POLITECNICO
MILANO 1863

SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Tensor-Based Compression and Interpolation of Electron-Phonon Matrix Elements: Towards AbInitio Diagrammatic Monte Carlo

Tesi di Laurea Magistrale in
Engineering Physics - Ingegneria Fisica

Author: **Davide Patricelli**

Student ID: 250933
Advisor: Prof. Paolo Biscari
Co-advisors: Cesare Franchini
Academic Year: 2024 - 25

Abstract

This thesis develops a computational framework bridging first-principles electron–phonon calculations and Diagrammatic Monte Carlo (DiagMC) simulations. While Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) provide accurate material-specific electron–phonon matrix elements on coarse Brillouin-zone grids, their direct use in many-body solvers is limited by the high dimensionality of the momentum- and band-dependent coupling tensor required on much finer grids.

We analyze the structure of this tensor in both Bloch and Wannier representations and show that the latter exhibits significant low-rank features. Exploiting this property, we develop tensor-based decomposition and interpolation strategies that enable accurate reconstruction of the full coupling from a compressed representation. In parallel, we implement an explicit momentum- and band-resolved DiagMC solver fully compatible with ab initio input.

Complementary to recent matrix-based approaches [1, 2], our method adopts a tensor formulation within a distinct DFT–DiagMC environment, providing a scalable route toward ab initio Diagrammatic Monte Carlo for realistic electron–phonon systems.

Abstract in lingua italiana

Questa tesi sviluppa uno schema computazionale che collega i calcoli elettrone–fonone basati sui primi principi alle simulazioni Diagrammatic Monte Carlo (DiagMC). Mentre Density Functional Theory (DFT) e Density Functional Perturbation Theory (DFPT) forniscono elementi di matrice elettrone–fonone specifici per il materiale su griglie a bassa risoluzione della zona di Brillouin, il loro utilizzo diretto nei metodi a molti corpi è limitato dall'elevata dimensionalità del tensore di accoppiamento dipendente dal momento, richiesto su griglie molto più dense, e dall'indice di banda .

Analizziamo la struttura di tale tensore nelle rappresentazioni di Bloch e di Wannier, mostrando che quest'ultima presenta marcate caratteristiche di basso rango. Sfruttando questa proprietà, sviluppiamo strategie di decomposizione e interpolazione basate su tecniche tensoriali che consentono una ricostruzione accurata dell'accoppiamento completo a partire da una rappresentazione compressa. Parallelamente, implementiamo un algoritmo DiagMC esplicitamente dipendente da momento e banda, pienamente compatibile con input ab initio.

In modo complementare ai recenti approcci basati su matrici [1, 2], il nostro metodo adotta una formulazione tensoriale all'interno di un distinto ambiente computazionale DFT–DiagMC, fornendo un percorso scalabile verso il Diagrammatic Monte Carlo ab initio per sistemi elettrone–fonone realistici.

Contents

Introduction

The aim of this thesis is to create and validate a bridge between two powerful methods in computational physics: Density Functional Theory (DFT), which allows the calculation of many quantities of interest *ab initio*, and Diagrammatic Monte Carlo (DiagMC), a stochastic method that can converge to practically exact theoretical results. The goal is therefore to motivate and develop a consistent framework that may be referred to as *ab initio* Diagrammatic Monte Carlo.

These methods are applied in particular to one of the fundamental interactions occurring in condensed matter: the interaction between electrons and phonons. This is an intrinsically interacting quantum many-body problem, at the basis of the accurate understanding of many physical phenomena and material properties, as well as of the formation of emergent quasiparticles such as the polaron.

The main obstacle in moving from DFT outputs to Monte Carlo simulations is that, in order to describe the interaction between these fermionic and bosonic degrees of freedom within an effective Hamiltonian, one needs access to a high-dimensional tensor encoding the electron–phonon coupling. Computing and storing this tensor in full is impractical. While interpolation techniques exist, their computational cost is typically too high to be compatible with the repeated evaluations required in a Diagrammatic Monte Carlo simulation.

To overcome this limitation, it is necessary to reformulate the problem at the level of its representation. In the Bloch basis, the electron–phonon coupling tensor is intrinsically high-dimensional and delocalized, making any direct compression ineffective. By transforming the problem to the Wannier representation, where spatial locality becomes explicit, the tensor acquires a structured form that reveals an intrinsic low-rank character. We then introduce techniques from numerical linear algebra, commonly employed in data analysis and machine learning to handle high-dimensional datasets, and adapt them to the specific structural properties of the problem. This enables a controlled dimensionality reduction of the coupling tensor, reducing the computational complexity of the interpolation step and significantly accelerating the overall algorithm while preserving physical

accuracy.

In order to arrive at this point, Chapters 1 and 2 introduce, in a reasonably detailed manner, the description of electronic and vibrational degrees of freedom, together with their mutual coupling. Although this presentation may initially appear somewhat distant from the final computational objective, many aspects of the transformations developed later rely precisely on these solid-state physics concepts. At the same time, the basic principles of DFT calculations for the relevant quantities are introduced, with further details provided in Appendix A. Particular attention is devoted to clarifying the passage from semiclassical or first-quantized descriptions to a fully second-quantized formulation, which is essential for embedding the problem within a many-body framework.

This provides the necessary foundation for Chapter 3, where the fundamental tools of quantum field theory in condensed matter physics are introduced, together with the concept of quantum correlators and Feynman diagrams. From this perspective, the construction of a Monte Carlo method based on the diagrammatic expansion of many-body theory follows naturally. The chapter is completed with the considerations required for an *ab initio* implementation that retains full momentum and band dependence.

This, in turn, highlights the necessity of not directly using raw DFT outputs, but instead defining techniques that allow the low-rank factorization, compression, and efficient interpolation of the electron–phonon tensor through advanced linear algebra tools and a generalized Fourier interpolation scheme. This central development is addressed in Chapter 4.

Finally, the last chapter discusses the effects and implications of inserting these methods into a DiagMC framework, outlining both the limitations encountered and possible directions for future developments.

The text presents the main theoretical foundations together with the corresponding implementation aspects. Given the strongly computational character of the thesis, implementation details are provided in the appendices: Appendix A contains the DFT calculations and the Python scripts used to process their outputs, while Appendix B describes the development of the Monte Carlo code.

Acronyms

ASR Acoustic Sum Rule. 32, 33, 102

DFPT Density Functional Perturbation Theory. 34–36

DFT Density Functional Theory. 1, 2, 6, 16, 18–22, 28, 34, 35, 38, 41, 77, 78, 80, 81, 102

DiagMC Diagrammatic Monte Carlo. 1, 2, 43, 58, 63, 65, 66, 74, 77, 87, 95, 107, 109, 111, 112

FBZ First Brillouin Zone. 10, 11, 13

IFC Interatomic Force Constants. 29, 30, 33, 34

MCMC Markov Chain Monte Carlo. 62, 65, 66, 72

PCA Principal Component Analysis. 90

SCF Self-Consistent Field. 20, 34

SVD Singular Value Decomposition. 90–96, 105