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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[†]
$\Longrightarrow$ *No generic implementation in generic software packages*

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* 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.

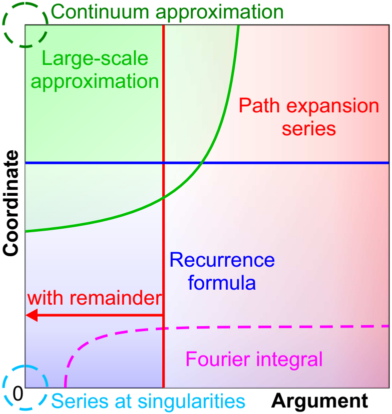
Lattice Green's function: definition and evaluation methods

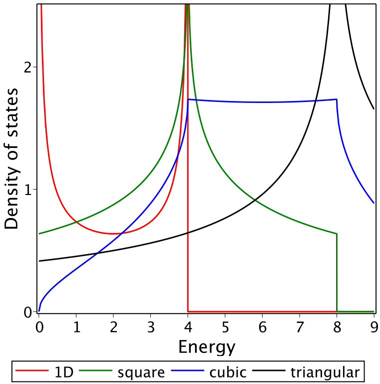
It is resolvent ("solution") of Laplace operator on lattice:

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

$$G_{xy}(s) = \int_0^\infty \tilde{G}_{xy}(t)\mathrm{e}^{-st}\,\mathrm{d}t,$$ where $\tilde{G}_{xy}(t)$ is propagator

(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)

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

- 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

Parameters			Exact	Number of terms		
s	(x, y, z)	precision	value	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)

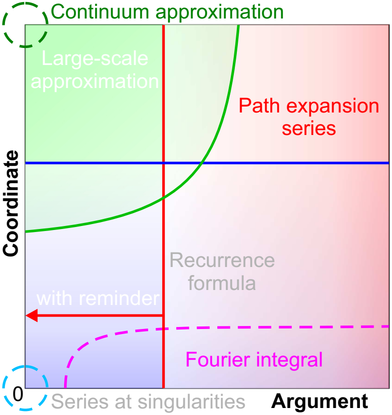
* double-precision is insufficient

State of the art and proposed advance

Before:*

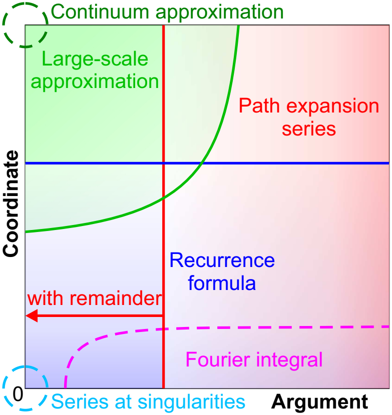
2D: square, triangular, honeycomb

3D: bcc, fcc, diamond, simple cubic



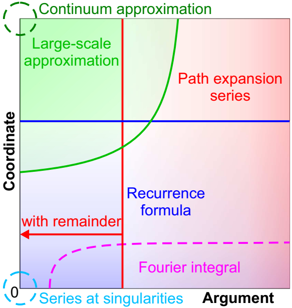
After:

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 *etal*]

2000 More efficient formulas in 3D & series at 0 for hypercubic [Joyce]

2010 Review and ideas for multiD lattices [Zucker, Guttmann]

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 ∼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 $S_\mu(k)$

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

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

For simplicity, let consider primitive lattices:

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

Result 1: Recurrence relations for primitive lattices

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

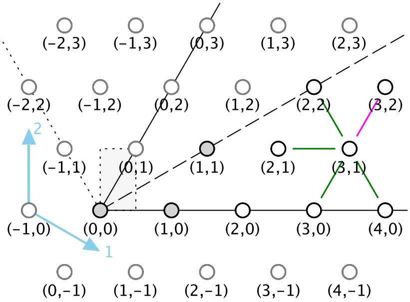
There is a hidden "space-time" symmetry:

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

producing d identities:

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

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 $G_x(s) = \sum_{n=0}^{d} P_n(s)\, G_{e_1+e_2+\ldots+e_n}(s)$ 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:

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

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

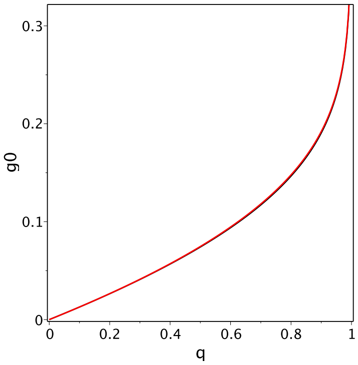
- No more than 1-summation formula for N_{yx} recursively in d

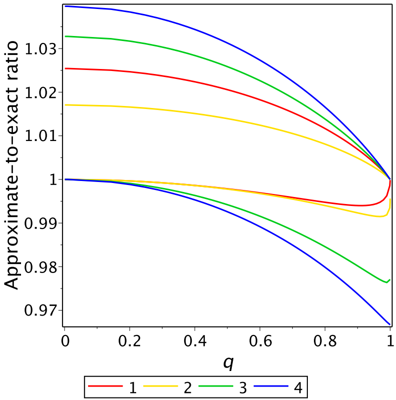
Result 2: Path expansion series remainder

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:





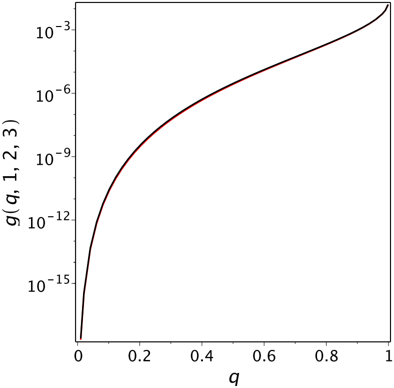
Result 2: Large-scale approximation

For translationally invariant lattice

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

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)