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# KPM.jl: A Julia Package for Kernel Polynomial Method in Condensed Matter Physics

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## Summary

The Kernel Polynomial Method (KPM) is a numerical technique for approximating spectral densities and response functions of large Hermitian operators without performing full diagonalization (Weisse et al., 2006). KPM expands spectral functions in Chebyshev polynomials and evaluates them via recursive matrix-vector multiplications. Reconstructing the moments of the Chebyshev expansion depends on the observable of interest and can be computed through either a single inner product or through a trace, which is computed using a stochastic trace (Skilling, 1988). Carefully chosen kernels (e.g., the Jackson) suppress Gibbs oscillations and improve convergence of the truncated Chebyshev series. Because the dominant cost is sparse matrix–vector products, KPM scales (nearly) linearly with the size of the Hilbert space, which for non-interacting systems scales like the volume, and can be applied to extremely large sparse Hamiltonians to compute quantities such as the density of states (DOS) and DC conductivity (João & Lopes, 2019).

`KPM.jl` is a Julia implementation (Bezanson et al., 2017) of KPM for tight-binding models in condensed matter physics, providing a high-performance, user-friendly toolbox. `KPM.jl` targets large sparse Hamiltonians, integrates with `CUDA.jl` for automatic GPU acceleration when available, and is designed for scalability and ease of integration into Julia-based workflows for large-scale spectral and transport calculations.

## Statement of need

`KPM.jl` provides a high-performance implementation of the Kernel Polynomial Method tailored to tight-binding models. The method avoids ever doing a full diagonalization and instead uses Chebyshev expansions, the package enables spectral and transport calculations on very large sparse Hamiltonians that are infeasible with exact diagonalization (ED). It fills the gap between low-level C/Fortran libraries and interactive, reproducible Julia workflows by offering:

1. **Scalability:** Capable of handling large sparse matrices representing realistic tight-binding models.
2. **Versatility:** Support for DOS and LDOS, as well the DC conductivity (both longitudinal and Hall) as well as linear and nonlinear optical response functions.
3. **Performance:** Automatic GPU acceleration via `CUDA.jl` when available.
4. **Integration:** As a Julia package, it easily interfaces with other tools in the Julia ecosystem for Hamiltonian generation and data analysis.

In condensed matter physics, understanding the effects of disorder, interactions, and complex lattice geometries often requires numerical simulations of very large Hamiltonians. Traditional ED methods for computing the full spectrum are limited to relatively small system sizes (typically $N \sim 10^4$ states), which can be insufficient to resolve the spectral features of disordered systems or incommensurate structures like twisted bilayer graphene. `KPM.jl` is especially useful for studies of disorder, moiré systems, and topological materials where large system sizes ($N \sim 10^7$ states) are essential to capture realistic spectral and transport behavior.

## Software design

`KPM.jl` is designed with modularity and performance in mind. The package operates on sparse Hamiltonians and computes Chebyshev moments using stochastic trace estimation with random vectors. The core functionality is divided into three main tiers corresponding to the complexity of the response function:

- **Density of States (1D):** The `KPM.kpm_1d` function computes the Chebyshev moments for the DOS. It supports stochastic estimation using multiple random vectors (`NR`) and allows users to supply custom input vectors to compute the LDOS. The moments are converted to the spectral density $\rho(E)$ using `KPM.dos`.
- **Linear Response (2D):** For transport properties like DC conductivity, `KPM.kpm_2d` calculates the moments required for the Kubo-Greenwood formula involving two current operators $(J_x, J_y)$. The function `KPM.d_dc_cond` processes these moments to obtain the energy-dependent conductivity $\sigma_{\alpha\beta}(E)$ with $\alpha, \beta = x, y, z$.
- **Nonlinear Response (3D):** The package includes specialized routines (`KPM.kpm_3d`) for frequency-dependent linear and nonlinear responses, such as the Circular Photogalvanic Effect (CPGE). This involves computing moments for three operators $(J_x, J_y, J_z)$ and post-processing them (`KPM.d_cpge`) to extract the second-order conductivity $\chi_{xyz}(\omega_1, \omega_2)$.

The software automatically detects available hardware and offloads matrix-vector multiplications to a GPU if a compatible CUDA device is present (`KPM.whichcore()`), ensuring efficient performance on modern clusters. Further memory can be saved by computing the matrix elements of $H$ and $\mathbf{J}$ on the fly, which is not implemented here.

## Example Usage

The following minimal example computes the DOS of a 1-D tight-binding chain using `KPM.jl`.

```
using KPM
using LinearAlgebra
using SparseArrays
using Plots

# Simple dense 1D tight-binding Hamiltonian (periodic)
function tb1dchain(N::Integer; t::Real=1.0)
    H = zeros(Float64, N, N)
    for i in 1:(N-1)
        H[i, i+1] = -t
        H[i+1, i] = -t
    end
    H[1, N] = -t
    H[N, 1] = -t
    return H
end
```

```julia
# Parameters
N = 500                # system size
NC = 256                # Chebyshev order
NR = 32                # number of random vectors for stochastic trace
nE = 1000              # output energy grid points

H = tb1dchain(N)
# Rescale H -> (-1, 1)
Hsparse = sparse(H.*(1+0*1im)) # make the Hamiltonian sparse under complex number
b, H_norm = KPM.normalizeH(Hsparse)

# Compute Chebyshev moments (DOS)
mu = KPM.kpm_1d(H_norm, NC, NR)    # returns moments (array-like)

# Reconstruct DOS on a grid and map energies back to physical scale
E, rho = KPM.dos(mu, b;kernel = KPM.JacksonKernel, N_tilde=nE)

# Analytical DOS
rho_exact = zeros(length(E))
mask = abs.(E) .< 2
rho_exact[mask] = 1.0 ./ (π * sqrt.(4 .- E[mask].^2))

# plot the DOS
plot(E, rho, xlabel="E", ylabel="DOS", label="KPM")
plot!(E, rho_exact, lw=1, ls=:dash, label="Analytic")
```

The final DOS is shown in Figure 1. Discrepancies between the KPM and analytic results arise from the finite system size, the truncated KPM expansion order, and stochastic trace estimation error.

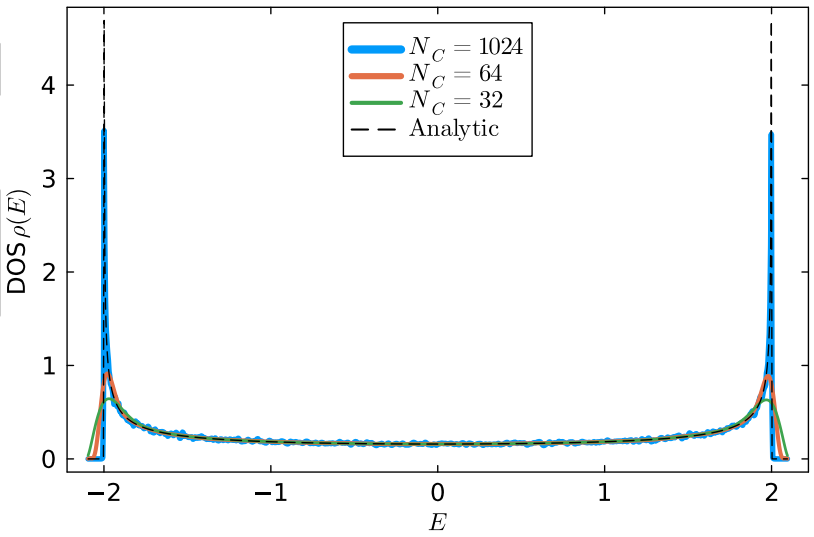


**Figure 1:** Density of states for a simple 1D tight-binding chain $L = 10^4$: KPM (solid) with variouns expansion order $N_C = 16, 32, 1024$ vs. analytic (dashed). The number of random vectors for the stochastic trace is $N_R = 10$.

## Research impact statement

KPM.jl has been utilized in numerous studies to investigate electronic structure and response in complex materials:

1. **Moiré systems and disorder:** Enabled large-scale simulations of twisted bilayer graphene and demonstrated how twist-angle disorder broadens flat bands and modifies spectral features (Chang et al., 2024; Chou et al., 2020; Fu et al., 2020; Wilson et al., 2020; Yi et al., 2022).
2. **Experimentally relevant transport calculations:** Applied to transport modeling based on tight-binding models derived from DFT+U to directly compare theory with experiment (Liu et al., 2021; L. Wu et al., 2020; T.-C. Wu et al., 2025).
3. **Effects of Quasiperodic potentials:** Used to compute conductivity and disorder-averaged spectral properties and Green's function in disordered materials (Fu et al., 2021; Yi et al., 2022).
4. **Nonlinear optical responses and disordered topological material:** Employed to calculate nonlinear responses such as the CPGE in disordered topological semimetals and to identify spectral signatures of surface and bulk phase transitions in disordered axion insulators (Grindall et al., 2025; A.-K. Wu et al., 2024).
5. **Method benchmarking and numerical validation:** Served as a reference implementation for comparing and validating new Chebyshev-regularization and spectral-density algorithms (Yi et al., 2025).

These applications demonstrate the package's capability to tackle cutting-edge problems in condensed matter theory.

## AI usage disclosure

GitHub Copilot was used to assist with updating CUDA-related code, improving tests and documentation, and polishing the manuscript for clarity and readability. The authors reviewed, edited, and validated all AI-assisted contributions and take full responsibility for the content of this publication.

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