Chapter 12: GWA Calculations in Practice

1 Introduction

GW calculations have become an essential part of computational condensed-matter physics, widely utilized for accurately predicting electronic properties such as band structures and spectral functions. Implementing GW methods involves significant computational efforts and choices related to approximations and numerical techniques. Initially, GW aimed at addressing electron correlations beyond Hartree–Fock by incorporating the concept of screening. The pioneering works established that correlation energies could be derived from the polarization response of the electron gas, notably illustrated by Hedin's seminal paper in 1965. Since then, practical GW methods have evolved through substantial algorithmic improvements and the exponential growth of computational power. Despite its success in improving Kohn–Sham density functional theory (DFT) bandgaps, GW calculations remain theoretically intricate and computationally demanding, especially for complex materials.

The GW method seeks accurate predictions and smaller error margins to become truly predictive. The core ambiguity of GW calculations lies in determining precisely which Green's function G and screened interaction W should be used. This ambiguity is intrinsic to many-body perturbation theory and requires thoughtful guidelines.

2 The Task: A Summary

The main objective of a GW calculation is computing the exchange-correlation self-energy:

$$\Sigma_{xc}(1,2) = iG(1,2)W(1^+,2) \tag{1}$$

Typically, matrix elements of the self-energy are evaluated within a basis set of independent-particle states:

$$\Sigma_{xc,k\ell}(t_1,t_2) = i\sum_{ij} G_{ij}(t_1,t_2)W_{ij}^{k\ell}(t_1^+,t_2) \tag{2}$$

The screened interaction W is obtained by solving the Dyson equation for W:

$$W(r_1,r_2) = v_c(r_1,r_2) + \int dr_3 dr_4\, v_c(r_1,r_3)P(r_3,r_4)W(r_4,r_2) \tag{3}$$

In the widely used Random Phase Approximation (RPA), the polarizability P is approximated as:

$$P \approx P_0(r_3,r_4) = -i\sum_{\sigma} G_\sigma(r_3,r_4)G_\sigma(r_4,r_3) \tag{4}$$

When the bare Coulomb interaction is spin-independent and no spin–orbit or non-collinear magnetism terms are present, the self-energy becomes spin-diagonal:

$$\Sigma_{xc,\sigma} = iG_\sigma W \tag{5}$$

In practice, calculations typically start from an initial guess, G_0, derived from a static mean-field calculation (often Kohn–Sham). The Dyson equation is then solved separately for each spin component σ:

$$G_\sigma = G_\sigma^0 + G_\sigma^0(\Sigma_{xc,\sigma} - v_{xc,\sigma})G_\sigma \tag{6}$$

Here, $v_{xc,\sigma}$ represents the already included exchange-correlation potential, which must be subtracted from the self-energy calculation to avoid double counting.

The frequency Fourier transform of the self-energy is given as:

$$\Sigma_{xc,\sigma}(r, r'; \omega) = \lim_{\eta \to 0^+} \frac{i}{2\pi} \int d\omega' G_\sigma(r, r'; \omega + \omega') W(r, r'; \omega') e^{i\eta\omega'} \tag{7}$$

GW calculations thus follow these essential steps:

1. Determine the starting Green's function, G_0.
2. Calculate polarizability P from G_0.
3. Solve the Dyson equation for W.
4. Compute the self-energy Σ_{xc} by the convolution of G and W.
5. Solve the Dyson equation or the quasi-particle equation to obtain updated Green's functions or quasi-particle energies:

$$(\hat{h} + \text{Re } \hat{\Sigma}(\varepsilon_\ell))|\psi_\ell(\varepsilon_\ell)\rangle = \varepsilon_\ell|\psi_\ell(\varepsilon_\ell)\rangle \tag{8}$$

The computational process involves careful consideration of spin structure, basis sets, and frequency integration techniques, making GW calculations methodologically challenging yet highly valuable for predicting and understanding electronic properties of materials.

3 Frequently Used Approximations

3.1 Building on a Single-Particle Green's Function G_0

In GW calculations, the exchange-correlation self-energy $\Sigma_{xc} = iGW$ is constructed using a single-particle Green's function G_0, typically derived from a mean-field approximation or a static self-energy calculation. The Green's function G_0 is represented as:

$$G_0^\sigma(r_1, r_2; z) = \lim_{\eta \to 0^+} \sum_\ell \frac{\psi_\ell^\sigma(r_1)\psi_\ell^{\sigma*}(r_2)}{z - \varepsilon_\ell^\sigma + i\eta\,\text{sgn}(\varepsilon_\ell^\sigma - \mu)}, \tag{9}$$

where ψ_ℓ^σ and ε_ℓ^σ represent single-particle eigenfunctions and eigenvalues, respectively, and μ is the chemical potential.

The next essential quantity is the irreducible polarizability P_0, calculated from G_0:

$$P_0(r, r'; z) = \sum_{ij\sigma} \frac{(f_{i\sigma} - f_{j\sigma})\psi_{i\sigma}^{0*}(r)\psi_{j\sigma}^0(r)\psi_{i\sigma}^0(r')\psi_{j\sigma}^{0*}(r')}{z - (\varepsilon_{j\sigma}^0 - \varepsilon_{i\sigma}^0)}. \tag{10}$$

From P_0, the screened Coulomb interaction W_0 and subsequently the self-energy $\Sigma_{xc} = iG_0W_0$ are obtained, known as the G_0W_0 approximation.

3.1.1 Choice of Starting Hamiltonian $\hat{h}$

The quality and accuracy of G_0W_0 calculations significantly depend on the initial independent-particle Hamiltonian $\hat{h}$ selected. Ideally, the starting Hamiltonian should yield either a band structure or density very close to the quasi-particle results of the subsequent GW calculation, serving as an approximate self-consistency condition. Typical choices include:

- **Kohn–Sham Hamiltonian:** Initially adopted in the earliest ab initio GW calculations, the KS Hamiltonian—particularly within the local density approximation (LDA) or generalized gradient approximation (GGA)—is frequently used due to its pragmatic convenience and good density predictions. However, KS-LDA tends to underestimate quasi-particle band gaps significantly (typically 50-100%), and the density might suffer from over-delocalization, excess hybridization, and magnetic moment underestimation. Nevertheless, for simple semiconductors, KS wavefunctions remain good approximations for quasi-particle wavefunctions, often with overlaps greater than 95%.

- **Hartree–Fock Hamiltonian:** Provides a conceptual advantage by assigning physically meaningful eigenvalues directly linked to electron addition and removal energies through Koopmans' theorem. However, due to its significantly larger bandgap predictions, this Hamiltonian is recommended mainly for large-gap semiconductors and atomic systems where screening is modest.

- **Generalized Kohn–Sham Hamiltonian:** Extends the Kohn–Sham approach by including non-local exchange potentials, particularly hybrid functionals. Such Hamiltonians maintain exact exchange contributions and provide significantly improved band structures and ground-state properties, making them suitable starting points for GW calculations, especially when combined with range-separated hybrid functionals.

- **DFT+U:** Introduces an empirical gap of magnitude U between localized states, suitable for systems with strongly correlated electrons such as transition-metal oxides or lanthanide compounds. This practical approach provides a convenient yet semi-empirical starting point.

Each choice of Hamiltonian comes with its benefits and drawbacks, and the appropriate selection depends significantly on the characteristics of the material under study and the computational resources available.

3.2 Choice of the Screened Interaction W_0

In the GW approximation (GWA), the screened Coulomb interaction W is typically calculated within the Random Phase Approximation (RPA). However, alternative choices and refinements beyond RPA are possible. The primary consideration for choosing W_0 is linked to the potential benefit from error cancellation between neglected vertex corrections in the polarizability P and the self-energy Σ_{xc}. Often, RPA calculations using Kohn–Sham (KS) inputs provide a good approximation for the inverse dielectric function, yielding results close to experimental data. This makes the KS-based RPA a strong candidate for W_0.

To further refine W, one could employ time-dependent density functional theory (TDDFT) or Bethe–Salpeter equation (BSE) methods, although the latter is typically computationally demanding except for small systems.

3.2.1 Plasmon Pole Models

A significant computational challenge in GWA is the frequency integration involved in calculating W_0. To simplify this, W_0 can be represented approximately as a sum over discrete poles. Such a representation transforms the self-energy calculation into a double sum over poles of G_0 and W_0.

Early GWA calculations approximated the imaginary part of W_0 by a single-plasmon branch characterized by a dispersion relation $\omega_p(q)$. In crystals, this approach is motivated by the behavior of the loss function $-\mathrm{Im}\,\epsilon^{-1}_{G,G}(q;\omega)$, typically dominated by a single plasmon peak at low momentum transfer.

The single-plasmon pole approximation is expressed as:

$$\mathrm{Im}\,\epsilon^{-1}_{GG'}(q;\omega) = -A_{GG'}(q)\left[\delta(\omega - \omega^p_{GG'}(q)) + \delta(\omega + \omega^p_{GG'}(q))\right], \tag{11}$$

where ω_p is the effective plasmon frequency and $A_{GG'}(q)$ is the strength.

Using the Kramers–Kronig relations, the real part of the inverse dielectric function is given by:

$$\mathrm{Re}\,\epsilon^{-1}_{GG'}(q;\omega) = \delta_{GG'} + \frac{2}{\pi}\frac{A_{GG'}(q)\,\omega^p_{GG'}(q)}{\omega^2 - [\omega^p_{GG'}(q)]^2}. \tag{12}$$

Parameters A and ω_p can be determined through various fitting approaches. One commonly used method involves fitting the inverse dielectric function along the imaginary axis at selected frequencies, typically at $\omega = 0$ and at a frequency of the order of the plasmon energy. This fitting method is advantageous because it allows quick assessments of model reliability by varying the fit frequency.

Extensions of the plasmon pole model to multiple poles are also possible through methods such as the band Lanczos approach, providing higher precision at the cost of increased computational effort.

4 Restricting Calculations to Quasi-Particle Properties

In many GW calculations, the primary interest lies in determining quasi-particle (QP) properties, such as band structures and lifetime broadenings. For such purposes, the full self-energy $\Sigma(\omega)$, which is generally non-hermitian and complex, is simplified to a real, energy-dependent approximation. The resulting equation has the structure of a one-body Schrödinger equation for each quasi-particle state ℓ:

$$\left(\hat{h} + \mathrm{Re}\,\hat{\Sigma}(\varepsilon_\ell)\right)|\psi_\ell(\varepsilon_\ell)\rangle = \varepsilon_\ell|\psi_\ell(\varepsilon_\ell)\rangle. \tag{13}$$

This quasi-particle equation, when solved near the Fermi level, provides sufficient information for most practical GW band structure calculations.

4.1 Solving the Quasi-Particle Equation to First Order

For an appropriate initial Green's function G_0, solving the quasi-particle equation to first order in the difference between the GW self-energy Σ_{xc} and the exchange-correlation potential v_{xc} is justified. The first-order corrected quasi-particle energies ε_ℓ are given by:

$$\varepsilon_\ell = \varepsilon^0_\ell + \langle\psi^0_\ell|\hat{\Sigma}_{xc}(\varepsilon_\ell) - \hat{v}_{xc}|\psi^0_\ell\rangle, \tag{14}$$

where $|\psi^0_\ell\rangle$ are eigenstates of the independent-particle Hamiltonian $\hat{h}$.

4.2 Linearizing the Self-Energy

To simplify the evaluation, the self-energy $\Sigma_{xc}(\omega)$ can be linearly expanded around the initial energies ε_ℓ^0. This yields the linearized quasi-particle equation:

$$\varepsilon_\ell = \varepsilon_\ell^0 + Z_\ell \langle \psi_\ell^0 | \hat{\Sigma}_{xc}(\varepsilon_\ell^0) - \hat{v}_{xc} | \psi_\ell^0 \rangle, \tag{15}$$

where the renormalization factor Z_ℓ is defined by:

$$Z_\ell^{-1} = 1 - \langle \psi_\ell^0 | \frac{\partial \hat{\Sigma}_{xc}}{\partial \omega} \bigg|_{\varepsilon_\ell^0} | \psi_\ell^0 \rangle. \tag{16}$$

The factor Z_ℓ, representing the weight of the quasi-particle in the spectral function, effectively reduces the magnitude of the self-energy correction, stabilizing and simplifying the computational treatment of the quasi-particle states.

5 Different Levels of Self-Consistency in GW Calculations

The standard GW approximation (GWA), specifically the G_0W_0 approach, relies on an initial Green's function G_0 derived from a static mean-field approximation. However, G_0W_0 is inherently dependent on the starting point and can exhibit significant limitations, such as:

- Dependence on initial Hamiltonian choice
- Violation of particle number conservation
- Poor satellite description
- Unphysical spectral functions due to improper gap representation

To mitigate these issues, various degrees of self-consistency have been introduced.

5.1 Alignment of the Chemical Potential

The simplest self-consistency step is aligning the chemical potentials between the initial Green's function G_0 and the resulting GW calculation by introducing an energy shift $\Delta\varepsilon$:

$$\mu = \mu_0 + \Delta\varepsilon = \mu_0 + \Sigma_{k_F}(\mu). \tag{17}$$

The adjusted Green's function becomes:

$$G_0^\sigma(r_1, r_2; z) = \sum_n \frac{\psi_{n\sigma}(r_1)\psi_{n\sigma}^*(r_2)}{z - \varepsilon_{n\sigma}^0 - \Delta\varepsilon}, \tag{18}$$

with the corresponding frequency shift in the self-energy:

$$\Sigma(z) \to \Sigma(z - \Delta\varepsilon). \tag{19}$$

5.2 Z = 1 Approximation

By assuming each state undergoes a uniform shift $\Delta\varepsilon$, one can simplify the self-consistency condition by evaluating the self-energy without the renormalization factor Z:

$$\varepsilon_\ell = \varepsilon_\ell^0 + \langle\psi_\ell^0|\hat{\Sigma}(\varepsilon_\ell^0) - \hat{v}_{xc}|\psi_\ell^0\rangle. \tag{20}$$

This approximation avoids the detailed calculation of quasi-particle renormalization factors.

5.3 Self-Consistent Update of Quasi-Particle Energies

A more comprehensive approach involves updating quasi-particle energies iteratively, which adjusts screening effects and typically increases the calculated gap closer to Hartree–Fock results. Such updates are crucial for accurate spectral predictions, especially if significant reordering of states occurs.

5.4 Self-Consistent COHSEX

For systems where Kohn–Sham wavefunctions differ significantly from quasi-particle wavefunctions, self-consistency can be introduced using the static COHSEX approximation. COHSEX employs a static self-energy constructed only from occupied states, simplifying the computational effort compared to fully dynamical self-consistency.

5.5 Quasi-Particle Self-Consistent GW (QSGW)

The QSGW method constructs an optimized static, non-local Hamiltonian H^{QP}, closely matching the GW-derived quasi-particle eigenvalues and wavefunctions. The effective Hamiltonian is defined as:

$$H^{QP} = \frac{1}{2}\sum_{ij} |\psi_i^{QP}\rangle \left[\mathrm{Re}\Sigma_{ij}(\varepsilon_i^{QP}) + \mathrm{Re}\Sigma_{ij}(\varepsilon_j^{QP})\right] \langle\psi_j^{QP}|. \tag{21}$$

QSGW generally provides improved predictions for quasi-particle energies and wavefunctions compared to G_0W_0.

5.6 GW0 Approach

The GW0 approach performs full self-consistency in G while keeping W_0 fixed. This method conserves particle number and maintains better satellite spectra accuracy compared to fully self-consistent GW. However, it leads to results closer to Hartree–Fock due to reduced screening.

5.7 Fully Self-Consistent GW

Fully self-consistent GW calculations iteratively solve the Dyson equation for both G and W. While this method is essential for accurate total energy calculations, it may degrade spectral quality due to inadequate treatment of vertex corrections.

5.8 Rules of Thumb

Practically, the choice of self-consistency depends on the targeted properties. GW0 with "best W" is often recommended for accurate spectra, combining realistic screening and correct analytical properties. For total energies, fully self-consistent GW within RPA may offer preferable results.

6 Frequency Integrations in GW Calculations

Frequency integrations represent one of the most challenging aspects of GW calculations due to the presence of poles near the real axis. Various approaches to effectively carry out these integrations are summarized here.

6.1 Calculation of P_0

The irreducible polarizability P_0 can be calculated via frequency Fourier transforms as:

$$P_0(\omega) = -\frac{i}{2\pi} \lim_{\eta \to 0^+} \sum_\sigma \int d\omega' G_\sigma(\omega + \omega') G_\sigma(\omega') e^{i\eta\omega'}, \tag{22}$$

or for finite temperatures using Matsubara frequencies:

$$P_0(z_n) = \frac{1}{\beta} \sum_m \sum_\sigma G_\sigma(z_m) G_\sigma(z_n + z_m). \tag{23}$$

These equations simplify to known forms when using independent-particle Green's functions.

6.2 Plasmon Pole Approximation

A simplified integration for the self-energy Σ involves approximating the screened Coulomb interaction W using plasmon poles, particularly useful for evaluating real parts of the self-energy near the Fermi level. This approach significantly reduces computational complexity.

6.3 Full Frequency Integration

Direct numerical integration of the full frequency-dependent self-energy $\Sigma(\omega)$ on the real axis is computationally demanding due to closely spaced poles. Alternatives to full real-axis integrations include:

- **Matsubara Frequencies**: At non-zero temperatures, self-energy calculations are typically performed using discrete Matsubara frequencies:

$$\Sigma(z_n) = -\frac{1}{\beta} \sum_m G(z_n - \nu_m) W(\nu_m). \tag{24}$$

- **Spectral Function Method**: At zero temperature, exploiting the analytic structure of Green's functions leads to integration via spectral functions $A(\omega)$ and $D(\omega)$:

$$\Sigma_c(\omega) = \int_{-\infty}^{+\infty} d\omega_1 \int_0^\infty d\omega_2 \frac{A(\omega_1) D(\omega_2)}{\omega + (\omega_2 - i\eta)\mathrm{sgn}(\mu - \omega_1) - \omega_1}. \tag{25}$$

- **Contour Integration**: Utilizing contour integration in the complex plane simplifies the evaluation significantly:

$$\Sigma_c(\omega) = -\frac{i}{2\pi} \int_{-i\infty}^{+i\infty} G(\omega + z) W_p(z) dz + \sum_i f_i(r) f_i^*(r') W_p(r', r, |\varepsilon_i - \omega| - i\eta) [\theta(\mu - \varepsilon_i)\theta(\varepsilon_i - \omega) - \theta(\varepsilon_i - \mu)\theta(\omega - \varepsilon_i)] \tag{26}$$

This method is more reliable as it avoids double-frequency integration.

- **Analytic Continuation**: Transitioning from imaginary-axis results to real-axis quantities can be done through analytic continuation, often employing Padé approximants:

$$R(z) = \frac{\sum_{i=0}^{n} a_i z^i}{\sum_{j=0}^{m} b_j z^j}, \tag{27}$$

  with appropriately chosen parameters to achieve desired precision near energy gaps.

6.4 GW Total Energy Calculations

Total energy calculations within GW methods involve an additional frequency integration, typically via the Galitskii–Migdal formula:

$$E = \frac{1}{2\beta} \sum_{\ell\sigma} \sum_{\nu} (\varepsilon^0_{\ell\sigma} + z_\nu) G_{\ell\ell\sigma}(z_\nu), \quad \text{for } T \neq 0, \tag{28}$$

$$E = \frac{1}{2} \sum_{\ell\sigma} \int_{-\infty}^{\mu} d\omega (\varepsilon^0_{\ell\sigma} + \omega) A_{\ell\ell\sigma}(\omega), \quad \text{for } T = 0. \tag{29}$$

Alternative evaluations using functional approaches, involving Matsubara frequencies and logarithmic functionals, are also common, especially in comparison to simpler DFT-RPA calculations.

7 GW Calculations in a Basis

GW calculations involve both frequency and spatial integrations. While frequency integrations are unique to many-body perturbation theory, spatial integrations share commonalities with standard mean-field methods. This section focuses specifically on spatial integrations, emphasizing basis-set approaches to solving GW equations.

7.1 Matrix Elements

GW equations are often solved using matrix formulations. Given a set of normalized basis functions $\chi_m(r)$, independent-particle or quasi-particle wavefunctions can be expanded as:

$$\psi_{i\sigma}(r) = \sum_m b^m_{i\sigma} \chi_m(r). \tag{30}$$

The two-point matrix elements in a general basis are defined as:

$$F_{n_1 n_2} = \int dr_1 dr_2 \chi^*_{n_1}(r_1) F(r_1, r_2) \chi_{n_2}(r_2). \tag{31}$$

Matrix elements in terms of independent-particle wavefunctions are given by:

$$F_{ij} = \int dr_1 dr_2 \psi^*_i(r_1) F(r_1, r_2) \psi_j(r_2). \tag{32}$$

Four-point functions transform according to:

$$F_{n_1 n_2 n_3 n_4} = \int dr_1 dr_2 dr_3 dr_4 \chi^*_{n_1}(r_1) \chi^*_{n_2}(r_2) F(r_1, r_2, r_3, r_4) \chi_{n_3}(r_3) \chi_{n_4}(r_4). \tag{33}$$

For the screened interaction W, we define matrix elements as:

$$W_{ki\ell j} = \int dr_1 dr_3 \psi_k^*(r_1)\psi_j(r_1)W(r_1, r_3)\psi_\ell(r_3)\psi_i^*(r_3). \tag{34}$$

The self-energy matrix elements become:

$$\Sigma_{xc,k\ell} = i \sum_{ij} G_{ij} W_{k\ell}^{ij}. \tag{35}$$

7.2 Choice of the Basis

7.2.1 Plane Waves

Plane-wave bases are preferred for periodic systems due to computational convenience and diagonalization of the bare Coulomb interaction. Key integrals, such as the polarizability, are efficiently computed using Fast Fourier Transforms:

$$\tilde{\rho}_{ijk\sigma}(q+G) = \frac{1}{\sqrt{\Omega}} \int dr\, \psi_{ik\sigma}^*(r)\psi_{jk+q\sigma}(r)e^{-i(q+G)r}. \tag{36}$$

7.2.2 Localized Orbitals

Localized-orbital bases (e.g., LCAO, LMTO, Gaussian orbitals) provide convenience in describing core and semi-core electrons. These bases have proven successful historically for various materials, especially those involving d and f electrons, as well as finite systems. Examples include the Linear Muffin-Tin Orbital (LMTO) and Numeric Atom-Centered Orbital (NAO) bases.

7.3 Optimized Basis for Polarizability

To reduce computational demands, the polarizability P_0 can be computed using an optimized product basis derived from pairs of orbitals. This significantly reduces the computational overhead by minimizing the number of required basis functions.

7.4 Basis for Self-Consistent Calculations

In self-consistent GW calculations, new quasi-particle wavefunctions are most conveniently expressed in the basis of eigenfunctions derived from the initial independent-particle Hamiltonian. Typically, only a small subset of eigenfunctions is required since the self-energy mixing is limited to a relatively small energy range and conserves crystal momentum.

8 Scaling and Convergence

8.1 The Coulomb Interaction

Careful treatment of the long-range Coulomb interaction is crucial in GW calculations. In plane-wave calculations for finite systems, simulations typically employ a large periodically repeated unit cell (supercell) containing the studied object surrounded by empty space. While ground-state calculations of neutral systems without dipole moments easily handle supercells, excited-state calculations suffer from convergence difficulties due to long-range interactions arising from electron additions, removals, or dipole creation. To alleviate this problem and reduce computational demands, modified Coulomb interactions cut off in real space can be employed.

In extended systems, the steep reciprocal-space Coulomb interaction $4\pi/q^2$ presents similar issues, necessitating fine q-meshes. An improved integration method uses two grids: a coarse grid for density and dielectric functions, and a finer grid for the Coulomb interaction. This enhanced integration technique improves convergence for both periodic and finite systems, effectively managing the divergence at $q = 0$.

8.2 Important Convergence Parameters

Spectroscopy calculations, including GW0 quasi-particle or spectral function computations, require careful consideration of convergence parameters that differ significantly from ground-state calculations:

- **k-points**: While convergence is less stringent than optical calculations, rigorous testing remains necessary due to pole integrations.
- **Empty States**: Convergence with empty states is typically slow, displaying an error scaling approximately as $E_{\text{cut}}^{-3/2}$. Iterative inversion methods circumvent explicit summation over bands, implicitly defining band numbers through Hamiltonian dimensions. Alternatively, the effective energy technique (EET) employs a state-independent "effective energy," significantly enhancing computational efficiency by utilizing closure relations.
- **Number of Basis Functions**: Practically, separate considerations for wavefunction expansions and self-energy summations are beneficial. Smaller inverse dielectric function components can suffice when crystal local field effects (LFE) are minimal, optimizing computational efficiency.

8.3 Scaling of GW Calculations

Typical GW calculations employ spectral representations in plane-wave bases, with key computational steps exhibiting varied scaling behaviors:

- Calculation of $\tilde{\rho}$ using fast Fourier transforms scales as $N_{\text{at}} \ln(N_{\text{at}})$.
- Polarizability matrix element calculations scale as $N_{\text{at}}^4 N_k^2$, simplifying to N_{at}^2 for smaller unit cells.
- Single self-energy matrix elements scale as $N_q N_{\text{at}}^3$ or N_{at}^2 in sufficiently small cells.

For large systems, significant scaling improvements are achievable by employing the nearsightedness principle, which assumes spatial localization of relevant quantities. Real-space methods, such as the space-time approach, calculate Green's functions directly, scaling as N_{at}^2, and compute polarizabilities from Green's function products, achieving linear scaling in atom numbers.