

Decay properties of the one-particle Green function in real space and imaginary time

Arno Schindlmayr*

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin-Dahlem, Germany

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The decay properties of the one-particle Green function in real space and imaginary time are systematically studied for solids. I present an analytic solution for the homogeneous electron gas at finite and at zero temperature as well as asymptotic formulas for real metals and insulators that allow an analytic treatment in electronic-structure calculations based on a space-time representation. The generic dependence of the decay constants on known system parameters is used to compare the scaling of reciprocal-space algorithms for the *GW* approximation and the space-time method.

I. INTRODUCTION

The *GW* approximation¹ for the electronic self-energy is known to produce quasiparticle band structures in very good agreement with experimental data for a wide range of crystalline materials that include semiconductors,^{2,3} simple metals,⁴ and even transition metals.⁵ It corresponds to a summation of ring diagrams to infinite order and may be thought of as an extended Hartree-Fock scheme with dynamically screened exchange. Despite the long-recognized success for bulk systems there are still comparably few applications to more complicated geometries, however, because of the rapid increase in computational cost. Unless additional simplifications like a plasmon-pole model² for the screened Coulomb interaction are employed, conventional reciprocal-space algorithms scale like N^4/b^2 for a calculation of the complete spectral function, where N is a measure of the system size, such as the number of atoms in a bulk material, and b is inversely proportional to the number of frequency mesh points.⁶ The scaling problem is further compounded if diagrammatic vertex corrections beyond the *GW* approximation are included.⁷ The design of more efficient implementations is therefore a pressing task.

In order to achieve a more favorable scaling, Rojas and co-workers recently proposed an algorithm based on an alternative representation of the Green function in real space and imaginary time.^{8,9} This approach allows the calculation of the irreducible polarizability and the self-energy as simple products rather than numerically expensive convolutions. Furthermore, it directly exploits locality, i.e., the fact that the Green function decays to zero as its spatial or temporal arguments move apart. As a result, with a fixed cutoff energy this so-called space-time method only scales like $N^2/\gamma^3 b$, where γ denotes the exponential decay constant in real space. Logarithmic terms are neglected. Under the assumption that the frequency mesh maps one-to-one onto the relevant region of the imaginary-time axis, b can there be identified with the inverse period $\frac{1}{2}k_B T$ in a finite-temperature formalism and with the exponential decay constant otherwise. The locality of the Green function is a manifestation of the more general “nearsightedness” principle¹⁰ and due to destructive quantum interference in many-electron systems.

While the behavior of the Green function in reciprocal space and the frequency domain has been analyzed in great

detail,¹¹ there has so far been no comprehensive study of the decay properties in real space and, for zero temperature, on the imaginary-time axis. In fact, even qualitative features are not always recognized correctly: Ref. 6, for instance, describes the asymptotic tail of the Green function as being proportional to $|\mathbf{r}-\mathbf{r}'|^{-2}$. While this assertion is correct for the homogeneous electron gas at zero temperature, I argue here that real materials in general exhibit exponential rather than algebraic decay. Attempts to model the self-energy using results obtained for the homogeneous electron gas,^{12–14} which are motivated by seemingly universal features in the short-range part of the nonlocality¹⁵ and the success of the local-density approximation¹⁶ in density-functional theory,¹⁷ should appreciate such fundamental differences.

The first objective of this paper is to systematically study the decay properties of the one-particle Green function in solids, separately for metals and insulators, and to obtain analytic expressions for the asymptotic behavior in real space and imaginary time. Besides intrinsic interest, these can be directly exploited in electronic-structure calculations. In the space-time method, for instance, an analytic treatment of the asymptotic tail on the imaginary time axis, in combination with a customized Gauss-Legendre grid, reduces the number of mesh points where the Green function must be evaluated numerically by one order of magnitude.¹⁸ I show here that the exponential fit proposed in Ref. 18 is only valid for systems with a finite band gap, however, while metals at zero temperature instead require an algebraic fitting function. The second objective is to relate the decay constants γ and b to known system parameters. This is then used for a more detailed scaling comparison between the space-time approach and conventional implementations.

Due to the central role of locality in $O(N)$ methods¹⁹ within density-functional theory, the spatial decay rate of the one-particle density matrix, which is a special element of the Green function, has recently received some attention.^{20,21} Physically, the nonlocality of the density matrix stems entirely from the delocalized quantum character of the wave functions, while the Green function also describes the actual transport of particles. The results obtained for the density matrix can therefore not be generalized in a straightforward way, although they are recovered here if the imaginary-time argument approaches zero from below. Furthermore, the one-particle density matrix contains no information about the

behavior of the Green function on the imaginary time axis.

This paper is organized as follows. Section II introduces the Green function in real space and imaginary time. In Sec. III an analytic solution for the homogeneous electron gas is presented. I derive asymptotic formulas for real metals and insulators in Secs. IV and V. The results are summarized in Sec. VI together with a discussion. Atomic units are used throughout.

II. THE GREEN FUNCTION

The imaginary-time or thermal Green function is defined as²²

$$\begin{aligned} \mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = & \Theta(-\tau) \langle e^{(\hat{H} - \mu \hat{N})\tau} \hat{\psi}^\dagger(\mathbf{r}') e^{-(\hat{H} - \mu \hat{N})\tau} \hat{\psi}(\mathbf{r}) \rangle \\ & - \Theta(\tau) \langle e^{-(\hat{H} - \mu \hat{N})\tau} \hat{\psi}(\mathbf{r}) e^{(\hat{H} - \mu \hat{N})\tau} \hat{\psi}^\dagger(\mathbf{r}') \rangle, \end{aligned} \quad (1)$$

where $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$ denote the creation and annihilation operator for an electron at \mathbf{r} . The Hamiltonian \hat{H} is modified by the chemical potential μ and the electron number operator \hat{N} , the angular brackets indicate the thermodynamic average, and $\Theta(\tau)$ denotes Heaviside's step function. Spin degrees of freedom are suppressed to simplify the notation. At finite temperature the real variable τ is restricted to $-\beta < \tau < 0$ with $\beta = 1/k_B T$ for the hole part and $0 < \tau < \beta$ for the electron part, and the Green function is periodically repeated. Due to the additional antiperiodicity $\mathcal{G}(\tau) = -\mathcal{G}(\tau + \beta)$ it suffices to examine the hole part. At zero temperature the period becomes infinite, however, and the properties of both parts must be studied separately. Note that Refs. 9 and 18 employ an alternative prefactor convention $G(i\tau) = i\mathcal{G}(-\tau)$ for the imaginary-time Green function at zero temperature, which stems from analytic continuation in the time domain rather than the frequency domain.

For real materials it is convenient to rewrite the hole part of the Green function in the form

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) = \sum_n \mathcal{G}_n(\mathbf{r}, \mathbf{r}'; \tau), \quad (2)$$

$$\mathcal{G}_n(\mathbf{r}, \mathbf{r}'; \tau) = \sum_{\mathbf{R}, \mathbf{R}'} w_n(\mathbf{r} - \mathbf{R}) F_n(\mathbf{R} - \mathbf{R}'; \tau) w_n^*(\mathbf{r}' - \mathbf{R}'), \quad (3)$$

$$w_n(\mathbf{r} - \mathbf{R}) = \frac{1}{\Omega_B} \int e^{-i\mathbf{k} \cdot \mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r}) d^3k, \quad (4)$$

$$F_n(\mathbf{R} - \mathbf{R}'; \tau) = \frac{1}{\Omega_B} \int e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} \frac{e^{-(\epsilon_{n\mathbf{k}} - \mu)\tau}}{1 + e^{(\epsilon_{n\mathbf{k}} - \mu)\beta}} d^3k \quad (5)$$

and analogous for the electron part. Here \mathbf{R} labels the lattice vectors, $w_n(\mathbf{r} - \mathbf{R})$ indicates the Wannier orbitals corresponding to a set of Bloch wave functions $\psi_{n\mathbf{k}}(\mathbf{r})$, and the integrals extend over the first Brillouin zone with volume Ω_B . Wannier orbitals are widely accepted to exhibit exponential localization. In addition to a rigorous proof for isolated bands,²³ there is compelling numerical evidence to this effect for the general case of composite bands.²⁴ Crucially,

the localization persists even if defects or surfaces break the periodicity of the solid.²⁵ As the decay length of Wannier orbitals is of the order of the interatomic spacing, only a small number of terms contributes significantly to the sum (3).

III. THE HOMOGENEOUS ELECTRON GAS

For the homogeneous electron gas, the hole part of the Green function is given by

$$\mathcal{G}(r, \tau) = \frac{1}{8\pi^3} \int e^{i\mathbf{k} \cdot \mathbf{r}} \frac{e^{-(\epsilon_k - \mu)\tau}}{1 + e^{(\epsilon_k - \mu)\beta}} d^3k \quad (6)$$

with $\epsilon_k = \frac{1}{2}k^2$. The range of integration can be extended to infinity, because the spherical Fermi surface is fully contained inside the Brillouin zone. The angular integrals are straightforward and lead to

$$\mathcal{G}(r, \tau) = -\frac{i}{4\pi^2 r} \int_{-\infty}^{\infty} k e^{ikr} \frac{e^{-(\epsilon_k - \mu)\tau}}{1 + e^{(\epsilon_k - \mu)\beta}} dk. \quad (7)$$

The remaining integral is most simply solved by closing the contour across the upper complex half-plane. The integrand has relevant first-order poles at $\pm k_l + i\gamma_l$ with

$$k_l = \sqrt{\mu + \sqrt{\mu^2 + \omega_l^2}}, \quad (8)$$

$$\gamma_l = \sqrt{-\mu + \sqrt{\mu^2 + \omega_l^2}}, \quad (9)$$

and the fermion Matsubara frequencies $\omega_l = (2l+1)\pi/\beta$. Evaluation of the residues yields the final result,

$$\mathcal{G}(r, \tau) = -\frac{1}{\pi\beta r} \sum_{l=0}^{\infty} e^{-\gamma_l r} \cos(k_l r - \omega_l \tau), \quad (10)$$

which explicitly shows the periodicity along the imaginary-time axis. At finite temperature the Green function is essentially a superposition of exponentially damped oscillations, whose long-range behavior is dominated by the $l=0$ contribution. For sufficiently small T the chemical potential approximately equals the Fermi energy $\epsilon_F = \frac{1}{2}k_F^2$. The damping constants are given by $\gamma_l \approx \omega_l/k_F$ in this regime, and the wave vectors of the corresponding oscillations become $k_l \approx k_F$. The overall decay constant is hence proportional to the temperature and given by $\gamma = \gamma_0 = \pi k_B T/k_F$.

As the limit $T \rightarrow 0$ is nontrivial, the Green function at zero temperature is most simply calculated from Eq. (6) with a step function instead of the Fermi distribution. The integral can be solved analytically and yields

$$\begin{aligned} \mathcal{G}(r, \tau) = & -\frac{\sin(k_F r)}{2\pi^2 r \tau} + \frac{1}{2(2\pi|\tau|)^{3/2}} \exp\left(\frac{k_F^2 \tau}{2} - \frac{r^2}{2\tau}\right) \\ & \times \left[\operatorname{erfi}\left(\frac{k_F \tau + ir}{\sqrt{2|\tau|}}\right) + \operatorname{erfi}\left(\frac{k_F \tau - ir}{\sqrt{2|\tau|}}\right) \right]. \end{aligned} \quad (11)$$

For the electron part $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$ replaces $\operatorname{erfi}(z) = \operatorname{erf}(iz)/i$. The limiting formulas are identical in either case

and follow from the asymptotic representation of the error function $\text{erf}(z)$ in the complex plane. For $r \rightarrow \infty$ the Green function becomes

$$\mathcal{G}(r, \tau) \sim -\frac{k_F \cos(k_F r)}{2\pi^2 r^2} + \frac{1 - k_F^2 \tau}{2\pi^2 r^3} \sin(k_F r), \quad (12)$$

which decays algebraically rather than exponentially. On the imaginary-time axis the Green function decays as

$$\mathcal{G}(r, \tau) \sim -\frac{\sin(k_F r)}{2\pi^2 r \tau} - \frac{\cos(k_F r)}{2\pi^2 k_F \tau^2} \quad (13)$$

for large positive or negative τ .

IV. METALS

The explicit solution for the homogeneous electron gas illustrates more general principles that also apply to real metals. Bands above or below the Fermi level yield contributions to the Green function analogous to the case of insulators, which is discussed below. They are short-ranged, so that for $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$ the sum (2) is dominated by terms arising from partially occupied bands that cross the Fermi level. Furthermore, the strong localization of the Wannier orbitals implies that the spatial decay properties of the relevant \mathcal{G}_n are in turn determined by F_n . If the homogeneous electron gas is used for guidance, then the decay length $1/\gamma$ for sodium with an average density $r_s = 3.99$ (Ref. 26) at room temperature $T = 298$ K may be estimated as 85.8 \AA . In contrast, the decay length of the temperature-independent Wannier orbitals is comparable to the interatomic spacing 3.72 \AA in the bcc cell and more than an order of magnitude smaller. The high-temperature region where F_n becomes sufficiently short-ranged such as not to dominate the asymptotic behavior is irrelevant for solid-state physics, because it lies above the melting point of the crystal lattice.

F_n has the mathematical form of a three-dimensional Fourier transform and is long-ranged because of rapid oscillations of the integrand in Eq. (5). Quantitatively, at finite temperature the integrand falls from near unity to zero in a narrow region around the Fermi surface. Its width is given by $\delta k \propto k_B T / |\nabla \epsilon_{n\mathbf{k}}|$, where the gradient is taken at the Fermi level. Directional effects due to the anisotropic crystal structure are ignored here, and it is assumed that the energy dispersion is analytic and smooth on the scale of δk . For sufficiently small T the latter condition is always fulfilled. According to basic Fourier analysis,²⁷ the extent of this rapid variation is directly proportional to the exponential decay constant of the transform, so that $\gamma \propto \delta k$ for F_n and hence for \mathcal{G} .

At $T = 0$ the integrand changes qualitatively, because the Fermi distribution has a discontinuity at the Fermi surface. As the Fourier transform of a discontinuous function decays algebraically rather than exponentially,²⁷ both the electron and the hole part of the Green function now assume the asymptotic form $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) \sim |\mathbf{r} - \mathbf{r}'|^{-\eta}$ with $\eta > 0$. Their decay on the imaginary-time axis is likewise algebraic $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau) \sim |\tau|^{-\kappa}$ with $\kappa > 0$, because the exponential $\exp(-\epsilon_{n\mathbf{k}}\tau)$ in the integrand reaches the Fermi level and thus exhausts the prefactor $\exp(\mu\tau)$.

V. INSULATORS

Temperature effects are negligible for insulators if the thermal energy $k_B T$ is much smaller than the band gap Δ . As this condition is almost always fulfilled below the melting point, it suffices to examine the case $T = 0$. If no band crosses the chemical potential, then all F_n are spatially short-ranged. For $\tau \rightarrow 0$ the integral (5) has the straightforward solution $F_n(\mathbf{R} - \mathbf{R}'; 0) = \delta_{\mathbf{R}, \mathbf{R}'}$. At finite imaginary times the only significant contribution comes from the vicinity of the band edges. The energy dispersion can hence be replaced by its harmonic approximation $|\epsilon_{n\mathbf{k}} - \mu| \approx \frac{1}{2} \Delta + \frac{1}{2} \sum_{i,j} k_i (m^*)_{ij}^{-1} k_j$, where m^* denotes the effective mass tensor at the top of the valence band for the hole part and at the bottom of the conduction band for the electron part. The range of integration may now be extended to infinity, and F_n is readily seen to be of Gaussian type. The overexponential falloff implies that for insulators the asymptotic properties of the Green function in real space are determined by the Wannier orbitals, which are exponentially localized. In the weak-binding case, where the band structure can be obtained by perturbation from that of the homogeneous electron gas, their decay rate is given by $\gamma \propto a \Delta$, where a is the lattice constant.²¹ Many common semiconductors have gaps substantially smaller than their bandwidth and are thus expected to fall into the weak-binding regime, e.g., for silicon $\Delta = 1.15$ eV (Ref. 26) as opposed to $\frac{1}{2}(2\pi/a)^2 = 5.1$ eV. The proportionality factor is direction-dependent but about unity, so that the decay length $1/\gamma$ may be estimated as 1.22 \AA , which is of the order of the interatomic spacing 2.35 \AA in silicon, as expected, and compatible with numerical calculations.²⁴ In the tight-binding regime the Wannier orbitals also decay exponentially, but the dependence of γ on the gap is indeterminate and subject to details of the atomic potential.²¹ This case may apply for large-gap Mott-Hubbard insulators like NiO but is less relevant in practice, because the GW approximation anyway shows serious deficiencies for such strongly correlated systems.²⁸ The falloff on the imaginary time axis is exponential with a decay constant $b = \frac{1}{2} \Delta$ both for the electron and the hole part, because the finite difference between the chemical potential and the band edges implies an incomplete cancellation of the prefactor $\exp(\mu\tau)$.

VI. SUMMARY

In this paper I have investigated the asymptotic properties of the one-particle Green function in real space and imaginary time. An analytic solution for the homogeneous electron gas shows the Green function as a superposition of damped harmonic oscillations with a wave vector approaching k_F as $T \rightarrow 0$. The damping $\mathcal{G} \sim \exp(-\gamma|\mathbf{r} - \mathbf{r}'|)$ is exponential at finite temperature but changes qualitatively to algebraic falloff $\mathcal{G} \sim |\mathbf{r} - \mathbf{r}'|^{-\eta}$ at $T = 0$. While the thermal Green function is by definition periodic on the imaginary time axis with the period 2β , it decays like $\mathcal{G} \sim |\tau|^{-\kappa}$ when the periodicity is lifted at $T = 0$. I have shown that these results also apply to real metals. In contrast, for insulators at zero temperature the Green function decays exponentially like $\mathcal{G} \sim \exp(-\gamma|\mathbf{r} - \mathbf{r}'|)$ in real space and $\mathcal{G} \sim \exp(-b|\tau|)$ in imaginary time.

The limiting formulas can be exploited in electronic-

structure calculations based on a space-time representation and allow an analytic treatment of the long-range tails. The asymptotic behavior of derived propagators within a perturbation scheme follows directly from the Green function. In particular, the self-energy in the GW approximation is the product of the Green function \mathcal{G} and the screened Coulomb interaction W . In insulators screening is incomplete with $W \sim 1/\epsilon|\mathbf{r}-\mathbf{r}'|$ at large distances, where ϵ is the dielectric constant, but the self-energy still decays exponentially in real space because the Green function does. On the other hand, for the homogeneous electron gas at zero temperature¹¹ $W \sim \cos(2k_F|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|^3$, so that the self-energy only decays algebraically. This distinct asymptotic behavior should

be appreciated if the electron-gas self-energy is applied to real materials. The problem is naturally solved by the *ad hoc* introduction of a gap in the otherwise metallic spectrum.¹³

Finally, the generic dependence $\gamma \propto k_B T/|\nabla \epsilon_{n\mathbf{k}}|$ and $b = \frac{1}{2}k_B T$ for metals as well as $\gamma \propto a\Delta$ and $b = \frac{1}{2}\Delta$ for insulators can be used to assess the scaling of different algorithms for self-energy calculations in the GW approximation. If all other parameters remain fixed, then conventional reciprocal-space implementations scale like N^4/T^2 for metals at finite temperature and N^4/Δ^2 for insulators at zero temperature, whereas the space-time method scales like N^2/T^4 and N^2/Δ^4 , respectively. This difference in efficiency gain as the temperature or the band gap increase is an important factor to be taken into account for benchmarking purposes.

*Electronic address: schindlmayr@fhi-berlin.mpg.de

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