

Tangent-Space Krylov Computation of Real-Frequency Spectral Functions: Influence of Density-Assisted Hopping on 2D Mott Physics

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We present a tangent-space Krylov method for efficient computation of zero-temperature real-frequency spectral functions on top of ground-state matrix product states obtained from the density matrix renormalization group. It relies on projecting the Hamiltonian to the tangent space of the ground-state matrix product states, where resolvents can be efficiently represented using Krylov space techniques. This enables direct computations of excitation energies and the corresponding spectral weights. We demonstrate the accuracy and efficiency of the tangent-space Krylov approach by showcasing spectral data for various models. These include the 1D Haldane-Shastry and Heisenberg models as benchmarks. As an interesting application, we study the Hubbard model on a cylinder at half filling, augmented by a density-assisted hopping (DAH) term. We find that DAH leads to particle-hole asymmetric single-particle mobilities and lifetimes in the resulting Mott insulator, and identify the responsible scattering processes. Furthermore, we find that DAH influences the dispersion of Green's function zeros beyond its range, which has a frustrating effect on the Mott insulator studied here.

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Introduction—Numerical methods based on matrix product states (MPSs) form a robust toolbox for studying strongly correlated systems. A prime example is the density matrix renormalization group (DMRG) [1,2] for ground-state searches. Numerous MPS tools are also available for computing ground-state dynamical correlators of the form $S[O_{\mathbf{k}}](\omega) = \int dt e^{i\omega t} \langle \Psi_{\mathbf{k}}(0) | \Psi_{\mathbf{k}}(t) \rangle$, with $|\Psi_{\mathbf{k}}(t)\rangle = e^{-i(H-E_g)t} O_{\mathbf{k}} |\Psi_g\rangle$, relevant for experiments that probe dynamical properties. One strategy is to time-evolve $|\Psi_{\mathbf{k}}(t)\rangle$ explicitly [3–10], but the inevitable growth of entanglement makes it difficult to reach the long times needed to access low frequencies. In a sense, when computing $|\Psi_{\mathbf{k}}(t)\rangle$ in full generality one works harder than necessary since only its overlap with $|\Psi_{\mathbf{k}}(0)\rangle$ is required.

An alternative strategy is to compute dynamical correlators directly in frequency space [11–19], where

$$S[O_{\mathbf{k}}](\omega) = \langle \Psi_g | O_{\mathbf{k}}^\dagger \delta(\omega - H + E_g) O_{\mathbf{k}} | \Psi_g \rangle. \quad (1)$$

An early approach, due to Hallberg [20], employed a Lanczos-based [21] continued fraction expansion. It

motivated further work [22–25] on formulating a Lanczos scheme in the MPS context—a task that proves challenging due to structural limitations. The core steps of any Lanczos implementation are applying the Hamiltonian to a quantum state, then orthogonalizing the result against other states. In the MPS framework, these steps increase the bond dimension and leave the manifold of MPSs of fixed bond dimension, which lacks a vector-space structure. To keep computational costs manageable, they must therefore be followed by compression. This introduces truncation errors that accumulate over iterations, leading to a global loss of orthogonality and convergence issues. These can be mitigated by reorthogonalization [23] or restarting procedures [24].

In this Letter, we introduce a novel tangent-space Krylov (TaSK) method, which restricts computations to the *tangent space* of the MPS manifold at the ground state, instead of the MPS manifold itself. Since the former has a *vector-space* structure, it enables us to formulate a Lanczos scheme devoid of orthogonality issues. Our approach uses a direct finite-size MPS adaptation [26,27] of the quasi-particle ansatz [28–35], which has been successfully employed to compute spectral functions on top of uniform MPSs. We further establish the two-site energy variance [27,36] as a novel means to estimate the projection errors due to the tangent space restriction.

We benchmark TaSK on the Haldane-Shastry and Heisenberg chains, finding excellent agreement with analytical results for the dynamical structure factor. As a

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challenging application offering new physical insight, we consider the Hubbard model on a cylinder, augmented by a density-assisted hopping (DAH) term [37–47]. The spectral functions and self-energies obtained for the Mott insulating phase exhibit strong particle-hole asymmetry, which is absent in a Hartree-Fock treatment of DAH. We identify scattering processes causing the mobility and lifetime asymmetries and find an emergent next-nearest-neighbor contribution to the Mott-pole dispersion.

Method—Consider a Hamiltonian H of an $\mathcal{L}$ -site system, represented as a matrix product operator,

$$H = \begin{array}{c} W_1 \quad W_2 \quad \dots \quad W_\ell \quad \dots \quad W_{\mathcal{L}-1} \quad W_{\mathcal{L}} \\ \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \square \text{---} \end{array} \quad (2)$$

Here, d denotes the dimension of the local Hilbert space and w the dimension of the internal virtual bond. Its ground-state wave function Ψ_g , found, e.g., via DMRG [48], can be expressed in site-canonical MPS form as

$$\Psi_g = \begin{array}{c} A_1 \quad A_{\ell-1} \quad C_\ell \quad B_{\ell+1} \quad B_{\mathcal{L}} \\ \text{---} \nabla \text{---} \nabla \text{---} D \text{---} D \text{---} \nabla \text{---} \nabla \text{---} \end{array}, \quad (3)$$

with internal bond dimension D , orthogonality center C_ℓ , and left and right isometries $A_{\ell'}(\nabla)$ and $B_{\ell'}(\nabla)$. The latter, together with their orthogonal complements, $\bar{A}_{\ell'}(\nabla)$ and $\bar{B}_{\ell'}(\nabla)$, can be used to explicitly construct [27] the tangent space $\mathbb{V}^{1s}$ of the ground-state MPS, spanned by one-site variations of Ψ_g , and the one-site projector

$$\mathcal{P}^{1\perp} = \sum_{\ell=1}^{\mathcal{L}} \begin{array}{c} \text{---} \nabla \text{---} \nabla \text{---} \\ \text{---} \nabla \text{---} \nabla \text{---} \end{array} \quad (4)$$

whose image $\mathbb{V}^{1\perp} = \mathbb{V}^{1s} / \text{span}(|\Psi_g\rangle)$ is the space of MPS tangent vectors orthogonal to $|\Psi_g\rangle$. Its dimension, $\dim \mathbb{V}^{1\perp}$, is equal to the number of independent variational parameters of Ψ_g and scales as $\mathcal{O}(\mathcal{L}D^2d)$. Wave functions of states in $\mathbb{V}^{1\perp}$ have the form

$$\Psi^{1\perp} = \sum_{\ell=1}^{\mathcal{L}} \begin{array}{c} T_\ell \\ \text{---} \nabla \text{---} \nabla \text{---} \\ \text{---} \nabla \text{---} \nabla \text{---} \end{array}, \quad \text{with} \quad \begin{array}{c} T_\ell \\ \text{---} \nabla \text{---} \nabla \text{---} \\ \text{---} \nabla \text{---} \nabla \text{---} \end{array} = 0. \quad (5)$$

In practice, the sum in Eq. (5) is never performed explicitly, and the gauge choice constraint on T_ℓ ensures that all terms in this sum are mutually orthogonal. As a result, overlaps, sums, and scalar multiplication of tangent vectors can be performed as operations involving only the tensors T_ℓ , at a computational cost of $\mathcal{O}(\mathcal{L}D^2d)$.

The vector-space structure of $\mathbb{V}^{1\perp}$ enables a controlled and efficient computation of spectral functions of the form (1) via the Lanczos algorithm [21], provided that we project all involved states to $\mathbb{V}^{1\perp}$. This projection is our main

approximation [further motivated in Sec. S-1 of Supplemental Material (SM) [49]]. Concretely, we use

$$S[O_{\mathbf{k}}](\omega) \approx \langle \Psi_0 | \delta(\omega - H^{1\perp}) | \Psi_0 \rangle + |\langle O_{\mathbf{k}} \rangle|^2 \delta(\omega), \quad (6)$$

with $\langle O_{\mathbf{k}} \rangle = \langle \Psi_g | O_{\mathbf{k}} | \Psi_g \rangle$. Here, we have introduced the projected Hamiltonian [69] $H^{1\perp} = \mathcal{P}^{1\perp}(H - E_g)\mathcal{P}^{1\perp}$ and initial state $|\Psi_0\rangle = \mathcal{P}^{1\perp} O_{\mathbf{k}} |\Psi_g\rangle$. Within the scope of this Letter, $O_{\mathbf{k}}$ is a sum of local operators with $O_{\mathbf{k}} |\Psi_g\rangle \in \mathbb{V}^{1s}$, thus the initial state projection is exact [70].

Equation (6) can be evaluated efficiently by means of a Lanczos scheme, which iteratively generates an orthonormal basis of the $(\mathcal{N}_{\text{kr}} + 1)$ -dimensional Krylov space

$$\mathcal{K}(\Psi_0) = \text{span}\{|\Psi_0\rangle, H^{1\perp}|\Psi_0\rangle, \dots, (H^{1\perp})^{\mathcal{N}_{\text{kr}}}|\Psi_0\rangle\}. \quad (7)$$

The resulting tridiagonal representation of $H^{1\perp}$ in $\mathcal{K}(\Psi_0)$ is diagonalized to obtain the approximate eigenpairs $(\omega_\alpha, |\Psi_\alpha^{1\perp}\rangle)$, which we then insert in Eq. (6),

$$S[O_{\mathbf{k}}](\omega) \approx \sum_{\alpha=0}^{\mathcal{N}_{\text{kr}}} S_\alpha \delta(\omega - \omega_\alpha) + |\langle O_{\mathbf{k}} \rangle|^2 \delta(\omega), \quad (8)$$

with $S_\alpha = |\langle \Psi_\alpha^{1\perp} | \Psi_0 \rangle|^2$. For $\mathcal{N}_{\text{kr}}$ large enough, the set of real discrete frequencies and spectral weights $\{\omega_\alpha, S_\alpha\}$ becomes an arbitrarily accurate approximation of Eq. (6) and can be broadened if desired (see Sec. S-2 B of SM [49]). We find that $\mathcal{N}_{\text{kr}} < 150$ is sufficient for the cases studied in this Letter.

The main computational cost of TaSK is the application of $H^{1\perp}$ to a tangent vector, done once per Krylov step. It scales as $\mathcal{O}(\mathcal{L}D^3dw)$, just as *one* single-site DMRG or time-dependent variational principle (TDVP) sweep. In practice, TaSK is considerably cheaper than TDVP for computing spectral functions (see Sec. S-5 of SM [49]).

The projection of the Hamiltonian to $\mathbb{V}^{1\perp}$, $H \rightarrow H^{1\perp}$, is the main source of error in TaSK. The distance of eigenstates $|\Psi_\alpha^{1\perp}\rangle$ of $H^{1\perp}$ from eigenstates of H can be quantified through their variance $\Delta_\alpha = \|(H - E_0 - \omega_\alpha)|\Psi_\alpha^{1\perp}\rangle\|^2$. While evaluation of the full variance is challenging, its two-site contribution [27,36],

$$\Delta_\alpha^{2\perp} = \|\mathcal{P}^{2\perp} H |\Psi_\alpha^{1\perp}\rangle\|^2 = \sum_{\ell=1}^{\mathcal{L}-1} \left\| \sum_{\ell'=1}^{\mathcal{L}} \begin{array}{c} T_{\ell'} \\ \text{---} \nabla \text{---} \nabla \text{---} \\ \text{---} \nabla \text{---} \nabla \text{---} \end{array} \right\|^2, \quad (9)$$

can be computed at reasonable cost (Sec. S-1 E of SM [49]). We will use $\delta_\alpha = (\Delta_\alpha^{2\perp})^{1/2}$ as error estimate for ω_α . Since $\dim \mathbb{V}^{1\perp} \sim D^2$, increasing D reduces the projection error.

Spin chains—As the first benchmark, we consider the one-dimensional SU(2) Haldane-Shastry model (HSM) with periodic boundary conditions,

$$H_{\text{HSM}} = \sum_{\ell < \ell' \leq \mathcal{L}} \frac{\pi^2 \mathbf{S}_\ell \cdot \mathbf{S}_{\ell'}}{\mathcal{L}^2 \sin^2 \frac{\pi}{\mathcal{L}} (\ell - \ell')}. \quad (10)$$

The $1/r^2$ spin exchange yields a Luttinger liquid of free two-spinon excitations [71,72]. Unlike magnons, these fractionalized excitations are not naturally represented within $\mathbb{V}^{1\perp}$, since this space is spanned by MPSs that differ from the ground state at most on a single site. Thus, HSM is a challenging test for TaSK, despite its integrability.

The ground-state MPS is obtained using state-of-the-art single-site DMRG with controlled bond expansion [51]. Using the QSpace tensor library [73–75], we exploit the non-Abelian SU(2) symmetry, retaining at most $D^* = 700$ multiplets. We consider the dynamical structure factor $S_k(\omega) = S[S_k^z](\omega)$, where $S_k^z = (1/\sqrt{\mathcal{L}}) \sum_{\ell=1}^{\mathcal{L}} \exp(i\ell k) S_\ell^z$ is a spin-wave operator, with $k = m\pi/\mathcal{L}$, $m \in \mathbb{Z} \bmod \mathcal{L}$.

Figure 1(a) displays $S_\pi(\omega)$ for $\mathcal{L} = 40$, computed with TaSK (black circles) and from exact formulas [58,72,76] (blue dots). We use $\mathcal{N}_{\text{kr}} = 30$ (see Sec. S-3 of SM [49] for a convergence analysis). The analytical and numerical results agree very well. Slight deviations appear only at high frequencies (inset), but remain within the error bars, confirming the reliability of δ_α as an error estimate.

Figure 1(b) demonstrates the convergence of low-lying excitations: their error estimates δ_α decrease monotonically

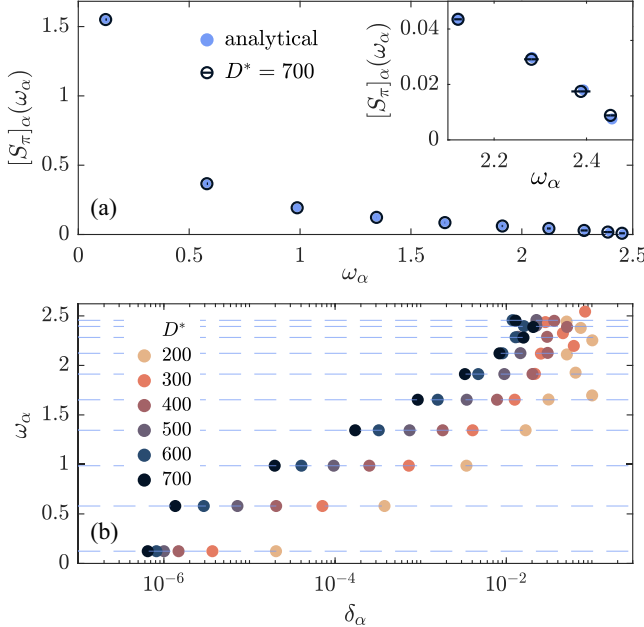


FIG. 1. Dynamical structure factor of the $\mathcal{L} = 40$ Haldane-Shastry model at $k = \pi$ and $\mathcal{N}_{\text{kr}} = 30$. (a) Comparison between analytical values (blue dots) and the TaSK result (black circles) for $D^* = 700$. Horizontal bars depict δ_α as error estimate for ω_α . Inset: enlargement to high frequencies. (b) Convergence trend across datasets with increasing D^* , relative to δ_α . Dashed lines indicate the analytical values from (a).

with increasing D^* . Thus, as expected, the projection error is reduced as $\dim \mathbb{V}^{1\perp} \propto D^2$ grows.

Next, we benchmark TaSK for the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg chain $H_{\text{Heis}} = \sum_{\ell=1}^{\mathcal{L}-1} \mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1}$. In contrast to the HSM, the spinons in this model interact, leading to multispinon contributions in $S_k(\omega)$ ($\sim 27\%$ of the total spectral weight [77]) and a broad distribution of spectral weight over the entire frequency range. This poses a particular challenge for Lanczos-based methods [11,20,23] as each new peak requires an additional iteration.

In Fig. 2 we present $S_\pi(\omega)$ computed for $\mathcal{L} = 64$ and $\mathcal{L} = 128$ and compared with Bethe ansatz results [77] in the thermodynamic limit. For both system sizes, we keep $D^* = 512$ SU(2) multiplets and define the spin-wave operator S_k^z as above. To approximate $S_\pi(\omega)$ in the thermodynamic limit, the two datasets of discrete frequencies ω_α are collapsed onto a single curve using the rescaling scheme described in Sec. IV D of Ref. [14] after preliminary binning (see Sec. S-3 of SM [49]). The resulting data points closely follow the Bethe ansatz curve corresponding to the full 2 + 4-spinon contribution.

Density-assisted hopping in the 2D Hubbard model—Because of its efficiency, TaSK can readily obtain spectra of interacting electrons on a 10×4 cylinder, where ground-state calculations are already challenging. Our goal is to study how DAH influences the physics of the 2D Hubbard model at half filling, where it describes a Mott insulator—the parent system from which superconductivity arises upon doping. Hirsch has argued that DAH is pivotal for high- T_c superconductivity in cuprates [37,38], and understanding its physical consequences is an active area of research [39–47].

A recent DMRG-based downfolding study of the Emery model [46] yielded a single-band Hubbard model augmented by a DAH term, $H = H_{t-U} + H_n$, with

$$H_{t-U} = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle, \sigma} (c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + \text{H.c.}) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (11a)$$

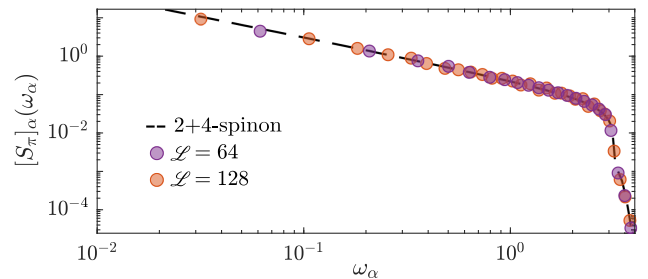


FIG. 2. Dynamical structure factor of the Heisenberg chain at $k = \pi$. We have used $\mathcal{N}_{\text{kr}} = 100$ and $\mathcal{N}_{\text{kr}} = 140$ for $\mathcal{L} = 64$ and $\mathcal{L} = 128$, respectively. Dashed line: the exact Bethe ansatz result for the full 2 + 4-spinon contribution from Ref. [77]. For other values of k , see Figs. S-7 and S-8 in SM [49].

$$H_n = -t_n \sum_{\langle \mathbf{r}\mathbf{r}' \rangle, \sigma} (c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + \text{H.c.}) (n_{\mathbf{r}\bar{\sigma}} + n_{\mathbf{r}'\bar{\sigma}}). \quad (11b)$$

Here, $c_{\mathbf{r}\sigma}^\dagger$ is a hole creation operator, $n_{\mathbf{r}\sigma} = c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}$ the hole-number operator, $\bar{\sigma}$ denotes the spin projection opposite to σ , and $\langle \mathbf{r}\mathbf{r}' \rangle$ denotes nearest neighbors. The DAH hopping rate was found [46] to be substantial, $t_n \simeq 0.6t$, significantly enhancing hole mobility *and* pairing. The latter finding cannot be understood within a simple Hartree-Fock (HF) treatment of DAH, which effectively replaces t by $t_{\text{eff}} = t + 2t_n \langle n_{\bar{\sigma}} \rangle$, thereby remaining a pure Hubbard model that does not exhibit superconductivity [78].

Here, we use TaSK to examine the (beyond-HF) effects of DAH on the single-particle spectral function, $A_{\mathbf{k}}(\omega) = S[c_{\mathbf{k}\sigma}^\dagger](\omega) + S[c_{\mathbf{k}\sigma}](-\omega)$, of the half-filled Mott insulator. We find a surprisingly strong particle-hole asymmetry in $A_{\mathbf{k}}(\omega)$ and a next-nearest-neighbor contribution to the dispersion of the self-energy pole.

We study the model (11) on a half-filled 10×4 cylinder, with $U = 12.6$ and either $t = 1.68$, $t_n = 0$ (denoted “ $t-U$ ”), or $t = 1$, $t_n = 0.6$ (denoted “ $t-t_n-U$ ”), matching the parameters of Fig. 4 of Ref. [46]. (For $t-t_n-U$, an HF treatment of DAH yields $t_{\text{eff}} = 1.6$, similar to our $t = 1.68$ for $t-U$.) We keep at least $D^* = 2000 \text{ U}(1) \times \text{SU}(2)$ multiplets. Figures 3(a) and 3(c) show $A_{\mathbf{k}}(\omega)$ for the Mott insulators obtained for $t-U$ or $t-t_n-U$, respectively, and Figs. 3(b) and 3(d) the imaginary parts of the corresponding self-energies $\Sigma_{\mathbf{k}}(\omega)$. To obtain smooth curves from the discrete spectral data $\{\omega_\alpha, S_\alpha\}$, we used a continued-fraction-based broadening scheme that conserves the first few spectral moments of $A_{\mathbf{k}}(\omega)$. This scheme and TaSK convergence properties are discussed in Secs. S-2 and S-3 of SM [49], respectively.

For $t-U$, $A_{\mathbf{k}}(\omega)$ [Fig. 3(a)] exhibits a Mott gap of size $6.67 < U$. Apart from broad incoherent features, the Hubbard bands exhibit dispersive coherent features, in particular at their inner edges. The self-energy [Fig. 3(b)] has a characteristic S-shaped spectrum [79], exhibiting broad horizontal bands connected by a sharp, dispersive pole. Both $A_{\mathbf{k}}(\omega)$ and $\text{Im} \Sigma_{\mathbf{k}}(\omega)$ are particle-hole symmetric, as expected, i.e., invariant under $\omega \rightarrow -\omega$, $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{\Pi}$, where $\mathbf{\Pi} = (\pi, \pi)$.

For $t-t_n-U$, the corresponding results are shown in Figs. 3(c) and 3(d). The overall features are similar to those of $t-U$, but t_n , though small ($t_n < 0.05U$), introduces a significant particle-hole asymmetry [see also Figs. 3(g)–3(i)], a dynamical effect that goes beyond HF. In particular, the particle part ($\omega < 0$) of $A_{\mathbf{k}}(\omega)$ is more coherent, i.e., dispersive features are sharper and exhibit smaller decay rates, and conversely for the hole spectrum ($\omega > 0$). $\text{Im} \Sigma_{\mathbf{k}}(\omega)$ shows corresponding weight redistributions. Moreover, the effective bandwidth is reduced or increased for particle or hole excitations, respectively, i.e., spectral features at $\omega < 0$ or > 0 are “squeezed” or “stretched” in ω . Thus, t_n dynamically enhances hole mobility compared to particle mobility (an effect also reported in Ref. [46]) and reduces hole lifetimes compared to particle lifetimes.

Which scattering events generate the particle-hole asymmetric features? A perturbative expansion of $\Sigma_{\mathbf{k}}(\omega)$ in t_n and U shows that at second order, they arise from *mixed* t_n-U scattering (see Sec. S-6 of SM [49]): a propagating particle or hole emits a particle-hole pair via the t_n vertex and reabsorbs it via the U vertex, or vice versa. Using this insight, and the fact that the U vertex and part of the t_n vertex do not depend on transfer momenta, we can estimate the latter’s contribution to the DAH-induced change in the self-energy, $\delta \Sigma_{\mathbf{k}}^{t_n}$, as follows (see Sec. S-7 of SM [49]): we use TaSK to compute the self-energy of the $t-U$ Hubbard

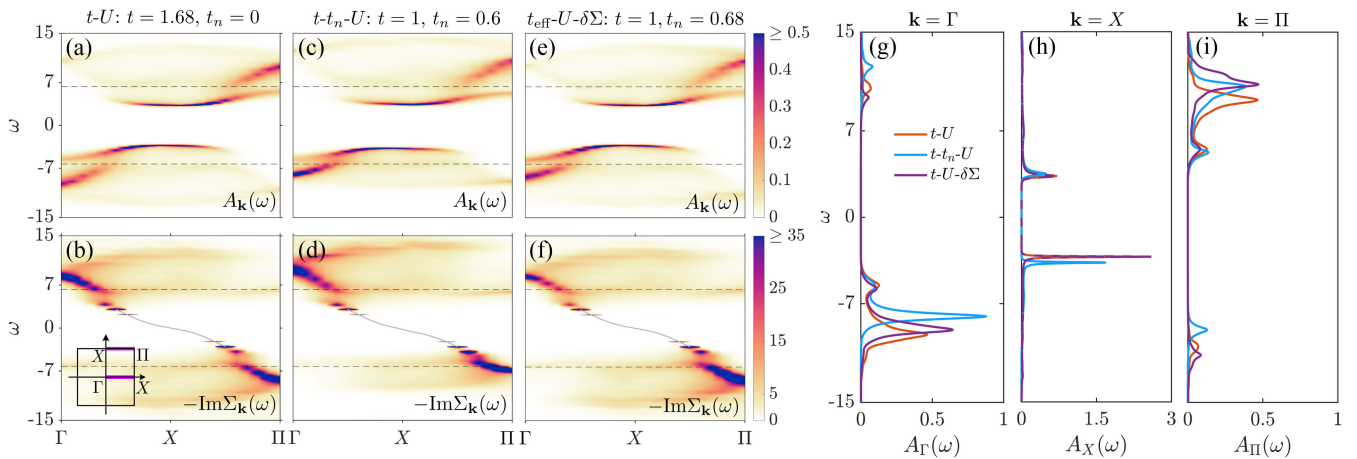


FIG. 3. Comparison of $A_{\mathbf{k}}(\omega)$ and $-\text{Im} \Sigma_{\mathbf{k}}(\omega)$ for the Hubbard model on a 10×4 cylinder, computed via TaSK (a), (b) without and (c), (d) with DAH, and (e), (f) computed by treating DAH simplistically via Eq. (12). Solid gray lines in (b), (d), (f) mark the self-energy pole where it becomes too sharp for the frequency resolution of our grid. Dashed gray lines indicate $\omega = \pm U/2$. Inset in (b): purple lines show the Brillouin zone paths $\Gamma \rightarrow X$ and $X \rightarrow \Pi$. (g)–(i) Line cuts of $A_{\mathbf{k}}(\omega)$ for $\mathbf{k} = \Gamma, X, \Pi$.

model with hopping t_{eff} , denoted $\Sigma_{\mathbf{k}}^{t_{\text{eff}}-U}$; from the latter, we obtain $\delta\Sigma_{\mathbf{k}}^{t_n}$ by replacing either the initial or final U vertex by the transfer-momentum-independent part of the t_n vertex. This yields

$$\delta\Sigma_{\mathbf{k}}^{t_n}(\omega) = -4 \frac{t_n \gamma_{\mathbf{k}}}{U} [\Sigma_{\mathbf{k}}^{t_{\text{eff}}-U}(\omega) - \Sigma_{\mathbf{k}}^{\text{HF}}], \quad (12)$$

where $\gamma_{\mathbf{k}} = \cos k_x + \cos k_y$ and $\Sigma_{\mathbf{k}}^{\text{HF}}$ is the HF self-energy. This “ $t_{\text{eff}}-U-\delta\Sigma$ ” scheme yields a total self-energy of $\Sigma_{\mathbf{k}}^{t_{\text{eff}}-U}(\omega) + \delta\Sigma_{\mathbf{k}}^{t_n}(\omega)$. It is shown in Fig. 3(f), computed using $t_{\text{eff}} = t + t_n = 1 + 0.68$ [so that $\Sigma_{\mathbf{k}}^{t_{\text{eff}}-U}(\omega)$ equals $\Sigma_{\mathbf{k}}(\omega)$ of Fig. 3(b)], almost matching the $t-t_n-U$ settings of Fig. 3(d) (where $t_{\text{eff}} = 1 + 0.6$). The corresponding $t_{\text{eff}}-U-\delta\Sigma$ spectral function [Fig. 3(e)] indeed reproduces several properties of the coherent features of $t-t_n-U$ in Fig. 3(c): reduced effective bandwidth and decay rate for particle excitations, and vice versa for hole excitations [see also Figs. 3(g)–3(i)]. By contrast, $\delta\Sigma^{t_n}$ hardly affects the incoherent background; reproducing the latter’s $t-t_n-U$ properties thus requires a more elaborate treatment.

A hallmark feature of Mott insulators is their self-energy poles [gray lines in Figs. 3(b) and 3(d)], which cause Green’s function zeros. Their generically dispersive nature, which has only recently been fully appreciated [54], is currently under active investigation, with interesting results ranging from topology [54,80–84] to possible connections to spinon physics [85–88]. If the interaction is purely Hubbard, it can be shown that the pole dispersion is directly inherited from the noninteracting dispersion [54].

Thus, for $t-U$, the Mott pole dispersion $\xi_{\mathbf{k}}$ should contain only nearest-neighbor terms. Indeed, using the ansatz $\xi_{\mathbf{k}} = -2\tau(\cos k_x + \cos k_y) - 4\tau' \cos k_x \cos k_y$ [89], where τ and τ' are nearest and next-nearest-neighbor amplitudes, we obtain a good fit with $\tau \simeq -2.03$ and $\tau' = 0$, confirming this expectation (see Sec. S-8 C of SM [49]). By contrast, for $t-t_n-U$ we find $\tau \simeq -1.86$ and $\tau' \simeq 0.17$. Hence *nearest-neighbor* DAH generates a sizeable *next-nearest-neighbor* term τ' —a remarkable result, arising from the fact that the DAH t_n vertex, unlike the U vertex, delocalizes electrons beyond single-particle hopping and HF (see Sec. S-8 of SM [49]). This emergence of nonzero τ' suggests that t_n may have a similar frustration effect as the much-studied next-nearest-neighbor hopping t' for the $t-t'$ Hubbard model, in particular if $\xi_{\mathbf{k}}$ can be interpreted as a spinon dispersion. Since frustration from t' can stabilize superconductivity in the Hubbard model [90,91], a similar effect from t_n may, together with the previously discussed mobility and lifetime effects, stabilize superconductivity in the $t-t_n$ Hubbard model [46].

Outlook—We showed that TaSK is an efficient and accurate method for computing real-frequency spectral functions. Its main source of error comes from the projection to the tangent space and can be estimated via the introduced two-site variance. Because of its relatively

light-weight nature, it is especially useful in cases where ground-state calculations are already challenging. These include strongly correlated electron systems on cylinders, geared, for instance, toward cuprates [92–95], heavy fermions [96–103], Moiré systems [104–106], or systems with strong electron-boson couplings [107–110].

As a first step in this direction, we have applied TaSK to a Hubbard cylinder exhibiting DAH, a problem relevant to cuprates. Our finding that mixed t_n-U scattering leads to enhanced hole mobilities and a possibly frustrating next-nearest-neighbor contribution to the dispersion of the self-energy pole may be relevant for high- T_c superconductivity. A more detailed study of this, which would include doping and the calculation of other dynamical properties such as spin or pair spectra, is left for future work.

While TaSK is designed to tackle challenging strongly correlated systems, it is, in its current form, less effective for models with exact or near-exact MPS ground states. There, the restricted tangent-space dimension may not adequately capture multiparticle continua. A generalization of TaSK that aims to overcome this limitation is proposed in Sec. S-1 F of SM [49] and will be pursued in future work.

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Data availability—The simulation data supporting these findings, including plotting scripts, are available via the Zenodo repository at Ref. [111].

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