

Short presentation of the article under review in J Phys A

Efficient evaluation of lattice Green's functions

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Lattice functions in physics

(theoretical physics (TP) and computational materials science (CMS))

- Lattice sums
 - ▶ Coulomb sums
 - CMS*: *Ewald summation*
 - TP: *exponential sums*
 - ▶ Dipole sums (e.g. infrared divergence of electron-phonon couplings in Frolich model [PRB 105, 214301 \(2022\)](#))
- Partial difference equations
 - ▶ Laplace equation on a lattice and tight-binding Hamiltonians
 - CMS: *Fourier transform*
 - TP: *subject of this study*
- Correlation functions of lattice models

These are special functions but essentially multidimensional[†]
⇒ No generic implementation in generic software packages

* CMS needs universal approach robust for *typical* values of parameters, TP needs arbitrary precision and analytic expressions for *any* values of parameters.

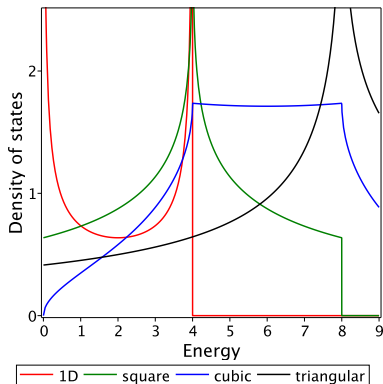
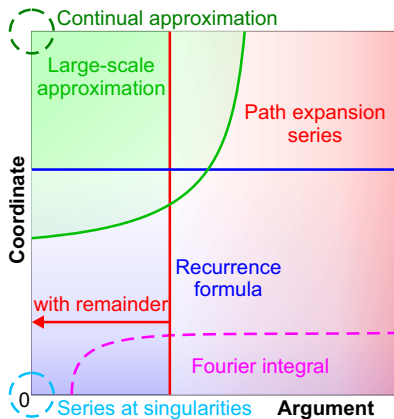
[†] Commonly used special functions are defined from 1D algebraic or difference or differential equations and 1D sums or integrals.

Lattice Green's function: definition and evaluation methods

It is resolvent ("solution") of Laplace operator on lattice:

$$G_{xy}(s) = [(s - \Delta)^{-1}]_{xy} \equiv G_{x-y}(s) \quad \hat{G}(s, k) \sim (s + k^2)^{-1}$$

$$G_{xy}(s) = \int_0^\infty \tilde{G}_{xy}(t) e^{-st} dt, \text{ where } \tilde{G}_{xy}(t) \text{ is propagator} \\ \text{(or transition probability of a random walk)}$$



Examples of use of lattice Green's function

(Evaluation efficiency is critical beyond mean-field because of summation of G)

$$G_{xy}(s) = [(s - \Delta)^{-1}]_{xy} \equiv G_{x-y}(s) \quad \hat{G}(s, k) \sim (s + k^2)^{-1}$$

- Electronic structure of crystals
- Quantum and statistical short-range lattice models
- Lattice models of disorder

What is wrong with Fourier integrals?

Benchmarking path expansion series and Fourier integral for evaluation of the Green's function of the simple cubic lattice

s	Parameters		Exact value	Number of terms		
	(x, y, z)	precision		series	sum	Fourier
1	(0,0,0)	single	0.170523807	0	40	100
1	(8,6,3)	single	$2.3 \cdot 10^{-7}$	—	70	1000
1	(80,60,30)	single	$2.0 \cdot 10^{-48}$	—	200	10^5*
0	(0,0,0)	1%	0.252731010	1	1000	4000
0	(0,0,0)	0.1%		1	?	$4 \cdot 10^6$
0	(0,0,0)	single		100	?	?
-4	(0,0,0)			—	—	?

'series' = 'sum' + series remainder (new result of this work)

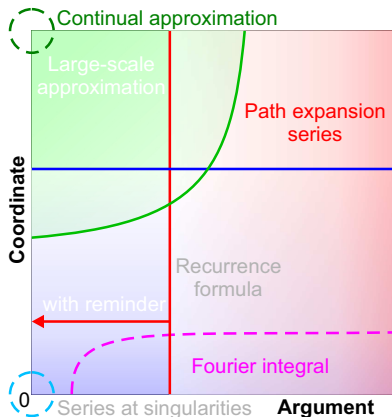
* double-precision is insufficient

State of the art and proposed advance

Before:*

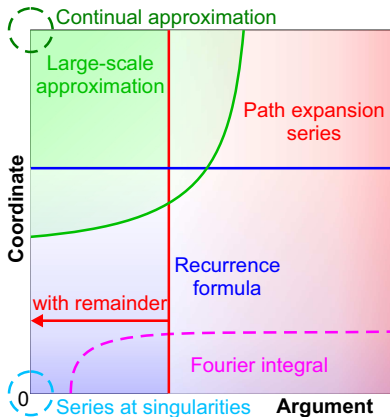
2D: square, triangular, honeycomb

3D: bcc, fcc, diamond, simple cubic



After:

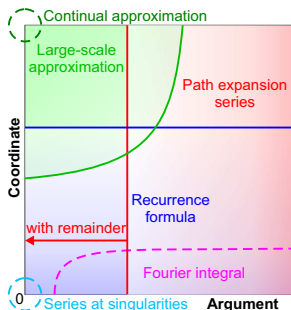
Any lattice with
root-free band dispersion



* Known recurrence formula in 3D are multi-page lattice-specific.
No efficient algorithm for regular part of series at singularities.

Milestones and current state of the art

- 1940 $G_{000}(0)$ for 3D* lattices [Watson]
- 1970 Efficient algorithms for 2D lattices & proof-of-principle results for 3D lattices [Katsura, Morita, Horiguchi *et al*]
- 2000 More efficient formulas in 3D & series at 0 for hypercubic [Joyce]
- 2010 Review and ideas for multiD lattices [Zucker, Guttman]



Open problems = targets of this study

- Efficient implementation (starting from 3D)
- Other lattices (starting from hypercubic, generic approaches)
- Series at singularity (partially solved for hypercubic [Joyce03])
- Series remainders
- Approximations (simple explicit formula with $\sim 5\%$ accuracy)

2D = square, triangular, honeycomb; 3D = bcc, fcc, diamond, simple cubic

Result 1: Recurrence relations and series at singularities

Two problems with existing recurrence schemes:

- cumbersome for analysis and implementation
- lattice-specific

There should be generic recurrence relations for “simple” lattices

“Simple” = translational invariance + root-free dispersion $S_\mu(k)$

$$G_{0x}(s) \equiv G_\xi^{\beta\alpha}(s) = \frac{1}{(2\pi)^d} \int \cdots \int_{-\pi}^{\pi} \hat{G}^{\beta\alpha}(s, k) e^{-ik\xi} dk$$

$$\hat{G}^{\beta\alpha}(s, k) = \sum_{\mu=1}^{\nu} \frac{P_\mu^{\beta\alpha}(k)}{s - S_\mu(k)}$$

For simplicity, let consider primitive lattices:

$$\hat{G}(s, k) = (s - S(k))^{-1}, \quad S(k) = \sum_{|z|=1} \cos kz + \text{const}$$

Result 1: Recurrence relations for primitive lattices

$$\hat{G}(s, k) = (s - S(k))^{-1} \quad \text{and propagator } \hat{\hat{G}}(t, k) = e^{tS(k)}$$

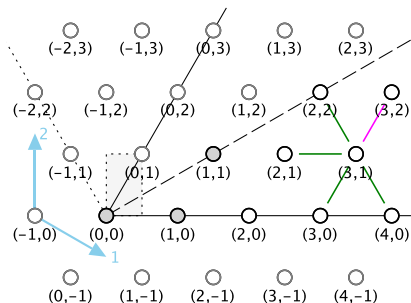
There is a hidden “space-time” symmetry:

$$\frac{\partial \hat{G}}{\partial k_i} = -\frac{\partial S}{\partial k_i} \hat{G}' \quad \text{and} \quad \frac{\partial \hat{\hat{G}}}{\partial k_i} = t \frac{\partial S}{\partial k_i} \hat{\hat{G}}$$

producing d identities:

$$\sum_{|z|=1} \frac{z_i}{x_i} G_{x+z}(s) = - \int_s^\infty G_x(s') ds', \quad i = \overline{1, d}$$

Result 1: Recurrence relations – outcome



For any “simple” lattice we get

- Recursive evaluation of Green's function $G_x(s)$, i.e. quasi-1D structure of G_{xy}
- Finite basis $G_x(s) = \sum_{n=0}^d P_n(s) G_{e_1+e_2+\dots+e_n}(s)$ with polynomial coefficients, i.e. only d non-polynomial functions!
- d -order linear ODE with polynomial coefficients for $G_0(s)$,
 \implies series expansion at singular points

Result 2: Series, remainders, and approximations

Path expansion series in a general case:

$$G_{xx}(s) = \frac{1}{(s + w_x)} + \sum_{z: |x-z|=1} \frac{t_{xz}t_{zx}}{(s + w_x)^2(s + w_z)} + \dots$$

and for lattice of identical sites:

$$G_{yx}(s) = \sum_{n=0}^{\infty} \frac{N_{yx}(n)}{(s + w)^{n+1+|x-y|}}$$

where $N_{yx}(n)$ is number of paths of length n and w is number of neighbors.

For any “simple” lattice we get

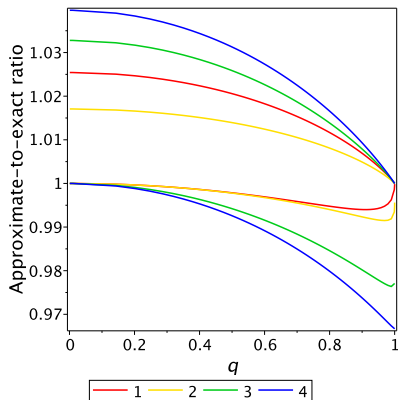
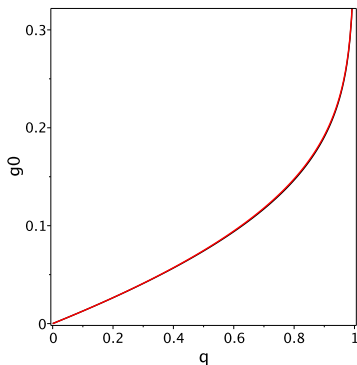
- No more than 1-summation formula for N_{yx} recursively in d

Result 2: Path expansion series remainder

By approximating $N_{yx}(n)$ at large n using Stirling's formula we get

$$R_{yx}^n = Cq^{n+1+|x-y|}\Phi(q, \alpha, n + \varepsilon), \text{ where } q = \frac{w}{s+w}$$

and Φ is Lerch transcendent. Good results even for $n = 0$ or -1 :



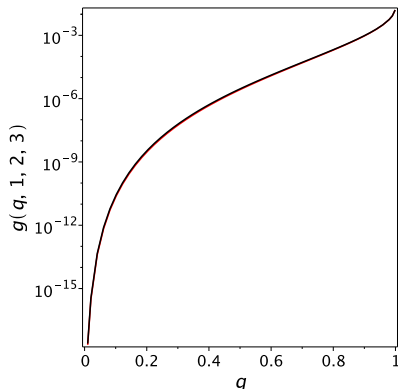
Result 2: Large-scale approximation

For translationally invariant lattice

$$\tilde{G}_x(t) = \frac{1}{(2\pi)^d} \int \cdots \int_{-\pi}^{\pi} e^{tS(k) - ikx} dk$$

can be evaluated with saddle point method.

Good results even for small x :



Result 3: Implementation in LatticeTools package

- Open-source Maple code, 1000 lines for 100 functions
- Documented in Maple notebooks
- Hypercubic and triangular lattices are fully implemented
- Efficient to evaluate 5D hypercubic lattice on a laptop
- Other functionalities include calculation of diffusion and mobility tensors as described in [JPCC 117, 4920 \(2013\)](#)