

The Revolutionary Dynamical Mean Field Theory: Unraveling the Secrets of Strongly Correlated Materials



Dynamical mean field theory (in practice)

Hubbard model $H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$

Make a guess for the host Green's function $\mathcal{G}_{\text{in}}(z)$

Solve impurity problem

$$S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{\sigma\uparrow}^\dagger(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{\sigma\uparrow}(\tau') + U \int_0^\beta d\tau n_{\sigma\uparrow}(\tau) n_{\sigma\downarrow}(\tau)$$

Dyson's equation

$$\mathcal{G}_0^{-1} = G^{-1} + \Sigma$$

$\Sigma_{\text{latt}} = \Sigma_{\text{imp}}$: Self-consistency

Impurity Self energy
 $\Sigma(z)$

$$G(z) = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)}{z - \epsilon + \mu - \Sigma(z)}$$

APS-IUSSTF lectures at Purdue - 2015

We live in a world filled with materials exhibiting complex behavior and surprising properties. From high-temperature superconductors to exotic magnetic materials, understanding the underlying physics behind these phenomena is crucial for technological advancements and scientific breakthroughs. However, the behavior of such materials often defies conventional theories and calls for a more sophisticated approach. This is where Dynamical Mean Field Theory (DMFT) steps in, revolutionizing our understanding of strongly correlated materials.

The Challenge of Strong Correlations

Strongly correlated materials, as the name suggests, are substances where the behavior of individual particles is greatly influenced by the interactions with their neighboring particles. This correlation effect can lead to dramatic changes in the material's properties, such as unconventional conductivity, magnetism, or even exotic phases of matter.

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Dynamical Mean-Field Theory for Strongly Correlated Materials

by Baby Professor (1st ed. 2021 Edition, Kindle Edition)

★★★★☆ 4.4 out of 5

Language : English

File size : 73755 KB

Text-to-Speech : Enabled

Enhanced typesetting : Enabled

Print length : 693 pages

Screen Reader : Supported



Conventional theoretical approaches, such as density functional theory (DFT), fail to accurately describe the behavior of strongly correlated materials. DFT, based on the concept of non-interacting electrons, overlooks the crucial role of electron-electron interactions in these complex systems. Therefore, a more sophisticated method is required to understand the underlying physics.

Enter Dynamical Mean Field Theory (DMFT)

Developed in the late 1980s, Dynamical Mean Field Theory has emerged as a powerful tool for investigating strongly correlated materials. It provides a framework to study the electronic structure and properties of these materials by

taking into account the local dynamical correlations. By considering the local behavior of electrons, DMFT successfully captures the essential physics that governs their collective behavior.

The key concept behind DMFT is to map the original lattice problem onto an effective impurity model. This simplification allows researchers to focus on the behavior of a single site and accurately describe its interactions. The local properties obtained from the impurity model are then combined with knowledge of the lattice structure to reconstruct the overall behavior of the material. This combination of local and non-local information is what makes DMFT so unique and powerful.

Unveiling the Mysteries

DMFT has proven to be a game-changer in the field of condensed matter physics. Its application has led to breakthroughs in the understanding of a wide range of materials, including high-temperature superconductors, heavy fermion metals, and transition metal oxides.

One of the remarkable achievements of DMFT is its ability to accurately describe the metal-insulator transition. In many materials, the transition between these two phases is not well understood. However, DMFT provides insights into the underlying mechanisms driving this transition, shedding light on the intricate balance between electron-electron interactions and disorder.

Another area where DMFT excels is the study of phase transitions in correlated materials. By investigating the behavior of individual sites and their interactions, DMFT has enabled researchers to understand the emergence of exotic phases, such as the Mott insulator phase or the strange metal behavior observed in high-temperature superconductors.

Advancing Technology through DMFT

DMFT is not only a theoretical tool but also a framework that can guide experimental investigations. Its ability to accurately capture the properties of strongly correlated materials has helped researchers design and discover new materials with enhanced functionalities.

For example, DMFT played a crucial role in the discovery of colossal magnetoresistance materials. These compounds exhibit a dramatic change in resistance when subjected to an external magnetic field, making them ideal for sensor and memory device applications. By combining insights from DMFT with experimental observations, researchers successfully identified the electronic properties that lead to this remarkable effect.

Looking Ahead

As technology continues to advance and our understanding of strongly correlated materials deepens, DMFT will undoubtedly play a crucial role in guiding future research. Its ability to capture the intricate interplay between local and non-local interactions makes it an invaluable tool for unraveling the mysteries of complex materials.

Through a synergy of theoretical and experimental efforts, we can expect further breakthroughs in our understanding of superconductivity, magnetism, and the emergence of exotic phases. The insights gained from DMFT will not only pave the way for new technological advancements but also offer profound insights into the fundamental principles of condensed matter physics.

Keywords: Dynamical Mean Field Theory, Strongly Correlated Materials, Electronic Structure, Phase Transitions, Condensed Matter Physics

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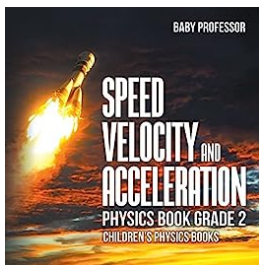
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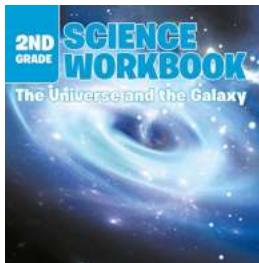
This is the first book that provides a detailed summary of one of the most successful new condensed matter theories - dynamical mean-field theory (DMFT) - in both static and dynamical cases of systems of different sizes. DMFT is one of the most successful approaches to describe the physical properties of systems with strong electron-electron correlations such as bulk materials, multi-layers, surfaces, 2D materials and nanostructures in both metallic and insulating phases. Strongly correlated materials usually include partially-filled localized d- or f-orbitals, and DMFT takes into account crucial for these systems time-resolved interaction between electrons when they “meet” on one atom and occupy one of these orbitals. The First Part of the book covers the general formalism of DMFT as a many-body theory, followed by generalizations of the approach on the cases of finite systems and out-of-equilibrium regime. In the last Chapter of the First Part we discuss generalizations of the approach on the case when the non-local interactions are taken into account. The Second Part of the book covers methodologies of merging DMFT with ab initio static Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) approaches. Such combined DFT+DMFT and DMFT+TDDFT computational techniques allow one to include

the effects of strong electron-electron correlations at the accurate ab initio level. These tools can be applied to complex multi-atom multi-orbital systems currently not accessible to DMFT. The book helps broad audiences of students and researchers from the theoretical and computational communities of condensed matter physics, material science, and chemistry to become familiar with this state-of-art approach and to use it for reaching a deeper understanding of the properties of strongly correlated systems and for synthesis of new technologically-important materials.



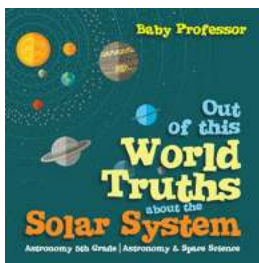
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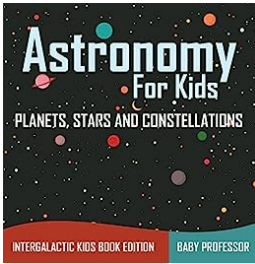
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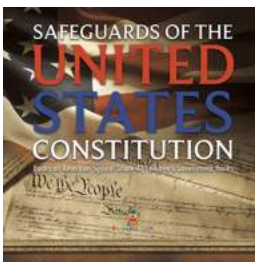
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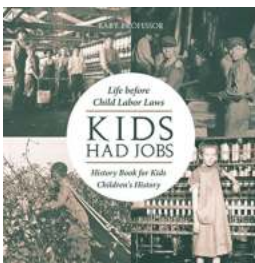
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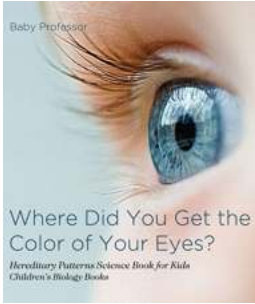
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