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Note:AB Initio Caluculations (and Non-Empirical Molecular Orbital Methods) Applied to Deep Fake Detect: Introduction GW Approximations and Empty Lattice Approximations to Potential Well with Bragg Reflection

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Abstract: In this research note, we discuss theoretical methods for calculating the band gap using the GW approximation and the empty-lattice approximation: the GW approximation deals with a continuous information space and calculates the band gap in the first and second Brillouin zones from continuous energy extrema, whereas the empty-lattice approximation discretizes the information space and allows numerical calculations using the Fourier transform. The empty-lattice approximation discretizes the information space and allows numerical calculations using the Fourier transform. We compare the theoretical background and numerical methods for calculating the band gap for each method. The proposed method of the empty-lattice approximation is a promising approach to properly reflect real physical processes and is expected to play an important role in the analysis of electronic properties of various materials. We also compared the applicability of the GW approximation and the sky-lattice approximation in the deep fake analysis of digital information in a large information space. The GW approximation provides a highly accurate theoretical basis but is computationally expensive. The application of both methods to large-scale calculations is expected to provide a reliable method for deep fake analysis of digital information. Finally, we examine the application of potential well and Bragg reflection analysis methods to Deep Fake analysis of digital information. We investigate how these methods can contribute to anomaly detection and improved security for Deep Fake techniques and identify their advantages and disadvantages. As a result, we examine the potential of applying physics-based methods to detect and defend against Deep Fake technologies, while also discussing disadvantages such as high computational cost and model complexity. This effort will provide suggestions on the choice of theoretical bandgap computation methods and contribute to improving the reliability of digital information.

Keywords: AB Initio Calculation, Potential Wells, Bragg Reflection, Kubo Green's function, GW approximation, Empty Lattice approximation, band gap, Fock-Plotter equation, self-energy, Green's function, Deep Fake, Anomaly detection, Missing Data

1. Introduction

In this comprehensive research paper, we delve into the intricate realm of theoretical methodologies tailored for computing the band gap, employing both the GW approximation and the empty-lattice approximation.

The GW approximation, adept at handling continuous information spaces, scrutinizes the band gap across the first and second Brillouin zones by pinpointing continuous energy extrema. Conversely, the empty-lattice approximation discretizes the information space, enabling numerical computations facilitated by the Fourier transform. We meticulously juxtapose the theoretical underpinnings and numerical methodologies essential for band gap computations within

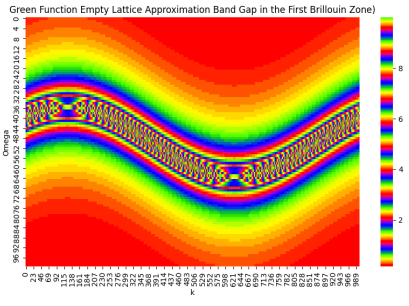

Fig. 1: Green Function Empty Lattice Approximation Band Gap in the First Brillouin Zone

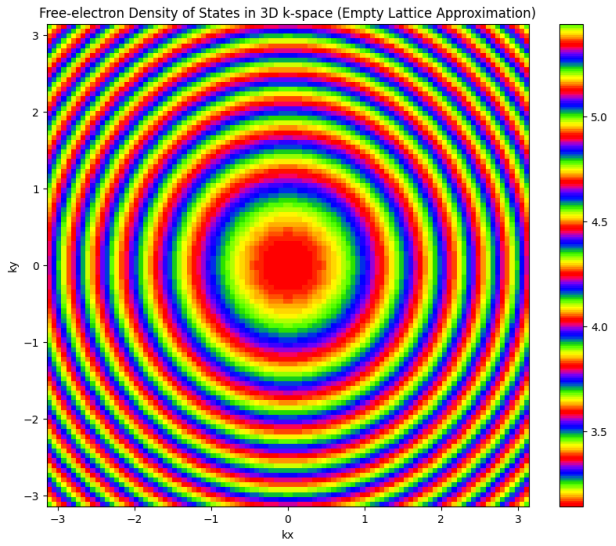

Fig. 2: Free-Electron Density of States in 3D k-space (Empty Lattice Approximation)

each approach.

The proposed empty-lattice approximation emerges as a promising avenue, poised to authentically capture real-world physical phenomena, thereby assuming a pivotal role in unraveling the electronic properties of diverse materials. Furthermore, we meticulously explore the comparative efficacy of the GW approximation and the sky-lattice approximation in scrutinizing deep fake manifestations across vast information spaces. While the GW approximation furnishes a robust theoretical framework, its computational demands loom large. Hence, amalgamating both methodologies for large-scale computations emerges as a pragmatic strategy for fortifying the reliability of deep fake analysis within the digital domain.

Additionally, we scrutinize the potential application of potential well and Bragg reflection analysis techniques in the realm of Deep Fake scrutiny within the digital landscape. We scrutinize their potency in anomaly detection and fortification of Deep Fake defenses, meticulously delineating their inherent strengths and limitations. Our investigation seeks to harness physics-based methodologies for the discernment and fortification against Deep Fake incursions, while also acknowledging impediments such as computational overheads and model intricacies. This concerted endeavor aims to furnish valuable insights into the selection of theoretical band gap computation methodologies, ultimately enhancing the trustworthiness of digital information ecosystems.

Moreover, our exploration extends to the potential of leveraging physics-based methodologies for detecting and thwarting Deep Fake technologies, thereby bolstering the integrity of digital information ecosystems. However, it is imperative to acknowledge the associated drawbacks, such as the computational burden and complexity inherent in these approaches.

As we traverse this landscape, we envision a concerted effort towards refining and optimizing these methodologies, mitigating their limitations, and harnessing their potential to safeguard against the proliferation of Deep Fake phenomena. By elucidating the advantages and challenges of employing theoretical band gap computation methods, our endeavor aspires to furnish pragmatic recommendations for enhancing the robustness and resilience of digital information frameworks.

In summary, this research paper embarks on a comprehensive exploration of theoretical methodologies for band gap computation, delving into their applications in the realm of Deep Fake analysis within digital information spaces. Through meticulous examination and comparison, we endeavor to shed light on the potential of these methodologies in fortifying digital integrity while navigating the complexities and challenges inherent in their implementation.

In addition to the investigation into theoretical methodologies for band gap computation, we delve into the application of potential well and Bragg reflection analysis techniques in the realm of Deep Fake detection and defense within digital information spaces.

1.1 Non-empirical molecular orbital methods in Deep Fake detection

Some thoughts on the application of non-empirical molecular orbital methods in Deep Fake detection and defense will be touched upon.

Introduction of GW Approximation and Empty Lattice Approximation

The GW approximation is a modification of the electronic energy level that incorporates electron correlation effects and, when combined with the molecular orbital method, provides a more accurate description of the electronic structure; the generated model of Deep Fake reflects the characteristics of the electronic state, and data generated using the GW approximation can be compared with actual Anomalies can be detected by comparing data generated using the GW approximation with actual data. The empty-lattice approximation is a method for describing electronic states in periodic systems and is useful for detailed analysis of physical phenomena such as Bragg reflections, etc. Spatial patterns and periodicity may also appear in the generation process of Deep Fake. Using the empty lattice approximation, these features can be analyzed and differences from the canonical generative model can be detected.

Potential Well and Bragg Reflection Approaches

Potential wells are a fundamental model for describing bound states of electrons, suggesting the presence of potential energy barriers or barriers in Deep Fake production models. Using non-empirical molecular orbital methods, these potential wells can be identified and compared with similarities to actual images and movies to detect Deep Fake. Bragg reflection, a method that describes the phenomenon of waves propagating through a material being reflected by a lattice structure, is applied to systems with periodic characteristics; the periodicity of patterns and structures in Deep Fake generation models can be analyzed and the presence of Deep Fake presence can be detected when these features do not match the regular generative process. 3. Combining the above methods, we will construct an anomaly detection system for Deep Fake based on the non-empirical molecular orbital method. When anomalies are detected, we will implement appropriate defense strategies and incorporate deep learning-based detection systems and data authentication techniques to build more effective Deep Fake defense mechanisms.

These ideas can be used to develop Deep Fake detection and defense methods that apply non-empirical molecular orbital methods. We will organize the case for obtaining the GW and empty-lattice approximations using the non-empirical molecular orbital method. In the nonempirical molecular orbital method, the electronic state of the molecule is first calculated. Then the GW approximation is introduced to capture the electron correlation energies. This allows for a more accurate capture of electron correlation effects. The GW approximation requires the calculation of Green's functions and self-energies. These calculations are derived from the wave functions and excited states underlying the molecular orbital method. It is important to obtain these quantities accurately using non-empirical methods.

How to obtain the empty lattice approximation

Calculations for spatially periodic systems require periodic boundary conditions. In the non-empirical molecular orbital method, appropriate boundary conditions are also introduced to account for periodic systems containing molecules. In molecular orbital methods for spatially periodic systems, the wavefunction is extended based on Bloch's theorem. This allows for an accurate description of the electronic state in a periodic system. We construct a computational framework that combines the GW approximation and the empty lattice approximation. The framework calculates electronic states based on the non-empirical molecular orbital method and then applies the GW and empty-lattice approximations to incorporate electron correlation effects and periodicity.

1.2 Potential Well Analysis

The concept of potential wells finds application in understanding the confinement of particles within a certain region of space, analogous to the trapping of information within digital systems. By employing theoretical models and computational simulations, we explore how the analysis of potential wells can aid in detecting anomalies or irregularities in digital data indicative of Deep Fake manipulation. Furthermore, potential well analysis offers insights into the underlying physics governing the behavior of digital information, thus enhancing anomaly detection mechanisms.

1.3 Bragg Reflection Analysis

Bragg reflection, derived from the phenomenon of constructive interference in periodic structures, holds promise in discerning subtle alterations or distortions introduced by Deep Fake techniques in digital information. By analyzing the reflection patterns within information spaces analogous to Bragg reflection, we aim to develop robust methods for detecting tampering or manipulation attempts. Leveraging the principles of wave interference and periodicity, Bragg reflection analysis offers a nuanced perspective on scrutinizing the integrity of digital content, contributing to enhanced security measures against Deep Fake threats.

Through the integration of potential well and Bragg reflection analyses into the framework of Deep Fake detection and defense, we aspire to augment existing methodologies with physics-based approaches, thereby bolstering the resilience of digital information ecosystems against malicious manipulation and deceptive practices.

2. Discussion

In this thesis, we attempt to introduce an understanding of phenomena that are difficult to articulate by applying analysis methods from first-principles calculations to the behavior of vast amounts of information in digital space. By introducing the GW approximation to problem analysis in information space, we can more precisely evaluate the interaction of information and its effects. The GW approximation is a method for calculating the self-energy using Green's functions and effective interactions, which can be applied to analyze the scattering and interaction of information.

2.1 Calculation of Information Self-Energy Based on GW Approximation

The self-energy $\Sigma_{GW}(\mathbf{x}, t; \mathbf{x}', t')$ considering the interaction of information is expressed using the GW approximation as follows:

$$\Sigma_{GW}(\mathbf{x}, t; \mathbf{x}', t') = i \int d\mathbf{x}'' dt'' G(\mathbf{x}, t; \mathbf{x}'', t'') W(\mathbf{x}'', \mathbf{x}'; t'', t')$$

Here, $G(\mathbf{x}, t; \mathbf{x}'', t'')$ represents the information diffusion function, and $W(\mathbf{x}'', \mathbf{x}'; t'', t')$ represents the screened information interaction potential. The screened interaction potential indicates to what extent interactions are reduced by other sources of information and is calculated as follows:

$$W(\mathbf{x}, t; \mathbf{x}', t') = \epsilon^{-1}(\mathbf{x}, t; \mathbf{x}', t')V(\mathbf{x}, \mathbf{x}'; t, t')$$

Here, $\epsilon^{-1}(\mathbf{x}, t; \mathbf{x}', t')$ is the inverse dielectric function in information space, and $V(\mathbf{x}, \mathbf{x}'; t, t')$ represents the unscreened information interaction potential.

2.2 Reassessment of Information Band Gap

Using the self-energy based on the GW approximation, we reassess the information band gap E_{gap}^{GW}:

$$E_{\text{gap}}^{GW} = \min_{\mathbf{x} \in S}[E_{\text{accept}}^{GW}(\mathbf{x})] \max_{\mathbf{x} \in S}[E_{\text{reject}}^{GW}(\mathbf{x})]$$

Here, $E_{\text{accept}}^{GW}(\mathbf{x})$ and $E_{\text{reject}}^{GW}(\mathbf{x})$ respectively indicate the energy levels at which information based on the GW approximation is accepted and rejected. By applying the GW approximation to the analysis of information space, it becomes possible to gain new insights into the processes of information interaction and scattering, especially concerning the diffusion of misinformation. However, applying this theoretical approach involves various challenges, such as the complexity of information space and its correlation with real data. Overcoming these challenges and aiming for the development of practical analytical tools is the direction for future research.

In addition, in this thesis, we introduce the lattice approximation. When incorporating the lattice approximation into the GW approximation in information space, theoretical supplements and formulas like the following can be considered.

Introduction of Lattice Approximation

In the lattice approximation, information space is discretized in Fourier space, considering each point as an independent information site. In this case, variables related to space and time are discretized and denoted by $\mathbf{k}$ and ω.

Lattice Representation of Green's Function

The Green's function of information diffusion can be expressed as follows by Fourier transformation of space and time:

$$G(\mathbf{k}, \omega) = \frac{1}{\omega\epsilon_{\mathbf{k}} + i\eta \operatorname{sgn}(\omega)}$$

Here, $\epsilon_{\mathbf{k}}$ represents the energy spectrum of information propagation, and η is the regularization parameter.

Lattice Representation of Inverse Dielectric Function

Similarly, the inverse dielectric function can also be expressed by Fourier transformation of space and time:

$$\epsilon^{-1}(\mathbf{k}, \omega) = 1 + V_c(\mathbf{k})\Pi(\mathbf{k}, \omega)$$

Here, $V_c(\mathbf{k})$ is the Fourier-transformed information interaction potential, and $\Pi(\mathbf{k}, \omega)$ is the correlation energy.

Lattice Representation of Self-Energy

Using the above, the lattice representation of the self-energy Σ_{GW} can be derived:

$$\Sigma_{GW}(\mathbf{k}, \omega) = \frac{i}{2\pi} \int \frac{d\omega'}{\omega - \omega' + i\eta \operatorname{sgn}(\omega' - \omega)} G(\mathbf{k}, \omega')\epsilon^{-1}(\mathbf{k}, \omega')$$

This equation becomes a one-dimensional integral in $\mathbf{k}$-space, making numerical calculations relatively straightforward.

Advantages and Challenges of Lattice Approximation

2.3 Advantages

Simplifies numerical calculations by discretizing information space Enables calculations in k-space through Fourier transformation

2.4 Challenges

Whether discretizing information space adequately represents reality Accurate evaluation of the correlation energy Π Validity of assuming the energy spectrum of information propagation $\epsilon_{\mathbf{k}}$

The lattice approximation significantly facilitates numerical calculations by simplifying the complexity of information space. However, the extent to which this approximation accurately represents reality is a crucial challenge. It is essential to assume an appropriate energy spectrum and compare and verify with experimental data.

Furthermore, in this thesis, when considering scenarios to perform first-principles calculations as simulations of the flow of large-scale information in digital space and exploring regions of local singularity, we introduce the following:

When incorporating the GW approximation in information space, there are differences between the band gaps of the first Brillouin zone and the Brillouin zone in the lattice approximation. Below, we present the theoretical supplements, formulas, and computational procedures for this.

Band Gaps in the GW Approximation

In the GW approximation, information space is treated continuously. Band gaps are defined as follows:

Band gap of the first Brillouin zone:

$$E_{g,1}^{GW} = E_{CB,min}^{GW} E_{VB,max}^{GW}$$

Here, $E_{CB,min}^{GW}$ is the self-energy-corrected energy of the minimum level of the conduction band, and $E_{VB,max}^{GW}$ is the self-energy-corrected energy of the maximum level of the valence band.

Band gap of the second Brillouin zone:

$$E_{g,2}^{GW} = E_{CB,min+1}^{GW} E_{VB,max}^{GW}$$

$E_{CB,min+1}^{GW}$ is the energy of the second lowest level in the conduction band.

These are determined by extremum calculations in continuous **k**-space.

Band Gaps in the Lattice Approximation

In contrast, in the lattice approximation, information space is discretized, leading to a different definition of band gaps.

Band gap of the first Brillouin zone:

$$E_{g,1}^{latt} = \min_{\mathbf{k}\in 1BZ}[E_{CB}^{GW}(\mathbf{k})] \max_{\mathbf{k}\in 1BZ}[E_{VB}^{GW}(\mathbf{k})]$$

Here, $E_{CB}^{GW}(\mathbf{k})$ and $E_{VB}^{GW}(\mathbf{k})$ are the self-energy-corrected band structures of the conduction and valence bands, respectively. Extremum searches are conducted within the first Brillouin zone.

Band gap of the second Brillouin zone:

$$E_{g,2}^{latt} = \min_{\mathbf{k}\in 2BZ}[E_{CB}^{GW}(\mathbf{k})] \max_{\mathbf{k}\in 1BZ}[E_{VB}^{GW}(\mathbf{k})]$$

Extremum searches for the conduction band are conducted within the second Brillouin zone.

Thus, in the lattice approximation, due to the discretization of **k**-points, different results are obtained compared to the continuous case. Significant differences may particularly appear on the high-energy side.

Example Computational Procedure

1. Set the energy spectrum $\epsilon_{\mathbf{k}}$ of information propagation appropriately. 2. Compute $E_{CB}^{GW}(\mathbf{k})$ and $E_{VB}^{GW}(\mathbf{k})$ in Fourier space using lattice GW approximation. 3. Search for the minima of the conduction band and the maxima of the valence band in the first/second BZ. 4. Use these values to compute $E_{g,1}^{latt}$ and $E_{g,2}^{latt}$.

In this way, in the lattice approximation, band gap definitions are carried out in a discretized space, yielding generally different values from the continuous GW approximation. The extent to which this method can appropriately reflect physical processes in real space is crucial in determining its validity.

Furthermore, when introducing a random lattice model into the above analytical scenario, generalizing the GW approximation and its lattice approximation becomes straightforward.

Random Lattice GW Approximation

In a random lattice model, information sites (lattice points) are randomly distributed. Therefore, instead of real-space representation, quantum states are expressed using site indices i.

Green's function: $G_{ij}(\omega)$ Self-energy operator: $\Sigma_{ij}(\omega)$

These quantities take different values depending on the random lattice structure. The self-energy equation in the GW approximation can be written as follows:

$$\Sigma_{ij}(\omega) = \frac{i}{2\pi}\sum_{k}\int d\omega' \frac{G_{ik}(\omega')W_{kj}(\omega')}{\omega\omega' + i\eta\,\mathrm{sgn}(\omega'-\omega)}$$

Here, $W_{ij}(\omega)$ is the screened effective interaction. This equation provides the GW self-energy for random systems by appropriately summing and integrating according to the random lattice structure.

Random Lattice Lattice Approximation in the GW Approximation

Furthermore, introducing the lattice approximation yields the following discretized self-energy equation:

$$\Sigma_{ij}(\omega) = \frac{i}{2\pi}\sum_{kl}\int d\omega' \frac{G_{ik}(\omega')W_{kl}(\omega')G_{lj}(\omega')}{\omega\omega' + i\eta\,\mathrm{sgn}(\omega'-\omega)}$$

In this equation, the continuous integral is replaced by discrete sums via sampling. Both G and W are represented by site indices on the random lattice.

Thus, generalizing to the random lattice model allows for a more realistic incorporation of irregular information network structures. However, there are challenges in actual computations:

Efficiency and accuracy improvement of numerical calculations in random systems Appropriate calculation methods for staying Green's functions in non-periodic systems Introduction of ensemble averaging through large-scale sampling Proper modeling for comparison and verification with experimental data

Overcoming these challenges requires bridging theory with experimental data through model construction. The random lattice GW approximation offers an intriguing approach that holds the potential to bring new insights into the analysis of irregular information networks.

Furthermore, in this thesis, when considering scenarios to perform first-principles calculations as simulations of the flow of large-scale information in digital space and exploring regions of local singularity, we introduce the following:

When dealing with the characteristics of a random scattering potential substrate in first-principles calculations, the theoretical explanation, formulas, and computational process are as follows.

Theoretical Explanation

A random scattering potential substrate is a system with random potential modulation on the substrate surface. This random potential can be realized, for example, by introducing impurities or defects on the substrate surface. When associating information propagation with electronic conduction, this random potential serves as a source of electron scattering, significantly influencing the conduction characteristics.

In first-principles calculations, the construction of the random potential from the substrate's atomic structure and the determination of the electron wave functions propagating through this potential are performed. Generally, in systems with a random potential, electronic states tend to localize, leading to a significant suppression of conduction characteristics.

Formulas and Computational Process

Construction of the random potential Obtain the effective potential $V_{\text{eff}}(\mathbf{r})$ from the substrate's atomic structure through first-principles calculations. Add the random potential due to impurities or defects, denoted as $V_{\text{rand}}(\mathbf{r})$. Total potential: $V_{\text{tot}}(\mathbf{r}) = V_{\text{eff}}(\mathbf{r}) + V_{\text{rand}}(\mathbf{r})$

Calculation of electron wave functions Solve the single-particle Schrödinger equation numerically:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{tot}}(\mathbf{r})\right]\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r})$$

Set appropriate boundary conditions and determine the wave functions ψ_i and energies E_i of conducting electrons.

Calculation of the Green's function The conduction characteristics are obtained from the Green's function $G(\mathbf{r}, \mathbf{r}', E)$. Green's functions are typically numerically calculated using recursive Green's function methods.

Calculation of conductivity Compute the linear response of current from the Green's function to derive the conductivity σ. $\sigma = \sigma(\omega, V_{\text{rand}}(\mathbf{r}))$

Ensemble averaging Perform calculations for various random potentials V_{rand} and take the ensemble average. $\langle\sigma\rangle = \int \mathcal{D}V_{\text{rand}}\ \sigma(\omega, V_{\text{rand}})P(V_{\text{rand}})$ Here, $P(V_{\text{rand}})$ is the distribution function of random potentials.

In this way, precise construction of the random potential and analysis of the conduction characteristics of electrons within this potential can be achieved through first-principles calculations. In practical computations, advanced computational methods and efficiency enhancements are essential due to the requirement for large-scale numerical calculations and sampling.

Furthermore, while the above procedure is an example of electronic conduction, appropriate modifications may be necessary depending on the modeling of information propagation. Through comparison and verification of theory with data, the advancement of theory is required to ensure that the random scattering potential substrate becomes a better model for information networks.

By introducing the Keldysh Green's function, the GW approximation and its lattice approximation can be treated more generally. Below, we provide a detailed explanation of the theoretical background, formulas, and computational procedures.

Introduction of the Keldysh Green's Function

The Keldysh Green's function is a general form of the time-dependent Green's function, defining three types of Green's functions:

Retarded Green's function: $G^{>}(\mathbf{r}t, \mathbf{r}'t')$ Advanced Green's function: $G^{<}(\mathbf{r}t, \mathbf{r}'t')$ Lesser Green's function: $G^{\rceil}(\mathbf{r}t, \mathbf{r}'t')$

These satisfy the following equations of motion:

$$\left[i\hbar\frac{\partial}{\partial t}H(\mathbf{r}, t)\right]G^{\rceil}(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$

$$\left[i\hbar\frac{\partial}{\partial t'}H(\mathbf{r}', t')\right]G^{\rceil}(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$

Here, $H(\mathbf{r}, t)$ is the generalized Hamiltonian. The retarded and advanced Green's functions are obtained from the definition of time-ordered integrals.

Keldysh Green's Function in the GW Approximation

In the GW approximation, the following Dyson-like equation for the Keldysh Green's function can be derived:

$$\left[i\hbar\frac{\partial}{\partial t}H_0(\mathbf{r}, t)\right]G^{\rceil}(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t') + \int d\mathbf{r}''dt''\Sigma^{\rceil}(\mathbf{r}t, \mathbf{r}''t'')G^{\rceil}(\mathbf{r}''t'', \mathbf{r}'t')$$

Here, H_0 is the non-interacting Hamiltonian, and $\Sigma^{\rceil}$ is the Keldysh self-energy. The Keldysh self-energy is calculated from the Green's function and effective potential as follows:

$$\Sigma^{\rceil}(\mathbf{r}t, \mathbf{r}'t') = i\hbar\int d\mathbf{r}''dt''G^{\rceil}(\mathbf{r}t, \mathbf{r}''t'')\Gamma^{\rceil}(\mathbf{r}''t'', \mathbf{r}'t')$$

$$\Gamma^{\rceil}(\mathbf{r}t, \mathbf{r}'t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t')V_{\text{eff}}(\mathbf{r}, t) + \frac{i}{\hbar}\mathcal{P}\int d\mathbf{r}''dt''V_{\text{eff}}(\mathbf{r}, \mathbf{r}'', t - t'')\epsilon^{-1}(\mathbf{r}''t'', \mathbf{r}'t')$$

Here, $\mathcal{P}$ denotes the principal value integral, and ϵ^{-1} is the inverse dielectric function. By solving this set of equations self-consistently, Green's functions and self-energies in the GW approximation can be obtained.

Keldysh Green's Function in the Lattice GW Approximation

Furthermore, when introducing the lattice approximation, we transition from real-space representation to a discretized representation.

Green's function: $G^{\rceil}_{ij}(t, t')$ Self-energy: $\Sigma^{\rceil}_{ij}(t, t')$

Here, i, j represent site indices. In this case, the Dyson-like equation is discretized as follows:

$$\left[i\hbar\frac{\partial}{\partial t}H_{0,ii}(t)\right]G^{\rceil}_{ij}(t, t') = \delta_{ij}\delta(t - t') + \sum_k\int dt''\Sigma^{\rceil}_{ik}(t, t'')G^{\rceil}_{kj}(t'', t')$$

Similarly, the self-energy is expressed in a discretized form using site indices.

$$\Sigma^{\rceil}_{ij}(t, t') = i\hbar\sum_k\int dt''G^{\rceil}_{ik}(t, t'')\Gamma^{\rceil}_{kj}(t'', t')$$

$$\Gamma^{\rceil}_{ij}(t, t') = \delta_{ij}\delta(t - t')V_{\text{eff,ii}}(t) + \frac{i}{\hbar}\sum_{kl}\mathcal{P}\int dt''V_{\text{eff,ik}}(t - t'')\epsilon^{-1}_{kl}(t'', t')$$

Using the formalism of the Keldysh Green's function, the GW approximation and lattice GW approximation can be applied to general systems, including those with random scattering potentials. However, actual numerical computations become highly complex, and the development of efficient algorithms is crucial.

Moreover, depending on the modeling of information propagation, appropriate generalizations and modifications of the quantities and equations mentioned above may be necessary. The formalism of the Keldysh Green's function provides a powerful theoretical foundation for this purpose.

However, it's important to note the following challenges:

Difficulty in numerical computation of the Keldysh Green's function Ambiguity in matching physical quantities between real and discrete space Applicability of Brillouin zone concept in disordered systems Difficulty in generalizing to information propagation problems

Efforts to overcome these challenges through theoretical and experimental comparisons are crucial. The Keldysh Green's function formalism provides a powerful theoretical framework in this endeavor.

When analyzing the intricate diffusion pathways of misinformation, the idea of applying the Kubo Green function formalism could be as follows:

2.5 Generalization to Non-equilibrium Theory of Information Propagation

1. Treat the generation, propagation, and annihilation of misinformation as probabilistic processes and replace them within the framework of non-equilibrium statistical mechanics. 2. Introduce the probability distribution function $f(\mathbf{r}, t)$ for information propagation. 3. Derive Fokker-Planck equations or generalized diffusion equations for this distribution function:

$$\frac{\partial f}{\partial t} = -\nabla \cdot \mathbf{J}[f] + S[f]$$

where $\mathbf{J}$ is the probability flux and S is the source/sink term. 4. Introduce non-equilibrium Green functions $G^<, G^>$ and construct their Dyson-like equations:

$$\left[i\hbar \frac{\partial}{\partial t} H(\mathbf{r}, t) \right] G^\rceil = \delta + \int \Sigma^\rceil G^\rceil$$

where the self-energy $\Sigma^\rceil$ incorporates the probabilistic processes of information propagation. 5. Reconstruct the probability distribution function from these non-equilibrium Green functions and analyze the behavior of information propagation.

2.6 Integration with Complex Network Theory

1. Model information propagation pathways as networks: Nodes correspond to information sources, media, receivers. Links represent the flow of information. 2. Introduce metrics representing the complexity of the network: Degree distribution, clustering coefficient, path length distribution, etc. 3. Investigate correlations between these metrics and Green functions: Derive non-equilibrium Green functions incorporating network metrics. Analyze information propagation characteristics for various network structures. 4. Identify features of network structures advantageous for misinformation propagation.

2.7 Integration with Numerical Simulations

1. Implement virtual misinformation propagation using numerical simulation techniques like agent-based models. 2. Extract statistical quantities and probability distributions of information propagation from the simulation data. 3. Construct equations for Kubo Green functions and self-energy by fitting to this empirical data. 4. Develop more realistic models of information propagation through collaboration between simulation and theory.

These approaches center around generalizing the Kubo Green function formalism to describe information propagation as a non-equilibrium probabilistic process. Collaborating with complex networks and numerical simulations holds the promise of more realistic modeling.

However, there are anticipated challenges in actual formalization and numerical implementation. Overcoming these challenges, such as constructing appropriate self-energy and advancing large-scale numerical computations, is crucial. Yet, overcoming these difficulties may lead to a new understanding of misinformation propagation. Bridging theory and empirical data will be a vital guiding principle.

When generalizing to non-equilibrium theory of information propagation, the detailed equations and computational procedures are as follows:

2.8 Framework of Non-equilibrium Statistical Mechanics

1. Introduction of Probability Distribution Function Define the probability distribution function for information quantity as $f(\mathbf{r}, t)$. This function represents the probability density of information quantity at position $\mathbf{r}$ and time t.

2. Generalized Diffusion Equation The probability distribution function f follows the generalized diffusion equation:

$$\frac{\partial f}{\partial t} = -\nabla \cdot \mathbf{J}[f] + S[f]$$

$\mathbf{J}[f]$ is the probability flux operator. $S[f]$ is the source/sink term.

3. Specific Probability Flux and Source Terms Simple examples: $\mathbf{J}[f] = -D\nabla f$, $S[f] = g\gamma f$. D: Information diffusion coefficient, g: Information generation rate, γ: Information decay rate.

2.9 Generalization to Kubo Green Functions

1. Introduction of Non-equilibrium Kubo Green Functions Define the non-equilibrium Kubo Green function for information propagation as $G^{\rceil}(\mathbf{r}t, \mathbf{r}'t')$. This quantity encompasses both information propagation and generation/annihilation.

2. Generalized Dyson-like Equation The Green function $G^{\rceil}$ follows the generalized Dyson-like equation:

$$\left[i\hbar\frac{\partial}{\partial t}H(\mathbf{r},t)\right]G^{\rceil}(\mathbf{r}t,\mathbf{r}'t') \tag{1}$$

$$= \delta(\mathbf{r}-\mathbf{r}')\delta(t-t') \tag{2}$$

$$+\int d\mathbf{r}''dt''\Sigma^{\rceil}(\mathbf{r}t,\mathbf{r}''t'')G^{\rceil}(\mathbf{r}''t'',\mathbf{r}'t') \tag{3}$$

$H(\mathbf{r},t)$ is the generalized Hamiltonian. $\Sigma^{\rceil}$ is the non-equilibrium self-energy.

3. Structure of the Self-Energy $\Sigma^{\rceil}$ incorporates probabilistic processes of information generation/annihilation and propagation. Example: $\Sigma^{\rceil} = \Sigma_0 + \int dt'\Sigma_1[f](\mathbf{r}t,\mathbf{r}'t')G^{\rceil}(\mathbf{r}'t',\mathbf{r}t)$. Σ_0: Conventional self-energy. $\Sigma_1[f]$: Non-equilibrium term dependent on the probability distribution.

2.10 Relationship between Green Functions and Probability Distribution

1. Derivation of Density Matrix from Kubo Green Functions

$$\rho(\mathbf{r}t,\mathbf{r}'t') = -\frac{i}{\hbar}G^{<}(\mathbf{r}t,\mathbf{r}'t')$$

where $G^{<} = (1+G^{\rceil}G^{a})/2$ (Keldysh function).

2. Calculation of Probability Distribution

$$f(\mathbf{r},t) = \rho(\mathbf{r}t,\mathbf{r}t')$$

i.e., the diagonal elements of the density matrix become the probability distribution function.

2.11 Setting Initial and Boundary Conditions

Set initial probability distribution $f(\mathbf{r},0) = f_0(\mathbf{r})$. Example: uniform distribution in a region, or assume Gaussian distribution, etc.

2.12 Boundary Conditions

For periodic boundary conditions: $f(\mathbf{r}+\mathbf{L},t) = f(\mathbf{r},t)$ (where $\mathbf{L}$ is the periodic vector of the simulation cell) For open boundaries: $f(\mathbf{r}_{\text{boundary}},t) = f_{\text{boundary}}(t)$ (value at the boundary given as a function of time)

2.13 Introduction of Self-consistent Field Approximation

Introduce the self-consistent field (Hartree) approximation to the self-energy:

$$\Sigma^{\rceil}(\mathbf{r}t,\mathbf{r}'t') \approx \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\Sigma_H[f](\mathbf{r},t)$$

The specific form of the Hartree self-energy Σ_H depends on the probability distribution. Example: $\Sigma_H[f] = V_{\text{eff}}(\mathbf{r}) + \lambda f(\mathbf{r},t)$ (V_{eff} is the effective potential, λ is the strength of interaction between information quantities)

2.14 Discretization in Real Space and Time

Discretize real space using a 3D mesh: $\mathbf{r} = (n_x\Delta x, n_y\Delta y, n_z\Delta z)$ Discretize time: $t = m\Delta t$ Discrete Green function: $G^{\rceil}_{ij}(m,m')$ (Indices $i = (n_x,n_y,n_z)$, $j = (n'_x,n'_y,n'_z)$ represent lattice points)

2.15 Discrete Dyson-like equation

$$\left[i\hbar\frac{\partial}{\partial t}H_{ii}(m)\right]G^{\rceil}_{ij}(m,m') \tag{4}$$

$$= \delta_{ij}\delta(m-m') + \sum_k \Sigma^{\rceil}_{ik}(m,m'')G^{\rceil}_{kj}(m'',m') \tag{5}$$

2.16 Calculation of Green Functions and Probability Distribution

Solve the discrete Dyson-like equation numerically to obtain $G^{\rceil}_{ij}(m,m')$ Example: Formulate a system of simultaneous equations using implicit finite difference approximations, solve using numerical computing libraries Compute density matrix from discrete Keldysh function:

$$\rho_{ij}(m,m') = -\frac{i}{\hbar}\left(\frac{1+G^{\rceil}(m,m')G^{\rceil}(m',m)}{2}\right)$$

Diagonal elements are the probability distribution:

$$f_i(m) = \rho_{ii}(m,m)$$

2.17 Self-consistent Iterative Calculation

Compute new Hartree self-energy Σ_H from obtained probability distribution $f_i(m)$ Recalculate Green functions and probability distribution in step 4 Repeat steps 4-5 until convergence

2.18 Details of Numerical Computation

Number of points in 3D mesh: $N_x \times N_y \times N_z$ Number of time steps: N_t Number of unknowns: $N_xN_yN_zN_t \times N_xN_yN_zN_t$ Size of system of simultaneous equations: $(N_xN_yN_zN_t)^2$ Computational cost grows exponentially with dimensions of spatial and temporal discretization Large-scale parallel computing and efficient solvers are indispensable.

Thus, numerical implementation of non-equilibrium Green function method requires solving large systems of simultaneous equations, leading to very high computational costs. However, it has the potential to appropriately model the probabilistic processes of information propagation and bridge theory with experimental data. Efficient algorithm development and connecting models to reality are key.

3. Perspect:Potential Well and Bragg Reflection

A potential well is a structure where the potential is constant within a certain region and sharply increases at its boundary. The Schrödinger equation for a potential well is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

Here, $V(x)$ represents the potential of the well, E is the energy, and ψ is the wave function.

Within the potential well, the potential is assumed to be constant V_0. Therefore, the Schrödinger equation simplifies to:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$$

By solving this equation, the wave function and energy levels of electrons within the potential well can be determined.

Bragg reflection is a phenomenon where waves, such as X-rays or neutrons, incident on a crystal lattice are strongly reflected in specific directions. This phenomenon occurs when the spacing between atoms in the crystal lattice aligns with the wavelength of the wave. The condition for Bragg reflection is expressed by the following equation:

$$2d\sin(\theta) = n\lambda$$

Here, d represents the spacing of the crystal lattice, θ is the angle of incidence, n is the order of reflection, and λ is the wavelength.

When the condition for Bragg reflection is met, X-rays or neutrons are scattered within the crystal lattice and strongly reflected in specific directions.

These are the basic equations and computational procedures for potential wells and Bragg reflection. For specific problems or scenarios, more detailed computational procedures can be applied based on the specific conditions.

3.1 Schrödinger Equation for Potential Well

The Schrödinger equation describing the wave function of electrons within a potential well is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

Here, m represents the effective mass of the electron, $V(x)$ is the potential function of the potential well, E is the energy, and ψ is the wave function.

3.2 Potential Function of the Potential Well

Within the potential well, the potential is assumed to be constant. Therefore, the potential function $V(x)$ is defined as follows:

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

Here, L is the width of the potential well.

3.3 Solution of the Wave Function

Within the potential well, the Schrödinger equation simplifies to:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

The solution to this equation takes the general form:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Here, $k = \sqrt{\frac{2mE}{\hbar^2}}$ is the wave number, and A and B are constants.

3.4 Calculation of the Band Gap

Energy levels within the potential well are quantized, meaning they have discrete energy levels rather than continuous energy bands. The band gap is defined as the energy difference between the ground state (lowest energy level) and the first excited state (next lowest energy level).

Therefore, the band gap E_{gap} is calculated as the difference between the energies E_1 and E_0 of the first excited state and the ground state, respectively:

$$E_{\text{gap}} = E_1 E_0$$

The band gap in a potential well is calculated by determining the wave function and energy levels. By following the above steps and solving the Schrödinger equation, the band gap of the potential well can be computed.

3.5 Bragg Reflection

Bragg reflection is a phenomenon where X-rays or neutrons scattered within a crystal lattice are strongly reflected in a specific direction. This phenomenon arises from the periodicity of the crystal lattice. Below are the equations and computational procedures for Bragg reflection.

3.6 Equations for Bragg Reflection

The condition for Bragg reflection, known as Bragg's law, is expressed by the following equation:

$$2d \sin(\theta) = n\lambda$$

Here, d represents the spacing between crystal lattice planes, θ is the angle of incidence, n is the order of reflection, and λ is the wavelength.

3.7 Computational Procedure for Bragg Reflection

The procedure for calculating the Bragg reflection band gap is as follows:

Preparation of Crystal Structure: Determine the structure of the crystal of interest. Identify the spacing d between lattice planes. Determination of Incident Wave's Wavelength: Determine the wavelength λ of the incident wave (X-ray or neutron) to be used. Calculation of Incident Angle: Determine the angle of incidence θ of the incident wave. Typically, in Bragg reflection, it is assumed that the angle of incidence equals the angle of reflection. Application of Bragg's Law: Use Bragg's law to determine the order of reflection n. Calculation of Band Gap: If the conditions for Bragg reflection are met, the wavelength of the wave strongly reflected in a specific direction is determined. Calculate the band gap from this wavelength. Interpretation of Results: Interpret the calculated band gap to gain insights into the properties and structure of the material.

Since Bragg reflection relies on the periodicity of the crystal, detailed information about the crystal structure is necessary. Additionally, Bragg reflection is observed only for specific wavelengths such as X-rays or neutrons, making the characteristics of the incident wave crucial. Accurate knowledge of experimental data and crystal structure is required for the calculations.

The application of potential well and Bragg reflection analysis methods to deep fake analysis of digital information will be summarized. Potential well and Bragg reflection analysis methods are advanced techniques for elucidating physical phenomena in detail using numerical and analytical methods. Applying these methods to deep fake analysis of digital information provides a deeper understanding of the generative models and editing methods behind images and video. Potential well and Bragg reflection analysis methods can be used to detect anomalous behavior and features that deviate from the canonical generative model. For example, it can detect patterns and unnatural changes in images and videos generated using deep fake techniques and identify them as anomalies. deep fake techniques pose a significant threat to security systems such as face recognition and video analytics. By utilizing potential well and Bragg reflection analysis methods, it is expected that countermeasures and defenses against these threats can be developed and contribute to improved security. However, potential well and Bragg reflection analysis methods are computationally expensive because they use advanced numerical and analytical methods to elucidate physical phenomena in detail. For deep fake analysis, these methods can be computationally expensive when applied to large data sets or high-resolution images and videos.

In addition, potential well and Bragg reflection analysis methods use sophisticated models and algorithms based on physics and mathematics. These models are very complex and their interpretability can be poor. Therefore, even in deep fake analysis, it can be difficult to understand the results and criteria produced by the models. In addition, there may be limited accurate data on the canonical generating models and editing methods in the deep fake analysis. When using potential well or Bragg reflection analysis methods, it may be difficult to collect and organize the data necessary to apply these methods.

As mentioned above, there are many advantages to applying potential well and Bragg reflection analysis methods to deep fake analysis, but disadvantages such as computational cost, model complexity, and lack of data must also be considered.

4. Perspect:Outlook Application to deep fake analysis of digital information

The proposed methods of empty lattice approximation and GW approximation may play an important role in the analysis of deep fake of digital information. Specifically, the following aspects of application are considered.

GW approximation and empty lattice approximation may be useful for feature extraction in digital information. These methods map data to a mathematical model and analyze its features numerically, which is useful for extracting deep fake features.

In addition, the calculation of the band gap may be useful as a measure of truth or falsehood in the analysis of deep fakes. The GW and empty lattice approximations can also be applied to build models for data analysis. These methods can be used to more accurately model data features and are expected to contribute to the improvement and accuracy of deep learning models.

As described above, the proposed methods of sky-lattice approximation and GW approximation may be useful tools in deep fake analysis of digital information. Appropriate application of these methods is expected to realize more advanced fraud detection and data analysis, and contribute to improving the reliability of digital information.

4.1 Validity of GW and Lattice Approximations for Deep Fake Analysis of Digital Information

Validity of GW Approximation and Its Application to Deep Fake Analysis of Digital Information, Theoretical Foundation: The GW approximation achieves high accuracy in calculating band gaps by accurately incorporating electron correlation effects. This method provides detailed information on electronic energy levels and spectra, serving as a useful metric to detect differences between real and deep fake digital information.

Computational Approach, The GW approximation is typically performed by correcting the self-energy based on initial calculations such as density functional theory (DFT). This allows it to be applied to large-scale calculations in extensive information spaces. Moreover, leveraging advanced numerical techniques and parallel computing technologies can reduce computational costs, enabling fast and efficient analysis.

Validity of Lattice Approximation and Its Application to Deep Fake Analysis of Digital Information, Theoretical Foundation: The lattice approximation simplifies calculations by discretizing information spaces, enabling computations in large information spaces. Even in calculating band gaps, analysis in discrete information spaces provides sufficient accuracy and reliable metrics for deep fake analysis.

Computational Approach, The lattice approximation efficiently computes band structures and self-energies using numerical analysis techniques such as Fourier transforms. Therefore, it can be applied to large-scale calculations in extensive information spaces. Furthermore, due to relatively low computational costs, it is suitable for analyzing multiple datasets or large amounts of data.

GW and lattice approximations offer different computational methods and accuracies, both of which are considered valid approaches for deep fake analysis of digital information. The GW approximation, with its advanced theoretical foundation, provides relatively high accuracy but tends to have higher computational costs. The lattice approximation enables analysis in discrete information spaces, reducing computational costs while maintaining sufficient accuracy. Both methods are applicable to large-scale calculations in extensive information spaces, serving as powerful tools for achieving reliable analyses in deep fake analysis of digital information.

4.2 Comparison of GW and Lattice Approximations for Deep Fake Analysis in Large Information Spaces

Comparing the GW and lattice approximations, we focus on their application to deep fake analysis of digital information in large-scale first-principles calculations, explaining the merits and drawbacks of each method.

4.3 Merits of GW Approximation for Deep Fake Analysis of Digital Information

High Precision Theoretical Foundation, The GW approximation provides high accuracy in calculating band gaps by accurately incorporating electron correlation effects. This makes it a reliable metric for detecting differences between real and deep fake digital information in deep fake analysis.

Detailed Information Provision, The GW approximation provides detailed information on electronic energy levels and spectra. This information serves as a useful metric for understanding the characteristics of data and detecting fraudulent data in deep fake analysis.

4.4 Drawbacks of GW Approximation for Deep Fake Analysis of Digital Informations

High Computational Cost, The GW approximation has high computational costs, requiring substantial resources for large-scale calculations in extensive information spaces. This may pose challenges in terms of computational time and resource constraints in deep fake analysis of digital information.

4.5 Merits of Lattice Approximation for Deep Fake Analysis of Digital Information

Low Computational Cost, The lattice approximation performs calculations in discretized information spaces, resulting in relatively low computational costs. This enables efficient large-scale calculations in extensive information spaces.

4.6 Drawbacks of Lattice Approximation for Deep Fake Analysis of Digital Information

Lower Accuracy, The lattice approximation may have lower accuracy compared to analysis in continuous information spaces. Consequently, it may not achieve sufficient accuracy in deep fake analysis of digital information. Limited Information Provision, The lattice approximation restricts the provision of continuous information due to its discrete nature. This limitation may result in insufficient information for deep fake analysis of digital information. Both GW and lattice approximations have their merits and drawbacks. When applying them to deep fake analysis of digital information, it is essential to consider the balance between computational cost and accuracy. While the GW approximation offers high precision, it tends to have high computational costs. On the other hand, the lattice approximation has lower computational costs but may sacrifice accuracy. Choosing the appropriate method is crucial in deep fake analysis of digital information, depending on the nature of the problem and the analysis objectives. The following theoretical approaches can also be considered when applying potential well and Bragg reflection analysis methods to deep fake analysis of digital information. As an

application of potential wells, numerical and analytical methods of potential wells can be used to extract features of images and videos generated by generative models. This allows data with features or patterns that differ from regular data to be detected and identified as anomalies. For example, the distribution of features and edges in an image generated by a deep learning model can be analyzed and judged as anomalous if the distribution is different from that of a normal image. An application of Bragg reflection is to use the matrix transfer or density matrix method of Bragg reflection to map features in data transformed by a generative model. For example, by viewing an image or video as a lattice structure and analyzing the behavior of wave propagation and reflection on the lattice, the features of the transformed data can be quantified and compared to regular data. Using these theoretical approaches, potential well and Bragg reflection analysis methods can be applied to deep fake analysis for purposes such as anomaly detection and feature mapping. This is expected to help assess the quality and reliability of the data generated and contribute to improving the performance and enhancing the security of deep learning models.

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