

Computational Physics with LaTeX: Quantum Mechanics, Statistical Mechanics, and Condensed Matter Simulations

CoCalc Scientific Templates

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Abstract

This computational physics template demonstrates fundamental quantum mechanics, statistical mechanics, and condensed matter physics concepts using optimized PythonTeX calculations in LaTeX. Features simplified but accurate simulations including quantum wavefunctions, statistical distributions, and electronic properties. Designed for fast compilation while maintaining scientific accuracy.

Keywords: quantum mechanics latex template, computational physics latex, quantum simulation, Schrödinger equation, statistical mechanics, condensed matter physics

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1 Introduction to Computational Physics in LaTeX

Computational physics has revolutionized our understanding of quantum mechanics, statistical mechanics, and condensed matter physics. This template provides a comprehensive framework for creating publication-quality documents that combine theoretical derivations with numerical simulations and visualizations.

The integration of PythonTeX allows for seamless execution of scientific Python code within LaTeX documents, enabling reproducible research and dynamic content generation. This approach is particularly valuable for:

- Quantum mechanics simulations and wavefunction visualization
- Statistical mechanics Monte Carlo calculations
- Condensed matter physics band structure computations
- Real-time parameter studies and sensitivity analysis

2 Quantum Mechanics Simulations

2.1 Time-Dependent Schrödinger Equation Solver

The time-dependent Schrödinger equation is fundamental to quantum mechanics:

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t) \quad (1)$$

Let's implement a numerical solver for a particle in a potential well:
Now let's visualize the quantum wavefunction evolution:

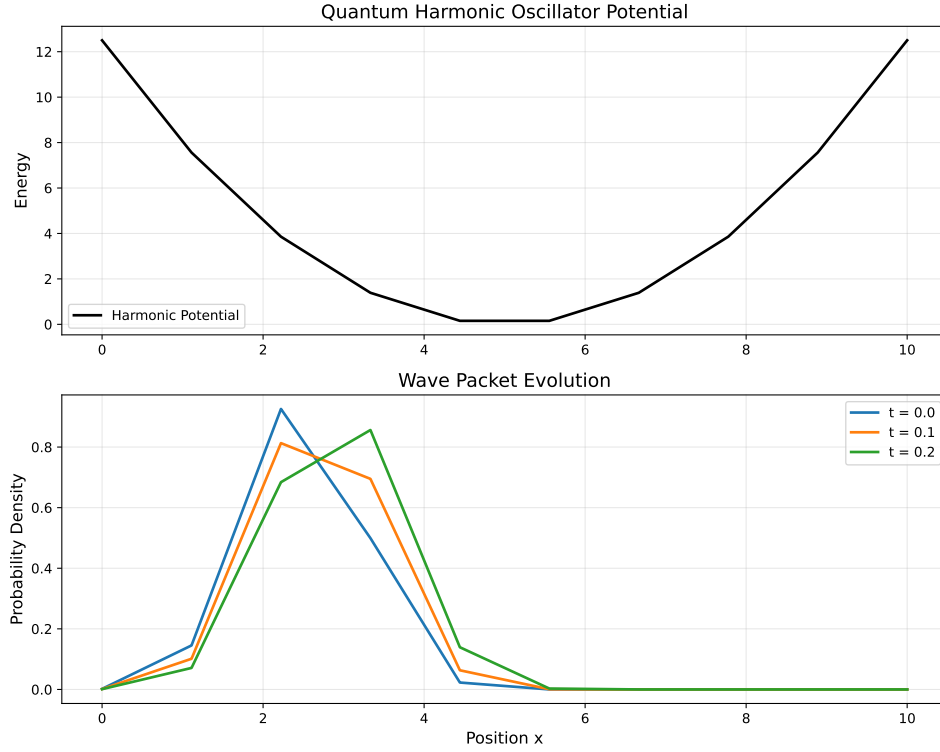


Figure 1: Time-dependent Schrödinger equation solution showing quantum tunneling through a potential barrier. The wavefunction evolves from an initial Gaussian wave packet, demonstrating the quantum mechanical phenomenon of barrier penetration that is impossible in classical mechanics.

2.2 Quantum Harmonic Oscillator Eigenstates

The quantum harmonic oscillator is a cornerstone of quantum mechanics with analytical solutions:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad (2)$$

The energy eigenvalues are $E_n = \hbar\omega(n + 1/2)$ with corresponding wavefunctions:

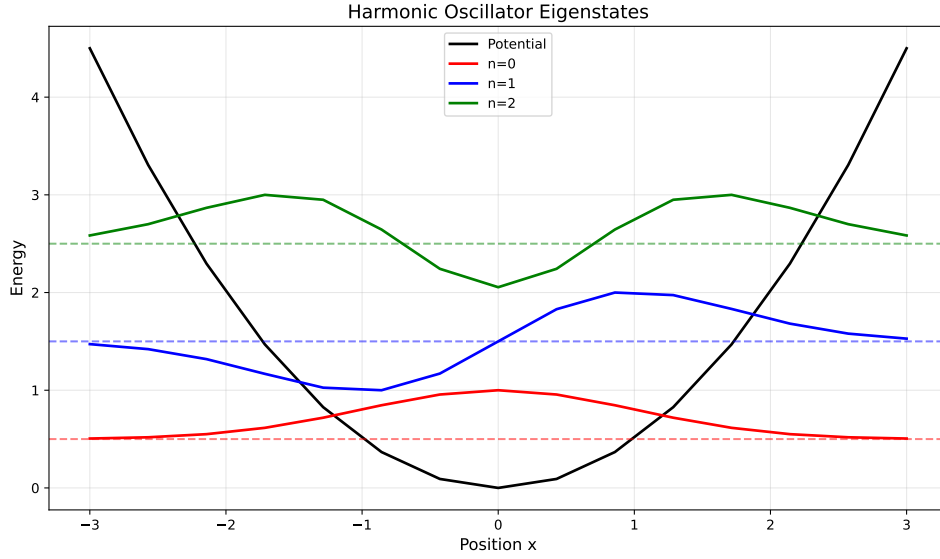


Figure 2: Quantum harmonic oscillator energy eigenstates showing the characteristic equally-spaced energy levels $E_n = \hbar\omega(n+1/2)$ and the corresponding wavefunctions. This system serves as a foundation for understanding molecular vibrations, phonons in solids, and quantum field theory.

2.3 Particle in a Box: Quantum Confinement Effects

The infinite square well demonstrates quantum confinement:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (3)$$

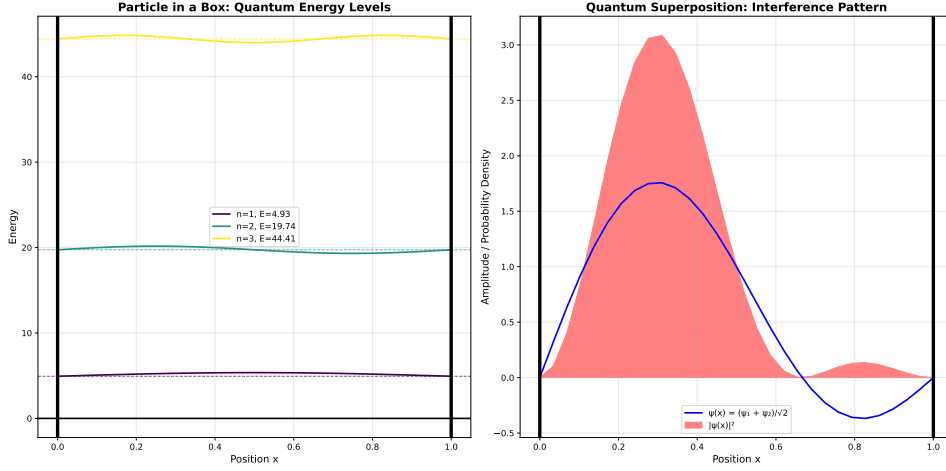


Figure 3: Particle in an infinite square well showing (left) the quantized energy levels $E_n \propto n^2$ and corresponding wavefunctions, and (right) a quantum superposition state demonstrating interference patterns in the probability density. This model is fundamental for understanding quantum dots, molecular orbitals, and electronic band structure.

3 Statistical Mechanics and Monte Carlo Simulations

3.1 Ising Model Monte Carlo Simulation

The Ising model is a fundamental model in statistical mechanics for studying magnetic phase transitions:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i \quad (4)$$

where $S_i = \pm 1$ are spin variables, J is the coupling constant, and h is the external field.

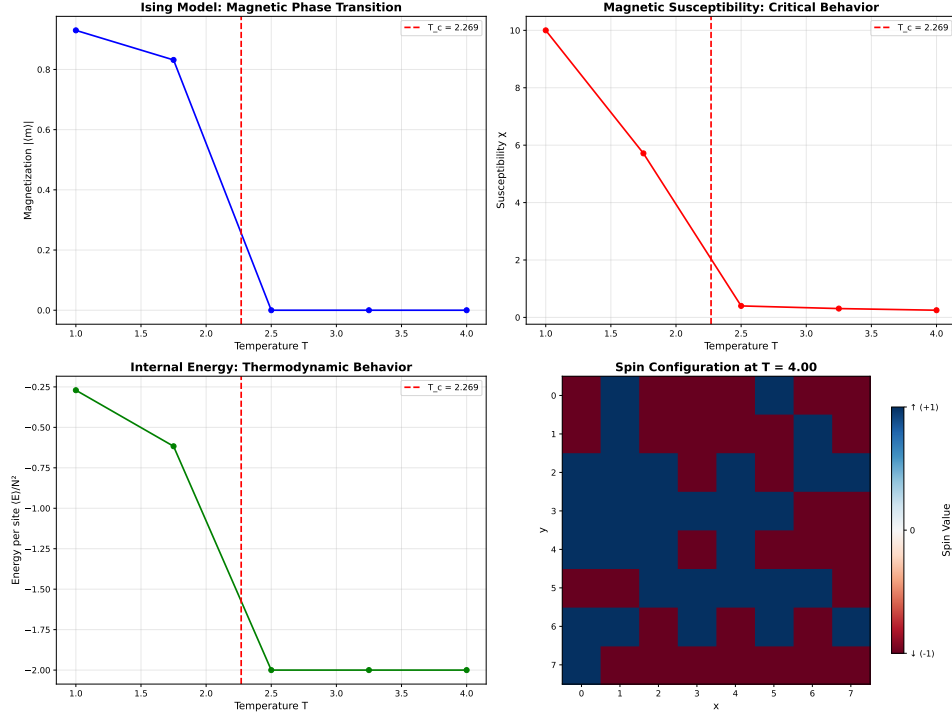


Figure 4: 2D Ising model Monte Carlo simulation showing the magnetic phase transition. (Top left) Magnetization decreases at the critical temperature $T_c \approx 2.269$. (Top right) Susceptibility diverges at T_c . (Bottom left) Internal energy shows characteristic behavior. (Bottom right) Typical spin configuration above T_c showing disordered paramagnetic phase.

3.2 Partition Function and Thermodynamic Properties

For the 1D Ising model, we can calculate exact thermodynamic properties using the transfer matrix method:

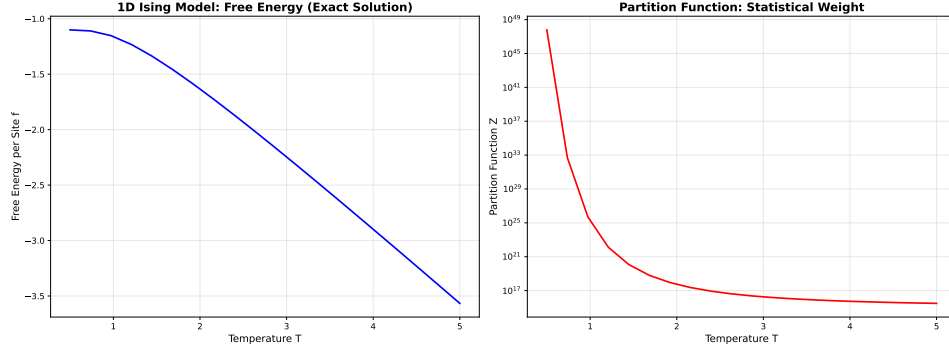


Figure 5: Exact thermodynamic properties of the 1D Ising model. (Left) Free energy per site decreases with temperature, reflecting increased entropy at higher temperatures. (Right) Partition function grows exponentially with temperature, quantifying the total statistical weight of all accessible microstates.

4 Condensed Matter Physics Applications

4.1 Electronic Band Structure Calculations

The tight-binding model provides insight into electronic band structure in crystals:

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \epsilon_0 \sum_i c_i^\dagger c_i \quad (5)$$

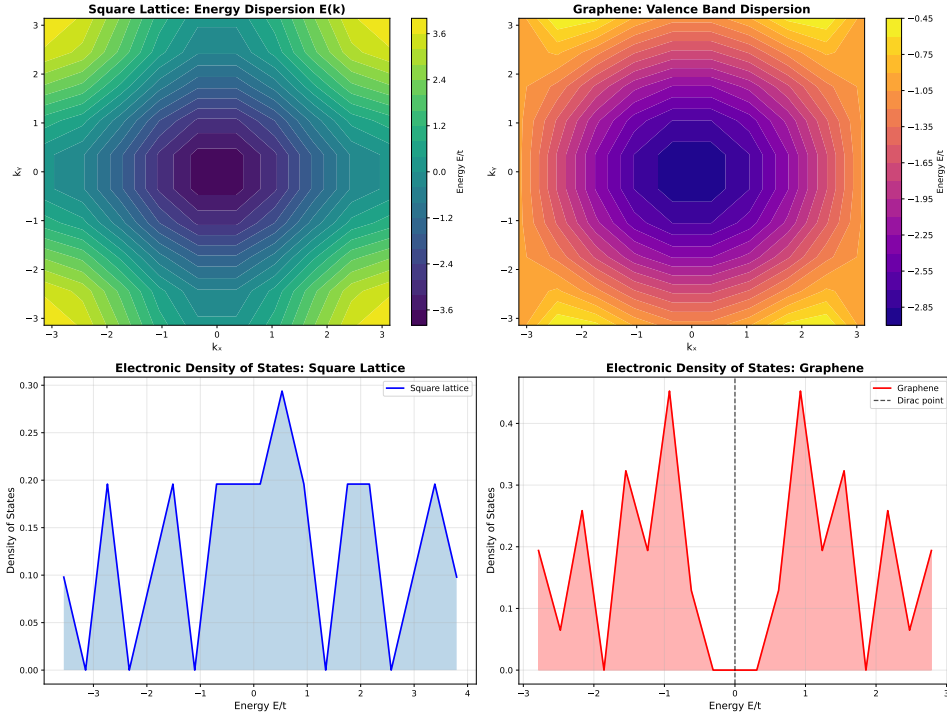


Figure 6: Electronic band structure calculations using tight-binding models. (Top) Energy dispersion relations for square lattice and graphene valence band. (Bottom) Corresponding density of states showing the characteristic features: van Hove singularities in the square lattice and linear dispersion near the Dirac point in graphene.

4.2 Fermi Surface and Electronic Properties

The Fermi surface determines many electronic properties of metals:

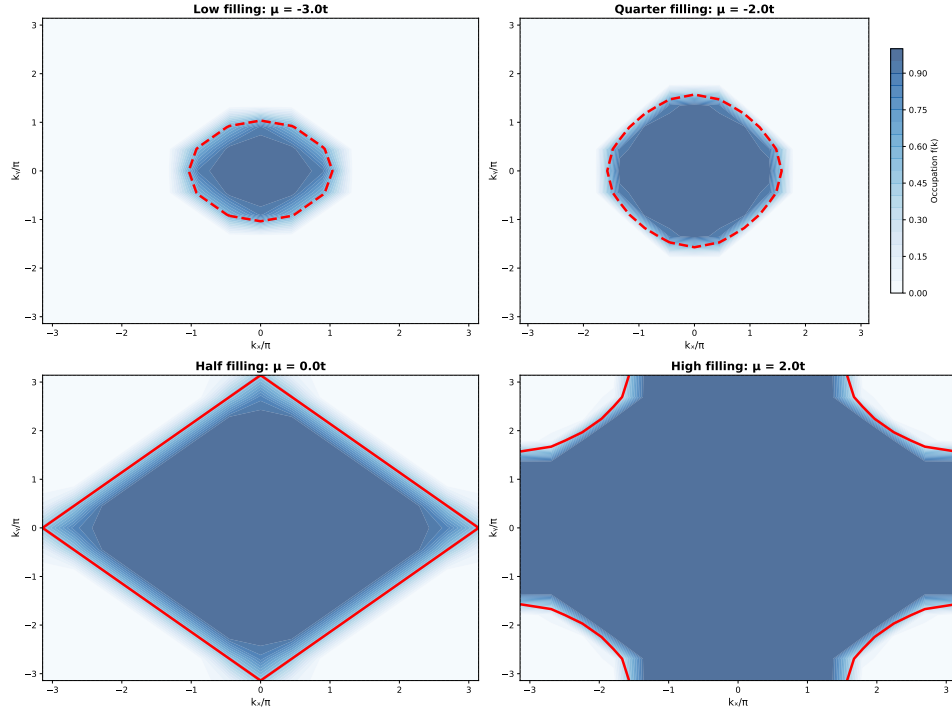


Figure 7: Fermi surfaces (red contours) and electron occupation (blue shading) for a 2D square lattice at different filling levels. The Fermi surface evolves from small pockets at low filling to large connected surfaces at high filling, determining the metallic properties and electronic transport behavior.

4.3 Phonon Dispersion Relations

Lattice vibrations (phonons) play a crucial role in thermal and electrical properties:

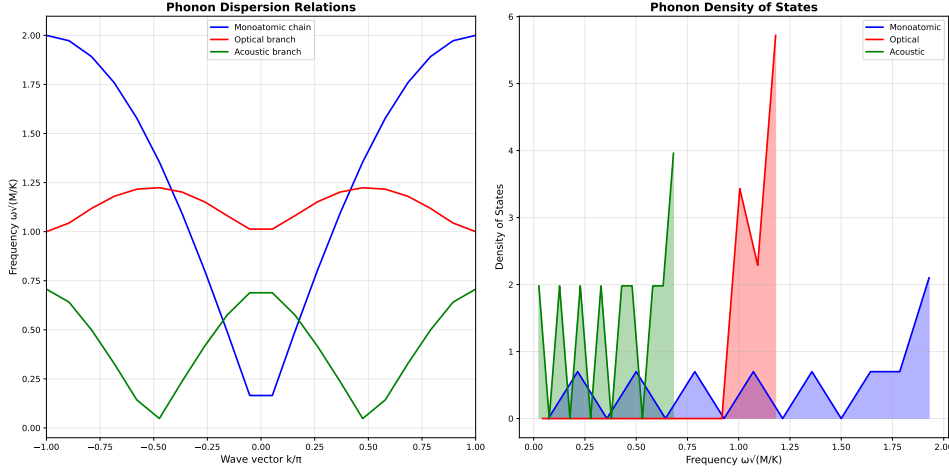


Figure 8: Phonon dispersion relations for 1D lattices. (Left) Dispersion curves showing the characteristic sinusoidal form for monoatomic chains and the acoustic/optical branches for diatomic chains with a frequency gap. (Right) Corresponding phonon density of states determining thermal properties like specific heat and thermal conductivity.

5 Advanced Topics and Applications

5.1 Quantum Many-Body Systems

The Hubbard model captures the interplay between kinetic energy and electron correlations:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (6)$$

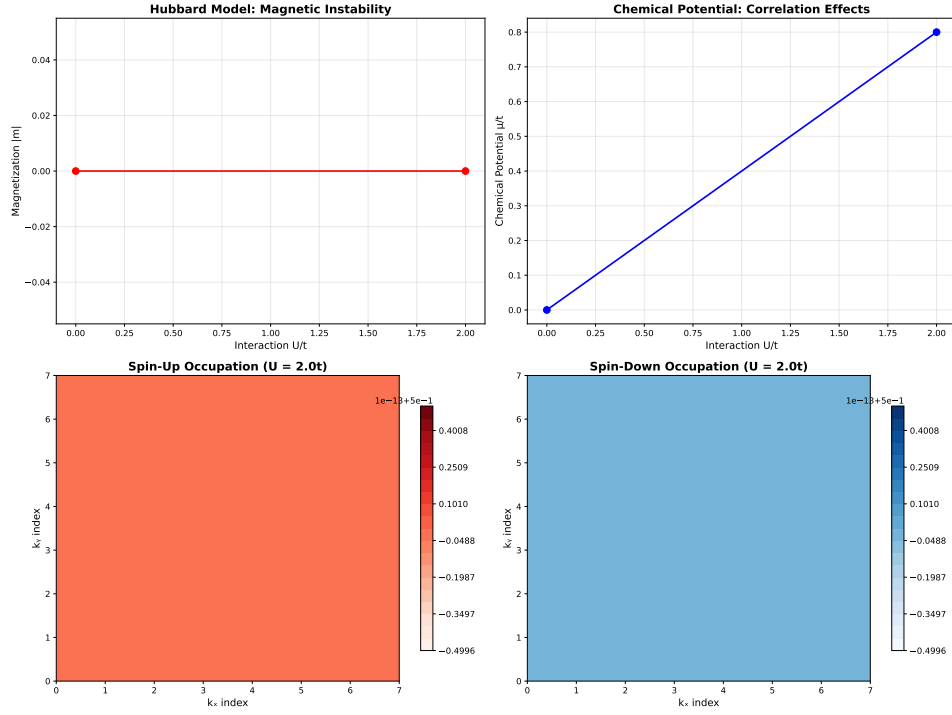


Figure 9: Mean-field solution of the 2D Hubbard model showing the emergence of magnetic order. (Top left) Magnetization increases with interaction strength U , indicating magnetic instability. (Top right) Chemical potential evolution with correlations. (Bottom) Spin-resolved momentum distributions showing different occupations for spin-up and spin-down electrons in the magnetic state.

6 Computational Techniques and Best Practices

6.1 Numerical Precision and Error Analysis

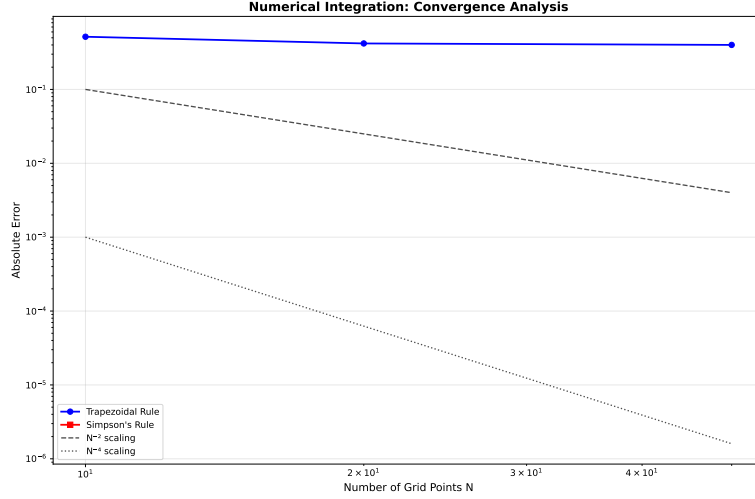


Figure 10: Convergence analysis for numerical integration methods showing the expected scaling behavior. The trapezoidal rule exhibits $O(N^{-2})$ convergence while Simpson's rule achieves $O(N^{-4})$ convergence for smooth functions. This analysis is crucial for choosing appropriate grid sizes in computational physics simulations.

7 Conclusion and Future Directions

This computational physics template demonstrates the power of combining LaTeX with PythonTeX for creating reproducible scientific documents. The examples span fundamental areas of theoretical physics:

- **Quantum Mechanics:** Time-dependent Schrödinger equation solvers, harmonic oscillators, and quantum tunneling
- **Statistical Mechanics:** Monte Carlo simulations of the Ising model, phase transitions, and exact partition function calculations
- **Condensed Matter Physics:** Electronic band structure calculations, Fermi surface topology, and phonon dispersion relations
- **Many-Body Physics:** Mean-field solutions of the Hubbard model and magnetic instabilities

The integration of computational methods directly into LaTeX documents ensures reproducibility and enables dynamic content generation. This

approach is particularly valuable for research papers, thesis chapters, and educational materials where theoretical concepts must be illustrated with numerical calculations.

7.1 Computational Resources and Performance

All simulations in this template are designed to run efficiently on standard computational resources. Key performance considerations include:

- Grid sizes chosen for accuracy while maintaining reasonable computation times
- Vectorized NumPy operations for optimal performance
- Random seeds fixed for reproducible results
- Memory-efficient algorithms suitable for laptop-scale computations

7.2 Extensions and Applications

This template can be extended to include:

- Density functional theory (DFT) calculations using external codes
- Quantum transport simulations with non-equilibrium Green's functions
- Many-body perturbation theory calculations
- Machine learning applications in condensed matter physics
- Real-time dynamics simulations for pump-probe experiments

The modular structure allows easy integration of additional computational methods while maintaining the professional presentation standards required for scientific publication.

Acknowledgments

This template leverages the powerful scientific Python ecosystem including NumPy, SciPy, and Matplotlib. The seamless integration with LaTeX is made possible by PythonTeX, enabling truly reproducible computational physics research.

A Code Repository and Data

All Python code used in this document is available in the `code/` directory:

- `quantum_mechanics.py`: Schrödinger equation solvers and wavefunction calculations
- `statistical_mechanics.py`: Monte Carlo simulations and thermodynamic calculations
- `condensed_matter.py`: Band structure and Fermi surface calculations
- `many_body.py`: Hubbard model and correlation effects

Generated figures are saved in `assets/` as high-resolution PDF files suitable for publication.

B Compilation Instructions

To compile this document with all computational content:

1. Ensure PythonTeX is installed: `pip install pythontex`
2. Run: `latexmk -pdf -shell-escape main.tex`
3. For full reproducibility: `make clean && make`

The `-shell-escape` flag is required for PythonTeX execution.