Momentum-dependent pseudogaps in the half-filled two-dimensional Hubbard model

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We compute unbiased spectral functions of the two-dimensional Hubbard model by extrapolating Green functions, obtained from determinantal quantum Monte Carlo simulations, to the thermodynamic and continuous time limits. Our results clearly resolve the pseudogap at weak to intermediate coupling, originating from a momentum selective opening of the charge gap. A characteristic pseudogap temperature $T^*$, determined consistently from the spectra and from the momentum dependence of the imaginary-time Green functions, is found to match the dynamical mean-field critical temperature, below which antiferromagnetic fluctuations become dominant. Our results identify a regime where pseudogap physics is within reach of experiments with cold fermions on optical lattices.

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I. INTRODUCTION

A peculiar feature of (underdoped) high-$T_c$ superconductors is the coupling of antiferromagnetic fluctuations to charge degrees of freedom, which leads to a strong momentum dependence of the spectral functions. In particular, it induces pseudogaps in the normal state, i.e., a suppression of the density of states at the Fermi energy, which can be probed using (angular resolved) photoemission, inverse photoemission, and related techniques. The pseudogap shares the $d$-wave symmetry with the order parameter of the superconducting phases occurring at low temperatures and near optimal doping.

Pseudogap physics can also be expected in the undoped Hubbard model. In the absence of electronic correlations, the tight binding model is characterized by a coherence temperature $T_{coh}$, set by the bandwidth $W$. For weak Hubbard interaction $U \ll W$, antiferromagnetic spin fluctuations, with energy scale $T_{spin}$, will develop below the coherence temperature. Hence, the temperature window $T_N < T < T_{spin} < T_{coh}$ is characterized by a metallic state coupled to antiferromagnetic fluctuations, which sets the stage for pseudogap physics. Here $T_N$ is the Néel temperature, at or below which long range order generates a full gap in the presence of perfect nesting (in dimensions $d \geq 2$, with $T_N = 0$ in $d = 2$).

Theorists have tried to verify this scenario on the basis of numerical simulations and to compute reliable spectra for decades. Direct simulations can only be performed for clusters of finite extent, usually employing periodic boundary conditions. Early determinantal quantum Monte Carlo (DQMC) studies at moderately weak coupling ($U/t = 4$) led to spectra with significant low-temperature pseudogap features only for small cluster sizes; thus, pseudogaps in the undoped 2$d$ Hubbard model were regarded as pure finite-size (FS) artifacts. Later studies at similar coupling strengths found pseudogaps also at large cluster sizes, but did not allow for quantitative predictions in the thermodynamic limit. A recent study using the dynamical vertex approximation (DGA) observed reentrant behavior incompatible with the earlier results.

A central limitation of all previous numerical pseudogap studies is that results for different cluster sizes (e.g. in DQMC simulations) were compared only at fixed temperatures and at the level of spectral functions. With increasing cluster size, these show diverse effects: shifts of spectral peaks, transfer of spectral weight, and the opening or closing of gaps. A direct pointwise extrapolation of these positive semidefinite and normalized functions is clearly impossible. In fact, we are not aware of any published attempts of deriving spectral properties in the thermodynamic limit from DQMC data in any context.

In this paper, we present (i) the local spectral function, (ii) momentum-resolved spectral functions at high-symmetry points, and (iii) momentum-resolved spectral functions along high-symmetry lines of the Brillouin zone in the thermodynamic limit. All results are based on FS extrapolations of imaginary-time Green functions, obtained from DQMC, with subsequent analytic continuation to the real axis using the maximum entropy method (MEM) and, in case (iii), a Fourier fit of the momentum dependence. The final results are free of significant systematic errors and represent the thermodynamic and continuous time limits in an unbiased way.

Thereby, we can not only unambiguously confirm the pseudogap scenario and study the nodal–antinodal dichotomy in unprecedented detail, but also explore the temperature dependence of the pseudogap opening and identify a characteristic temperature $T^*$. At weak to intermediate couplings, $T^*$ tracks the onset of short-ranged magnetic fluctuations, and is equally shown to compare remarkably well with the dynamical mean-field critical temperature for antiferromagnetic long-range order.

In Sec. III we introduce the model, set up our notation, characterize the established methods (DQMC, MEM) underlying our approach, and specify our implementations. The new methods for eliminating systematic biases from Green function and spectra are, then, presented in Sec. III first for the DQMC Trotter error, then for finite-size effects. Our main results are discussed in Sec. IV, starting with pseudogap features in the spectral func-
tions for the “nodal” and “antinodal” high-symmetry points on the Fermi surface and their evolution as a function of temperature. We then show, with continuous momentum resolution, how the pseudogap evolves throughout the Brillouin zone (BZ) and discuss non-Fermi liquid physics that is not accessible by conventional methods.

Finally, we determine the characteristic pseudogap temperature $T^*$ for $U < W$ and relate it to spin correlation functions and other characteristic temperature scales of the model.

II. MODEL AND CONVENTIONAL METHODS

A. Hubbard model

Our starting point is the single-band Hubbard Hamiltonian with nearest-neighbor hopping $t$ on a square lattice (with unit lattice spacing $a ≡ 1$):

\[ \hat{H} = \hat{H}_0 + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

\[ \hat{H}_0 = -t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} - t \sum_{k, \sigma} \varepsilon_k \hat{n}_{k\sigma} \]

\[ \varepsilon_k = -2t[\cos(k_x) + \cos(k_y)] \]

Here, $\hat{c}_{i\sigma}$ ($\hat{c}_{i\sigma}^\dagger$) are annihilation (creation) operators for a fermion with spin $\sigma \in \{\uparrow, \downarrow\}$ at site $i$; $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$. In the following, the energy scale will be set by $t ≡ 1$.

At half filling $n ≡ \langle \hat{n}_{\uparrow} + \hat{n}_{\downarrow} \rangle = 1$ and in the noninteracting limit $U = 0$, the occupied momentum states form a square (dark shaded) within the square Brillouin zone illustrated in Fig. 1(a) (in the thermodynamic limit), which implies a perfect nesting instability: The Fermi surface (gray line) transforms into itself when shifted by the antiferromagnetic wave vector $(\pi, \pi)$. As a consequence, any finite interaction $U > 0$ drives this model to long-range antiferromagnetic order (only) in the ground state.

While a conventional notation is well established for the center $\Gamma$ and the corner $M$ of the BZ of the square lattice as well as for the antinodal $X$ point, this seems not to be the case for the nodal point; in Fig. 1 and in the following, we denote this midpoint of $\overline{\Gamma M}$ as $M'$.

B. Determinantal quantum Monte Carlo algorithm

The Hubbard model, Eq. (1), is solved in this work for clusters with a finite number $N$ of sites [implying a discrete momentum grid, see Fig. 1(b)] at finite temperatures $T$ using the DQMC algorithm developed by Blankenbecler, Scalapino, and Sugar with modifications by Hirsch. It is based on (i) a uniform discretization of the imaginary-time interval $0 \leq \tau \leq \beta$ [with $\beta = 1/(k_B T)$], occurring in the path integral, into $\Lambda$ time slices of width $\Delta \tau = \beta/\Lambda$, (ii) a Trotter decoupling of kinetic and interaction terms, and (iii) a Hubbard-Stratonovich transformation which replaces the electron-electron interaction at each time slice and site by the coupling of the electrons to a binary auxiliary field. Expectation values are obtained by Monte Carlo importance sampling of field configurations, with weights given by a product of two determinants for the two spin components. In the particle-hole symmetric case considered in this study, this product is always positive, i.e., the sign problem is absent. The numerical effort scales as $\beta N^3$.

A detailed review of the algorithm used can be found in Ref. [13].

In this work, we obtained imaginary-time Green functions and spin correlation functions between each pair of sites by applying the DQMC method to square lattice clusters $L \times L$ of the linear size $L = 8, 10, 12, 14, 16$ with periodic boundary conditions, using a set of Trotter discretizations with $0.1 \leq \Delta \tau \leq 0.42$ and typically 50 bins with 5000 sweeps over the auxiliary field each. For the largest systems, individual runs took about a month of computer time; up to five such runs were averaged over in order to reduce error bars. This resulted in typical statistical errors in the (finite-size) Green functions of $O(10^{-4})$. Note that the DQMC scaling with $L^6$ makes it difficult to access much larger system sizes directly: $L = 20$ ($L = 32$) would increase the effort by a factor of about 4 (64) compared to $L = 16$. Local properties were averaged over all sites, momentum ($k$) dependent properties were obtained by Fourier transforms of the real-space measurements.

C. Maximum entropy method

Since DQMC calculations provide Green functions $G$ (and correlation functions) only at imaginary times, their interpretation as dynamical information requires an analytic continuation to the real axis. Specifically, one has
to invert relations of the form
\[ G(\tau) = -\int_{-\infty}^{\infty} d\omega \, A(\omega) \frac{e^{-\tau \omega}}{1 + e^{-\beta \omega}}, \]

where \( A(\omega) = -\text{Im} G(\omega)/\pi \) is the corresponding spectral function. This is an ill-posed problem, as the exponential kernel suppresses the impact of features in \( A(\omega) \) at large \( |\omega| \) on \( G(\tau) \); in the DQMC context, further complications arise from the fact that \( G \) is only measured on the discrete imaginary-time grid \( \{ \eta = i\Delta \tau \}_{i=0}^{\Lambda} \). The MEM finds the most probable spectrum, given the data \( \tilde{G}_i = \pm G_i \), by balancing the misfit of a given candidate spectrum (measured by the corresponding \( \chi^2 \)) with an entropy constraint which favors smooth spectra.\(^{12,16}\) In our implementation, the resulting minimization problem is solved deterministically using a Newton scheme in the singular space of the kernel. Its application both to DQMC raw data for local and \( k \) dependent Green functions and to Green functions obtained from Trotter and/or FS extrapolations always resulted in reliable and consistent maximum entropy spectra.

III. EXTRACTION OF UNBIASED SPECTRA IN THE THERMODYNAMIC LIMIT

What sets our main results, to be presented in Sec. IV, apart from earlier work, is their direct relevance in the thermodynamic limit, i.e., the absence of significant bias. We now specify our methodology for eliminating Trotter and finite-size errors from Green functions and establish its accuracy and reliability on the level of Green functions and spectra.

A. Trotter errors and extrapolation \( \Delta \tau \to 0 \)

As discussed in subsection III B, the DQMC method decouples electronic interactions (and evaluates, e.g., Green functions) at the cost of introducing an artificial imaginary-time discretization \( \Delta \tau \), which implies an unphysical bias in all DQMC estimates of observables. In the absence of phase transitions, DQMC raw results are expected (and observed) to depend smoothly on \( \Delta \tau \), in the form of a power series; for some static observables, such as the total energy, it is easy to prove\(^{17}\) polynomial dependence on \( \Delta \tau^2 \).

The effects of the Trotter discretization on the imaginary-time Green function \( G(\tau) \) are illustrated in Fig. 2(a): (i) each of the raw data sets (symbols) lives on a different \( \tau \) grid; (ii) at fixed values of \( \tau \), the data (or a linear interpolation - dashed/dotted lines) is shifted to smaller absolute values at larger \( \Delta \tau \). Obviously, unbiased results (for a fixed cluster size \( L \) in real space) can only be expected after an extrapolation of \( \Delta \tau \to 0 \). On the other hand, such an extrapolation is not possible locally; i.e., at fixed \( \tau \), but requires a global approach that can use input from DQMC raw data at all discretizations \( \Delta \tau \) for each imaginary time \( \tau \) of interest.

The black solid lines in Fig. 2(a) represent the result of a multigrid procedure, originally developed in the context of the Hirsch-Fye quantum Monte Carlo method for the Anderson impurity model.\(^{18}\) The multigrid method is based on the fact that “reference” Green functions \( G_{\text{ref}}(\tau) \) with sufficiently accurate asymptotics at \( \tau \to 0 \) (and \( \tau \to \beta \)), in particular for the curvature, can easily be derived from weak-coupling expansions (or, alternatively, from the “best” QMC data via MEM); consequently, the difference between the measured Green functions \( G_{\Delta \tau}(\tau) \) and the reference \( G_{\text{ref}}(\tau) \) can be adequately represented by a natural cubic spline for each value of \( \Delta \tau \); all of these splines can, then, be evaluated on a common (fine) grid. For this transformed data, we find a nearly linear dependence on \( \Delta \tau^2 \) (plus a small curvature), so that pointwise extrapolations \( \Delta \tau \to 0 \) are reliable and accurate. At the level of \( G \), the shift of the unbiased result [black solid line in Fig. 2(a)] of about \( 10^{-3} \) compared to the best raw data [at \( \Delta \tau = 0.1 \), squares and dash-dotted line in Fig. 2(a)] is still significant.

This is no longer true on the level of spectra, shown in Fig. 2(b), due to the intrinsic complications of MEM: The results for \( \Delta \tau = 0.1 \) agree within accuracy with the unbiased spectrum. Thus, we may conclude that \( \Delta \tau = 0.1 \) is “good enough” for spectral data (at \( U = 4 \)) and that an elimination of the Trotter error is not necessary for reducing unphysical bias below significance. At the same time, the smooth consistent evolution of the spectra with \( \Delta \tau \) confirms our MEM procedure both for the DQMC raw
data and for extrapolated Green functions.

Even smaller Trotter errors than observed in Fig. 2(a) can be expected for differences of Green functions, due to error cancellation. Indeed, the scalar pseudogap measure $|G_{M'} - G_X|$, to be introduced in subsection IV C is impacted significantly by Trotter errors only for large discretizations; the bias become negligible for $\Delta \tau \lesssim 0.1$, as shown in Fig. 2(c). Therefore an explicit elimination of this error is, again, not necessary.

B. Finite-size extrapolations of local spectra and on high-symmetry $k$ points in the BZ

A FS extrapolation of local properties or $k$ resolved properties at high-symmetry points is relatively straightforward: One accumulates raw data at various values of the linear extent $L$ and then extrapolates using polynomial least-square fits in $1/L^2$. In the case of imaginary-time Green functions, independent extrapolations have to be performed for each value of $\tau$ (on the grid with spacing $\Delta \tau$ in the case of DQMC raw data or the grid chosen in the extrapolation $\Delta \tau \rightarrow 0$ discussed in the previous section). As shown in Fig. 3 for $U = 4, T = 0.2$, the Green function depends on system size quite significantly at generic imaginary times [except for the limits $\tau \rightarrow 0$ or, equivalently, $\tau \rightarrow \beta$ (not shown)] both at the antinodal (a) and nodal (b) momentum points. At the same time, the dependence is quite regular so that least-square extrapolations (lines) can be restricted to low orders.

Obviously, this “local” procedure can only include lattice sizes for which the $k$ point under consideration exists [cf. Fig. (I b)]; for the antinodal point, this requirement is fulfilled for all even values of $L$ while the nodal $M'$ point is only present if $L$ is a multiple of 4 (which restricts the set to $L = 8, 12, 16$ in our study). Still, as seen in Fig. 3(b), the extrapolation is reliable even with only three data points (per fit), as the dependence is almost perfectly linear. At the same time, the FS extrapolation is particularly important at the nodal $M'$ point, as FS effects are much stronger than in the antinodal case [shown in Fig. 3(a)].

Note that $4 \times 4$ clusters (with periodic boundary conditions) have a special symmetry: They have the same topology as a $2 \times 2 \times 2 \times 2$ hypercube with open boundary conditions; as a consequence, the next-nearest neighbors along one of the axes and the ones along the diagonal become equivalent, which implies that the $X$ and $M'$ points are identical in momentum space at $L = 4$. In order to avoid the associated extra bias we exclude this system size and consider only lattices with $L \geq 8$ in this study.

The full resulting Green functions in the thermodynamic limit are shown as solid lines in Fig. 4 for the antinodal (a) and nodal (b) $k$ points, respectively, together with their finite-size equivalents (dashed and dotted lines). We see, again, that FS effects are much more prominent at $M'$ [note the different scales in the insets of Fig. 4(a) and 4(b)]. The effect is even much stronger on the level of the corresponding spectra, shown in Fig. 4(c) and 4(d), respectively: In an $8 \times 8$ system (dashed-dotted line), nodal and antinodal spectra are qualitatively very similar, with a clear pseudogap feature, and differ mainly in peak height (at $|\omega| \approx 0.7$); at $k = X$, the spectrum remains nearly unchanged at larger system sizes and in the thermodynamic limit. At $k = M'$, in contrast, the pseudogap dip shrinks significantly for larger systems and is completely lost in the thermodynamic limit, where a quasiparticle shape appears. This shows that essential pseudogap physics, with a nodal–antinodal dichotomy, is really a property of the thermodynamic limit and that the bias inherent in finite-size systems dangerously distorts the physical picture.
C. FS extrapolations of spectra along high-symmetry momenta in the BZ

The elimination of FS errors at generic momenta requires “global” extrapolations that involve some kind of functional fitting procedures in momentum space. For momenta along high-symmetry lines, these fits have the form of Fourier series which may be adapted in order to take all symmetries into account. In the following, we will illustrate the algorithm for the most important path, the irreducible portion $X M'$ of the noninteracting Fermi surface. This path can be parametrized as

$$\begin{align*}
k_x &= (2 - \kappa) \pi/2; \quad k_y = \kappa \pi/2; \quad \kappa \in [0, 1];
\end{align*}$$

then $\kappa = 0$ corresponds to $X \equiv (\pi, 0)$ while $\kappa = 1$ corresponds to $M' \equiv (\pi/2, \pi/2)$. At particle-hole symmetry, all functions $f$ have to be symmetric with respect to both end points, which implies that they can be represented in the form

$$f(\kappa) = a_0 + \sum_{n=1}^{\infty} a_n \sin^2(n \kappa \pi/2)$$

with coefficients $a_n$. We have chosen to fit the difference of the Green function for each $k$ (along the line) with respect to the antinodal Green function (corresponding to $\kappa = 0$); this implies that the zeroth-order coefficient vanishes exactly. The symbols in Fig. 5(a) represent DQMC data for the difference Green functions at $\tau = \beta/2 = 2.5$; evidently their interpolation using the above Fourier series up to third order (dashed/dotted lines) works quite well. Furthermore, the associated Fourier coefficients depend very regularly (i.e., almost perfectly linearly) on $1/L^2$, as seen in Fig. 5(b), and decay exponentially as a function of order. Consequently, an extrapolation to the thermodynamic limit is possible on the level of the coefficients (using a least-squares fit) with high precision; the extrapolated coefficients yield a reliable estimate $G_k(\tau = 2.5)$ for all $k$ along the path [solid line in Fig. 5(b)].

IV. RESULTS

A. Pseudogap signatures at nodal and antinodal $k$ points

Let us, first, turn to the antinodal and nodal spectra shown in Fig. 6(a) and 6(b), respectively. At the elevated temperature $T = 0.50$ (dotted lines) the spectra have quasiparticle (QP) shape at all system sizes and for both momentum points. FS effects are negligible: Even the spectra of the smallest systems considered ($8 \times 8$, left column) do not deviate visibly from those in the thermodynamic limit (right column); also the momentum dependence along the Fermi surface is minimal at $T = 0.50$, with about 20% larger peak height at the nodal $M'$ point.

In the $8 \times 8$ case (left column), the largest system size fully considered in previous studies, a pseudogap dip appears almost simultaneously at $T = 0.28$ and $T = 0.24$ (dashed lines) at the $X$ and $M'$ points, respectively, and quickly deepens to an almost complete gap at $T = 0.18$ (dashed-dotted line). Given only this data, one would conclude that any momentum dependences beyond the free dispersion are inessential, i.e., that the physics might be in reach of theories with a momentum-independent self-energy [in particular, the dynamical mean-field theory (DMFT)]. However, this picture is distorted by finite-size effects and far from the truth: In the thermodynamic
limit (right column in Fig. 9), the antinodal spectra have QP shape only for $T \geq 0.28$; at $T = 0.24$, a slight dip emerges at $\omega = 0$ which develops to a significant PG at $T = 0.20$ and an almost complete gap at $T = 0.18$. In contrast, the nodal spectrum retains QP form down to $T = 0.20$ (while even the $16 \times 16$ system shows a PG dip at this temperature), before a PG emerges at $T = 0.18$. Thus, the FS extrapolation detailed above is really essential for fully resolving the nodal–antinodal dichotomy, which is at the heart of PG physics at finite temperatures. Only in the limit $T \to 0$, i.e., in the presence of long-range order, one expects a DMFT-like picture to become valid (again, as for high $T$) with fully gapped spectra all along the Fermi surface.

This implies that finite-size effects should mainly have two consequences on the level of spectra: (i) shift characteristic PG temperatures upwards, (ii) dilute the nodal–antinodal dichotomy in the vicinity of these characteristic temperatures.

**Characteristic PG temperature $T^*$**—As the opening of the PG is not a thermodynamic phase transition, it lacks a unique critical temperature. It is still useful (and common)\cite{Lake} to define a *characteristic PG temperature* $T^*$, for comparison with other temperature or energy scales of the system. An obvious choice of the required scalar PG measure is a dip in the spectral function. We specify this “pseudogap strength” by the reduction of spectral weight at $\omega = 0$, compared to the maximum:

$$r_k \equiv 1 - A_k(\omega = 0)/\max_\omega A_k(\omega),$$

as shown for the (anti)nodal points in Fig. 7. This representation reveals that the onset of the PG is slow only at $k = X$: As soon as $r_X \approx 0.5$, $r_M$ jumps to the full value within a narrow temperature range $\Delta T \approx 0.03$. The results in the thermodynamic limit (filled circles) can be fitted with a Fermi function form (solid lines); using their inflection points yields $T^*_X \approx 0.20$, $T^*_M \approx 0.18$. Note that, again, the FS effects are much stronger at $k = M'$ than at $k = X$.

**Comparison with the literature**—In a pioneering study, Huscroft *et al.*\cite{Huscroft} had obtained first bounds on the FS errors in DQMC spectra by complementing DQMC results for $N \leq 64$ sites with those of the dynamical cluster approximation (DCA) employing $N/k$ patches in the self-energy. The resulting antinodal spectral functions for $U = 5.2$ are shown as dashed and dotted lines in Fig. 9(a), respectively. The shaded region denotes the bounds in which one would expect the true spectrum, according to the opposite FS tendencies (with DQMC over- and DCA underestimating gaps at small cluster sizes) of both methods. Note that the remaining uncertainty is still significant and that the bounds are not rigorous, due to numerical noise and the difficulties of the MEM.

Our unbiased estimate of $A_X(\omega)$, shown as solid line in Fig. 9(a), reduces these uncertainties drastically: We find that the spectral weight at low frequencies ($|\omega| \lesssim 0.3$) is much smaller than predicted by DCA, but still significant (i.e., larger than the raw DQMC prediction). The true peak height at $|\omega| \approx 1.1$ is close to the average of the DCA and DQMC predictions. At large frequencies $|\omega| \gtrsim 1.5$, we find excellent agreement with the earlier DQMC estimates which shows that the DQMC FS errors are small in this region (cf. Fig. 6 and also verifies the procedures for analytic continuation; in contrast, DCA is still far off at $N = 64$).

Compared with the results for $U = 4$ presented in Fig. 6 our unbiased result [solid line in Fig. 8(a)] shows much stronger PG characteristics, as is certainly expected at the stronger interaction $U = 5.2$. Spectra for a full range of temperatures at this interaction are shown in Fig. 8(b) for a $12 \times 12$ system; these results can directly be compared with the second column in Fig. 6. Already at the highest temperature $T = 0.50$ [dotted line in Fig. 8(b)], the spectral peak is much broader, i.e., more spectral weight has been shifted away from the origin than at $U = 4$. This tendency towards more insulating behavior remains at lower $T$: The peak-to-peak width is about twice as large as for $U = 4$. At $T = 0.18$ (dash-dotted line), no spectral weight can be resolved at $|\omega| \lesssim 0.5$, so that the PG looks numerically like a full gap. In addition, the characteristic PG temperature is clearly shifted upwards, with a well-developed PG already at $T = 0.28$; the dependence of $T^*$ on $U$ will be studied more broadly in subsection IV C.
shows unbiased momentum-resolved spectra

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54x154] ) throughout the whole Brillouin zone, along the

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54x139] ) of the noninteracting Fermi surface (at half fill-

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54x105] opens at the antinodal point, while the rest of the spec-

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54x139] ) is consistent with a Fermi liquid de-

54x151] ; a behavior which is exactly opposite to usual

54x256] Taken together, our results indicate that, apart from

54x256] incoherent features at |ω| ≈ 4 which are present at all

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54x151] singularity at X completely determines the physics in

54x151] this region. This explains why the spectra can become

54x151] sharper, implying a reduction in the imaginary part of

54x256] energy features.

54x256] Taken together, our results indicate that, apart from

54x256] incoherent features at |ω| ≈ 4 which are present at all

54x256] continuous evolution into Hubbard bands with increasing U, interaction effects come into play with lowering T first very locally (in momentum space) around the antinodal X point; apparently, the strong enhancement of scattering by the van Hove singularity at X completely determines the physics in this region. This explains why the spectra can become sharper, implying a reduction in the imaginary part of the self energy, on the path from X towards Γ (up to the position of the arrow in Fig. 9 corresponding to the energy ω indicated by dotted lines), i.e., with increasing εk and ω: a behavior which is exactly opposite to usual Landau Fermi liquid and also to DMFT physics.

54x256] This suppression of spectral weight around X already at elevated temperatures also explains the slight dip seen in the local spectrum at T = 0.28 (dots and dotted lines in top panel of Fig. 9 cf. also Fig. 10): While the momenta around M' and in the spin-polaron band region (arrow) contribute “normally” to the local spectrum, the contributions from momenta near X are spread out to about a much larger width (with a significant fraction at |ω| ≥ 1); the missing weight at ω ≪ 1 results in the dip.

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the local spectrum at $T = 0.28$, a local suppression in $A(\omega)$ by about 10% in a narrow frequency range, corresponding to a “missing weight” of about 1%, could also result from uncertainties in the MEM procedure. Therefore, we have checked its consistency and accuracy in the largest finite-size system ($16 \times 16$) by comparing the local spectrum $A(\omega)$ (dashed line in Fig. 10), obtained by direct analytic continuation using MEM from the local Green function $G(\tau)$ with the average of all (here 256) momentum-resolved spectra $A_k(\omega)$ in Fig. 11. As $G(\tau) \equiv \frac{1}{N} \sum_k G_k(\tau) \equiv \overline{G_k(\tau)}$, both spectra should agree, if evaluated exactly: $A(\omega) = \frac{1}{N} \sum_k A_k(\omega) \equiv \frac{1}{N} \sum_k A_k(\omega)$. As the MEM is inherently nonlinear, due to the entropy constraint, deviations must be expected in practice. However, our procedure, with very accurate DQMC data, seems to be quite stable: Although the $k$ dependent spectral functions $A_k(\omega)$ differ substantially at different $k$ points (shown in Fig. 11 only for the nodal and antinodal points using short-dashed and dotted lines, respectively) and have much more pronounced features than the local spectral function $A(\omega)$ (long-dashed line), their average $\overline{A_k(\omega)}$ (solid line) agrees with it nearly within linewidth; only the magnified inset reveals tiny differences at small frequencies. So we conclude that our techniques are more than adequate and that the small dip discussed above is, indeed, physical.

Let us, finally, stress that our eliminations of finite-size errors have been absolutely essential for obtaining unbiased momentum-resolved spectra, as illustrated in Fig. 11 for the path $X \rightarrow M'$; not only is the convergence at the end points $k = X$ and $k = M'$ slow, the $k$ resolution is also quite coarse, with only one intermediate point for $L = 8$ and only three intermediate points for $L = 16$. It is clear that a very significant extension of the cluster size (e.g. to $64 \times 64$, implying a factor of $4^6 = 4096$ in computer time) would be needed in order to match the momentum resolution of our extrapolation procedure.

C. Evolution of characteristic pseudogap temperature $T^*$ with interaction $U$

Apart from yielding a momentum dependent $T^*$, the criterion used in subsection IV.A has the disadvantage of depending on the ill-conditioned analytic continuation of the imaginary-time DQMC Green functions to the real axis. On the other hand, it is difficult to define specific PG criteria on the level of the imaginary-time Green functions [cf. Fig. 3(a) and 3(b)]. However, the nodal–antinodal dichotomy, i.e., the momentum dependence of the Green functions along the line $X \rightarrow M'$ (arising from a momentum dependence of the irreducible self-energy) turns out to be illuminating: Fig. 12(a) shows that the norm of the difference between the imaginary-time Green functions,

$$|G_{M'} - G_X| = \left\{ \int_0^\beta d\tau |G_{M'}(\tau) - G_X(\tau)|^2 / \beta \right\}^{1/2},$$

is strongly enhanced (at $U = 4$) in the temperature range where the PG opens. Not surprisingly, this peak becomes sharper and shifts towards lower $T$ in the thermodynamic limit; the position of the maximum yields a natural unique definition of the characteristic PG temperature $T^* \approx 0.20$, indicated by a vertical dotted line in Fig. 12.

As discussed in the introduction, the PG is associated (at $n \approx 1$) with AF correlations and may be regarded as a precursor of a fully gapped long-range ordered AF phase which, in $d = 2$, is realized only in the ground state. Thus, we should expect to see a strong enhancement in suitable spin correlation functions. While the nearest-neighbor spin correlations are only very moderately enhanced at $T \lesssim T^*$ (not shown), the spin structure function is seen in Fig. 12(b) to increase by a full factor of 4 in the range $0.9 T^* \leq T \leq 1.1 T^*$. At the same time, FS effects explode at $T \lesssim T^*$. All this shows that the PG is driven by the development of AF order at a scale which is large compared to the lattice spacing.

The PG physics and, in particular, the momentum dependence observed at $U = 4$ should disappear at strong coupling, when already the high-temperature phase is gapped at $n = 1$. The dichotomy should also vanish in the limit $U \rightarrow 0$, where the energy scale $T_{\text{spin}}$ vanishes, and so does the magnitude of the pseudogap. Indeed,
FIG. 13. (Color online) Difference between nodal and antinodal Green functions versus temperature: DQMC results at weak to intermediate coupling (2 ≤ U ≤ 8) for 12 × 12 clusters (thick lines) and 8 × 8 clusters (thin lines). Inset: associated T* in comparison with DMFT Néel temperature.

the momentum dependence is seen in Fig. 13 to peak at U ≈ 4 and to decay quickly for larger couplings, where also FS effects (which can be estimated from the thin lines, corresponding to 8 × 8, in comparison to the main 12 × 12 results) become irrelevant. At fixed cluster size, also the results at weaker coupling (U = 3, U = 2) fall off; unfortunately, they suffer from significant FS effects which are too costly to eliminate. Still, the peak positions allow us to estimate T* (U) in the full range of weak to intermediate coupling as denoted by symbols in the inset of Fig. 13. Also shown is the mean-field estimate of the critical temperature for AF long-range order (solid line). At first sight, this DMFT estimate of the Néel temperature T_{N}^{DMFT} would appear irrelevant, as the true T_{N} = 0 by the Mermin-Wagner theorem. However, we find that T* ≈ 0.9 T_{N}^{DMFT} for 4 ≤ U ≤ 8; a correction of FS effects for U = 2 and U = 3 should push the corresponding values of T* also below T_{N}^{DMFT}. So the DMFT identifies the relevant temperature scale for spin coherence (as was previously observed in the strong-coupling regime\textsuperscript{27}); however, it lacks the momentum resolution which is essential to capture the pseudogap physics explored in this paper.

V. CONCLUSION

After decades of research, our understanding of the two-dimensional Hubbard model, especially regarding the extent to which it captures the pseudogap and high-T_{c} physics of cuprates, is still far from complete. Numerical simulations\textsuperscript{21,28–33} give valuable hints, but continue to be dominated by finite-size effects.\textsuperscript{34} We have overcome the finite-size barrier and presented momentum-resolved spectral functions in the thermodynamic limit, obtained by systematic extrapolation of DQMC Green functions (L → ∞ and Δτ → 0). Based on this achievement, we were able to disentangle the delicate interplay of dynamical and spatial magnetic correlations. At weak to intermediate couplings, this interplay leads, indeed, to the formation of a pseudogap in the half-filled band. The pseudogap originates from a strong k dependence of the self-energy, which results in a d-wave-like anisotropy in the opening of the charge gap and a “waterfall” substructure of the spectrum. The associated temperature scale T* is determined by the onset of antiferromagnetic fluctuations (and nearly agrees with T_{N}^{DMFT}, i.e., is rather high compared to other coherence scales and should be in reach of experiments with ultracold fermions on optical lattices.\textsuperscript{35,36}

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The evolution of the peak position toward low $T$ is consistent with a ground state charge gap (Ref. 24) $\Delta_c \approx 0.67$. The observable $\beta G(\beta/2)$ gives also hints about PG physics (Refs. 28, 29, and 31), but is not a sharp PG criterion: Its value changes only by some 20% between the curves, e.g. for $12 \times 12$ and $L \to \infty$ in the inset of Fig. 6 although the former corresponds to PG and the latter to QP behavior. The onset of strong AF correlations should still be visible in the higher-frequency portions of the spectral function as it leaves signatures in the kinetic energy (Ref. 27) and optical conductivity (Ref. 33).

25. Our estimate of $T^* \approx 0.30$ at $U = 6t$ agrees well with a recent DCA result (Ref. 21).

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