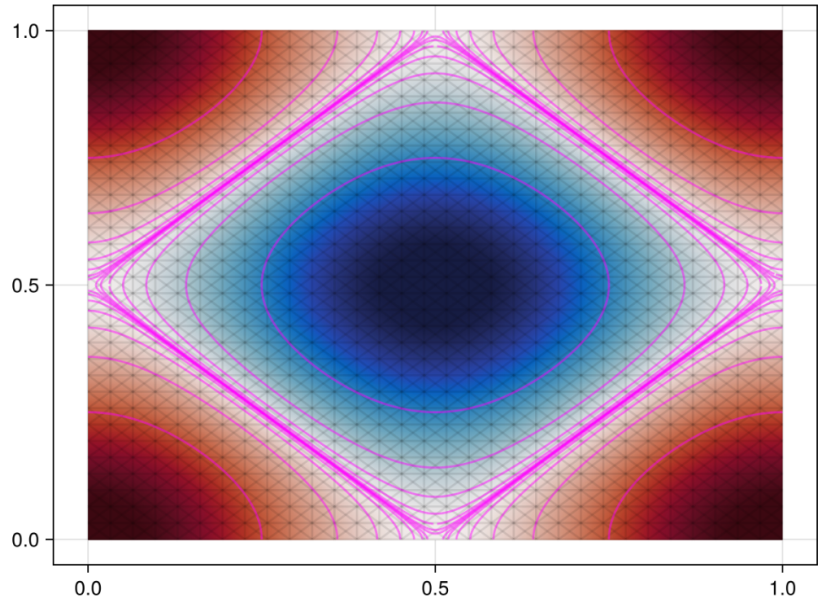
Real parts

1. For each triangle, find $q(x) = c$ using k-step newton-raphson method and return edge(s) ij
2. Approximate $|\nabla q(x)|$ for each faces with finite difference method
3. Integrate $p(x)/|\nabla q(x)|$ along ij using adaptive trapeziod rule and set to $F(c)$
4. Integrate $\int d\ln(c)\, F(c)$ using adaptive trapeziodal rule

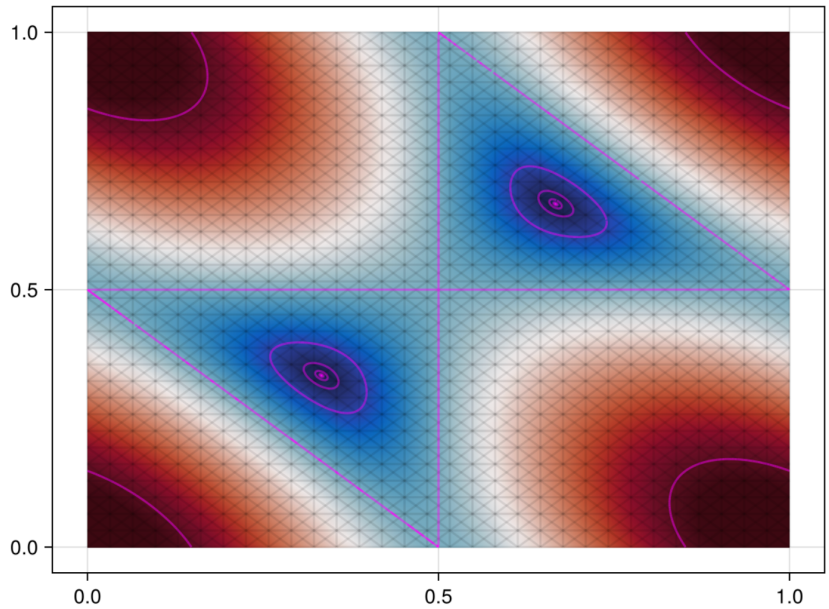
Results and Bachmarking

Level set i.e. Fermi Level

Square Lattice

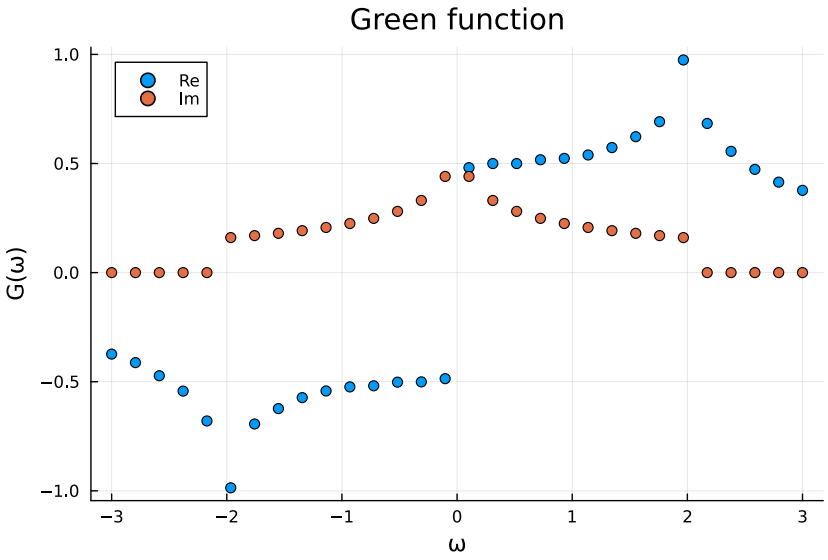


Graphene Band (with linear transformation)

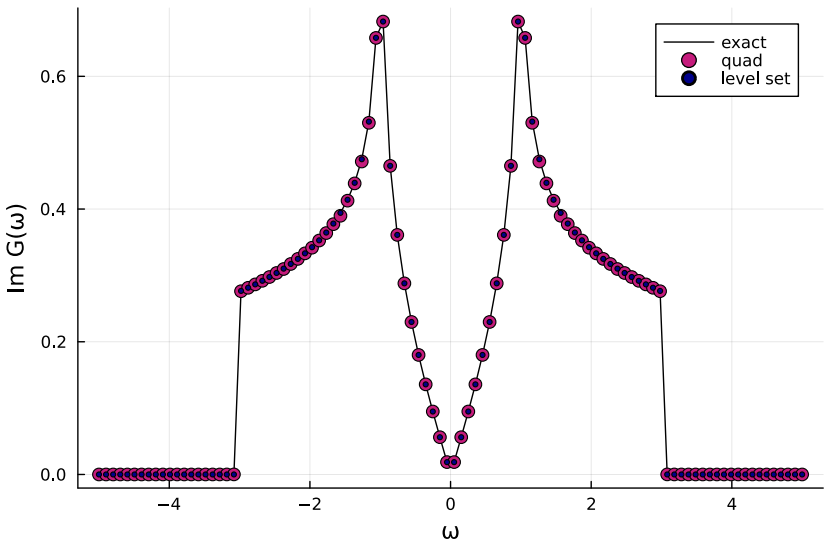


Density of state

DOS of square lattice



graphene DOS computed using exact, level set method, and quadruture method



Benchmarking

Here we compute the density of state of graphene band at $\omega = 2.0$ and compare the result with the 2d quadruture rule using error as a function of runtime as metric.