Pseudogap Formation in the
Symmetric Anderson Lattice Model

P.G. McQueen*, D.W. Hess,
Complex Systems Theory Branch,
Naval Research Laboratory, Washington, D.C. 20375-5345

and J.W. Serene
Department of Physics
Georgetown University
Washington, D.C. 20057

Abstract

We present self-consistent calculations for the self-energy and magnetic susceptibility of the 2D and 3D symmetric Anderson lattice Hamiltonian, in the fluctuation exchange approximation. At high temperatures, strong f-electron scattering leads to broad quasiparticle spectral functions, a reduced quasiparticle band gap, and a metallic density of states. As the temperature is lowered, the spectral functions narrow and a pseudogap forms at the characteristic temperature $T_x$ at which the width of the quasiparticle spectral function at the gap edge is comparable to the renormalized activation energy. For $T << T_x$, the pseudogap is approximately equal to the hybridization gap in the bare band structure. The opening of the pseudogap is clearly apparent in both the spin susceptibility and the compressibility.

PACS numbers: 71.28.+d, 75.20.hr
It is well known that heavy electron systems may be superconducting, magnetic or paramagnetic at the lowest temperatures [1]. Recent discoveries of cerium and uranium based compounds with quasiparticle gaps or pseudogaps $E_g \sim 10 - 100K$ have generally been interpreted as evidence that the zoo of heavy electron systems includes semiconductors as well [2]. However, the interpretation of the data is not unambiguous, and it is not yet clear whether these systems should be understood simply as ordinary semiconductors with unusually small gaps and strongly correlated electronic quasiparticles. An alternate interpretation of the resistivity, susceptibility, specific heat, and neutron scattering data is that at high temperatures ($T >> E_g$) these materials most closely resemble a heavy fermion metal above its coherence temperature, and as the temperature drops a pseudogap opens in the density of states at roughly the coherence temperature as estimated from high temperature properties.

A natural explanation of the existence of the narrow-gap semiconductors is that the high temperature band structure is semiconducting, and as the temperature is lowered, the effective hybridization of the f-levels with the conduction band is reduced as strong electronic correlations develop, just as in heavy electron metals. The reduced effective hybridization then leads directly to a dramatic reduction of the gap from its bare value. This picture is supported by slave boson calculations for the Anderson lattice Hamiltonian with infinite on-site repulsion $U$, for $T$ below the bose condensation temperature [3]. The mean field approach of those calculations does not include the finite quasiparticle lifetime resulting from strong electron-electron scattering. We have previously reported calculations of the self-energy and magnetic susceptibility for the symmetric Anderson lattice model in 2D with finite $U$, including the quasiparticle lifetime [4]. From the susceptibility and DOS we concluded that, on account of the temperature dependent quasiparticle lifetime, a pseudogap formed with decreasing temperature at a characteristic temperature much smaller than the hybridization gap in the bare band structure. Jarrell et al. reported essentially exact calculations for the $D = \infty$ symmetric Anderson lattice model with finite $U$ [5]. They also observe a metallic high temperature state and the formation of a pseudogap with decreasing temperature.

Here we present additional results and a detailed analysis of the formation of the pseu-
dogap in the symmetric Anderson lattice model with $U \sim W/2$, where $W$ is the bare conduction bandwidth; our results in 2D and 3D are qualitatively similar. The Anderson lattice Hamiltonian is 

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_{i\sigma} \{ V (f_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger f_{i\sigma}) + e_f n_{i\uparrow}^f - h \sigma (n_{i\sigma}^c + n_{i\sigma}^f) \} + U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f , \quad (1)$$

where $c_{i\sigma}$ ($f_{i\sigma}$) annihilates a conduction (f) electron at site $i$ with spin $\sigma$, $t$ is the nearest-neighbor conduction electron hopping energy, $e_f$ is the f-level energy, $V$ is the onsite hybridization energy between conduction and f electrons, $U$ is the Coulomb energy of two f-electrons on the same site, and $h$ is a homogeneous magnetic field coupled to the electron spin. For the symmetric model $\mu = 0$, and $e_f$ is chosen so that there are exactly two electrons per lattice site at all temperatures. The chemical potential is then at the middle of the indirect hybridization gap in the bare band structure, between the $\Gamma$ and $M$ points. The bare activation energy $\Delta_0$ is half the hybridization gap, and given by

$$\Delta_0 = \sqrt{(tD)^2 + V^2 - Dt} . \quad (2)$$

The fully renormalized single particle dispersion relations determined from the poles of the retarded Green’s function show a temperature dependent gap $E_g(T)$, which at high temperatures is close to the bare hybridization gap. The high-temperature density of states does not have a gap, however, because the quasiparticle width at the band edges, $\Gamma(T)$, is large compared to the temperature dependent activation energy $\Delta(T) = E_g(T)/2$. In this sense the system is effectively metallic (though with a poor conductivity). As the temperature is lowered, increasing correlations in the metallic state renormalize $\Delta(T)$ and the gap decreases, but $\Gamma(T)$ decreases even more rapidly than $\Delta(T)$ until $T$ eventually reaches a crossover temperature $T_x$ where $\Gamma(T_x) \sim \Delta(T_x)$. At this point the pseudogap begins to open in the single particle density of states. The opening of the pseudogap feeds back into the calculation of the self-energy and leads to a more rapid decrease of $\Gamma(T)$ and a rapid growth of $\Delta(T)$; these in turn accelerate the reduction of the density of states in the pseudogap
with decreasing temperature. At the lowest temperatures, \( \Delta(T) \sim \Delta_0 \). The opening of the pseudogap is reflected in the temperature dependence of the spin susceptibility, which drops faster than is possible for a semiconductor with a fixed gap when \( T \lesssim T_x \). We also note that for \( T > T_x \) the self-energy is to an excellent approximation independent of momentum, but as \( T \) is reduced through \( T_x \), the self-energy becomes increasingly momentum dependent. This is reflected in a strong flattening of the quasiparticle dispersion at low energy. With decreasing \( U \), \( T_x \) increases and the explicit temperature dependence of the opening of the pseudogap becomes more important; the temperature dependences of the thermodynamic and single particle properties are less dramatic and begin to resemble those of ordinary semiconductors. A crossover temperature \( T_x \) can still be identified from temperature dependence of the self-energy, and insofar as \( T_x(U) \) is meaningful for all \( U \), we expect that for \( T_x(U) \gg \Delta_0 \), \( \Delta(T) \) will not differ much from \( \Delta_0 \) and the system will behave essentially like an ordinary insulator. Here we focus on the more interesting cases \( T_x(U) < \Delta_0 \).

We have carried out fully self-consistent calculations for the 2D and 3D symmetric Anderson lattice Hamiltonian using a self-consistent perturbation theory known as the fluctuation exchange approximation (FEA) [12]. Here we present a highly abbreviated description of the FEA as applied to the Anderson lattice model and refer the reader to Ref. [17] for a more complete description. In a self-consistent perturbation theory, the fully renormalized temperature Green’s function \( G \) is related to the self-energy \( \Sigma \) through Dyson’s equation,

\[
G(k, \varepsilon_n) = \left[ G_0^{-1}(k, \varepsilon_n) - \Sigma(k, \varepsilon_n) \right]^{-1}.
\]  

(3)

The self-energy is obtained from a generating functional \( \Phi[G] \),

\[
\Sigma(k, \varepsilon_n) = \frac{1}{2} \frac{\delta \Phi[G]}{\delta G(k, \varepsilon_n)},
\]  

(4)

and the grand thermodynamic potential is given by [8]

\[
\Omega(T, \mu, h) = - \text{Tr} \left[ \Sigma G + \ln(-G_0^{-1} + \Sigma) \right] + \Phi[G],
\]  

(5)

which the appealing property of being stationary with respect to independent variations in \( G \) and \( \Sigma \). Here ‘Tr’ denotes a generalized trace over all arguments of the Green’s function.
and $G_0$ is the Green’s function of the non-interacting system. With the spin-quantization axis along the field, the Green’s functions and self-energies are spin diagonal, and because the Hubbard interaction acts only between f-electrons, $\Phi$ is a functional of the f-electron Green’s function $G_f$ alone and only the f-electron self-energy $\Sigma_f$ is nonzero. This greatly simplifies the solution of Dyson’s equation for $G$. The practical application of self-consistent perturbation theory entails the selection of a specific (possibly infinite) subset of the diagrams for $\Phi$. The diagrams that define the FEA are those that generate the Hartree-Fock and second-order self-energies together with contributions from the exchange of longitudinal spin and density fluctuations, transverse spin fluctuations, and singlet pair fluctuations. Explicit expressions for these contributions to $\Phi[G]$ for the Anderson lattice model appear in Ref. [7]. For the results presented below, the contribution to $\Phi$ from spin fluctuations is within 10% of that from the second order diagram; contributions from pair fluctuations and from density fluctuations are smaller by factors of roughly $-1/5$ and $-1/10$ respectively.

We calculate $\Sigma_f$ using an algorithm originally developed for the Hubbard model [13], on a $32^D$ lattice with spot-checks on lattices as large as $128 \times 128$ in 2D, and using a frequency cutoff at least six times the unhybridized conduction band width, $W = 4Dt$.

The magnetic susceptibility $\chi_s(T)$ was found from the slope of $\text{Tr}[\sigma_z G]$ versus $h$ for small fields (typically 0.005$t$ and 0.01$t$); this calculation of $\chi_s(T)$ is equivalent to solving an integral equation for the response function with irreducible vertices comprising particle-particle and particle-hole bubble-chains and Aslamazov-Larkin-type diagrams [14].

The retarded self-energy on the real axis was obtained from N-point Padé approximants [15]. This self-energy was then used to construct the spectral functions and quasiparticle dispersion relations along symmetry directions in the Brillouin zone. The densities of states were found by analytic continuation of the $\mathbf{k}$-summed imaginary-frequency Green’s functions using a variant of the N-point Padé approximant method of Vidberg and Serene [16]. These densities of states satisfy sum rules to better than 1% accuracy. At some temperatures in the transition region between the metallic and insulating states (see below), it is difficult
to obtain reliable analytic continuations. For example, Fig. 1 compares three different Padé continuations for the DOS at two temperatures: $T = 0.055t$, where the gap is opening, and $0.035t$ where the gap is well formed. The three analytic continuations for $T = 0.035t$ are essentially indistinguishable for all frequencies. At low energy, the analytic continuations for $T = 0.055t$ agree well except very near $\varepsilon = 0$; for $2t \leq \varepsilon \leq 8t$, two of the three continuations nearly coincide while the third shows qualitatively different behavior. To investigate this variability, we computed the rms deviation of the original imaginary frequency data from the data generated by using the candidate analytic continuation as a spectral function. For this purpose we use only frequencies less than half the high frequency cutoff to avoid cutoff-dependent artifacts. For $T = 0.035t$, the curves shown have rms deviations of $1.3 \times 10^{-4}$, $1.1 \times 10^{-4}$ and $1.3 \times 10^{-4}$ for $N = 57, 59, \text{and } 61$ respectively. At the temperature where the pseudogap is opening, qualitative differences in the structure of the DOS at energies $\sim W/2$ are often weakly reflected in the rms deviation as seen for the $T = 0.055t$ DOS shown in Fig. 1. There the rms deviations are $5.4 \times 10^{-5}$, $5.4 \times 10^{-5}$ and $6.1 \times 10^{-5}$ for $N = 35, 37, \text{and } 39$ respectively; the qualitatively different continuation shows only a slightly larger rms deviation. The DOS results presented below will include only those temperatures at which the analytic continuations for a given (reasonable) $N$ agree well with those over a range of $N$ and have the smallest rms deviations. In all cases the rms deviation is less than $2 \times 10^{-4}$.

For the calculations in 2D reported here, we used $\mu = 0$, $V = t$ and $\tilde{e}_f = 0$, where $\tilde{e}_f = e_f + \frac{1}{2}U(n^f_\uparrow + n^f_\downarrow)$ is the ($h = 0$) Hartree-renormalized f-level. With this choice of parameters the bare activation energy $\Delta_0$ is $0.236t$. For the 3D model, we took $V = 1.5t$ so that the ratio of the bare hybridization gap to the conduction electron bandwidth is the same in 3D as in 2D. We found that in this case the spin susceptibility and density of states for the symmetric Anderson lattice model in 3D may be roughly scaled to those in 2D by scaling all energies with respect to the bandwidth. An example of this scaling for the spin susceptibilities $\chi_s$ for $U = W/2$ is shown in Fig. 2. In the following we present primarily 2D data.

As the temperature is decreased through $T_x$, a pseudogap opens in the single particle
excitation spectrum. Pseudogap formation is reflected in $\chi_s$ and in the density $n(\mu, T)$; analytic continuation is not needed to calculate either of these. Fig. 3a shows $\chi_s(T)$ for various $U$ including $U = 0$. The form of $\chi_s(T)$ for finite $U$ strongly suggests the existence of a gap that apparently decreases with increasing $U$. For the largest $U$ shown, $U = 4t = W/2$, the rapid decrease in $\chi_s(T)$ occurs at a temperature $\sim \Delta_0/4$. For $U > 0$, $\chi_s(T)$ cannot be scaled to the $U = 0$ result by a simple renormalization of the gap. The dependence of $n$ on $\mu$ also shows a clear signature of pseudogap formation, as shown in Fig. 3b. For $U = 0$ and $T \gtrsim \Delta_0$, $dn/d\mu$ is constant over $-0.3t \lesssim \mu \lesssim 0.3t$ whereas for $T = 0.0625t$, $dn/d\mu$ shows substantial curvature. As the temperature is reduced, the gap in the single particle excitation spectrum becomes more apparent and $dn/d\mu$ essentially vanishes for $\mu \lesssim \Delta_0$. In contrast, for $U = W/2$ and $T = 0.0625t$, $dn/d\mu$ is essentially constant for $-0.3 < \mu < 0.3$, consistent with a metallic state or a semiconducting state with a gap $\lesssim 0.0625t$. At the lower temperature of $T = 0.055t$, $n(\mu)$ shows slight curvature. As the temperature is lowered, $dn/d\mu \to 0$ for a region of $\mu$ about $\mu = 0$ as expected in the presence of a pseudogap. At the lowest temperature, the region where $dn/d\mu$ nearly vanishes is about the size of the bare hybridization gap. From $n(\mu)$ and $\chi_s(T)$ one estimates essentially the same characteristic temperature $T_x$ for pseudogap formation.

The formation of the pseudogap can be seen explicitly in the single-particle (tunneling) density of states shown for various temperatures in Fig. 4. For $T = 0.125t$ and $T = 0.03125t$, Fig. 4a shows the total DOS over a wide energy range, from which one sees that the density of states is smoothly varying over most of the bandwidth. For $T = 0.125t$ there is no sign of a gap at low energy, but for $T = 0.03125$ a pseudogap centered at $\varepsilon = 0$ is clearly evident. Over the narrower range $-t \leq \varepsilon \leq t$ shown in Fig. 4b there is still no evidence of a hybridization gap at the highest temperatures, but as the temperature is lowered, a sharp asymmetric peak signals the pile up of states at the pseudogap edge. The density of states at zero energy decreases rapidly with decreasing temperature. We have shown previously that this decrease closely tracks that of $\chi_s(T)$ [1,17].

To illustrate how the pseudogap forms, we plot in Fig. 5a the spectral functions as
a function of $\varepsilon$ at the $\Gamma$ and $M$ points which lie on either side of the pseudogap. At high temperature, the spectral functions are very broad due to strong electron-electron scattering. The tails of the two spectral functions, centered close to the bare gap edges, extend well into the gap where they overlap and form the observed maximum. As the temperature is decreased, the spectral functions at the $\Gamma$ and $M$ points sharpen as shown in Fig. 5b. In contrast to the relatively strong $T$ dependence of the width of the spectral function $\Gamma(T)$, the position of the quasiparticle band at the $\Gamma$ point $\Delta(T)$ (as determined from the peak of the spectral function), also shown in Fig. 5b, is weakly $T$ dependent until $\Gamma(T) \sim \Delta(T)$, which sets the crossover temperature $T_x$. At this point the dramatic rapid decrease in $\chi_s(T)$ and the low energy DOS begins, with a correspondingly rapid renormalization of the quasiparticle energy at the gap edge.

The correlations above $T_x$ are apparent in the large renormalization of the band structure at low energy; the peak positions of the spectral functions at the gap edges at $T_x$ are at about $\Delta_0/4$. The sharpening of the spectral functions with decreasing temperature above $T_x$ reflects the evolution toward coherent quasiparticle excitations. The quasiparticle renormalization factor provides another measure of the strength of correlations. In a metal, the quantity $\text{Im} \Sigma(k,\varepsilon_0)/\varepsilon_0 = D_k(T)$ can be used to construct a reasonable estimate of the quasiparticle renormalization factor $a_k = (1 - \partial \text{Re} \Sigma(k,\varepsilon)/\partial \varepsilon|_{\varepsilon=0})^{-1}$; for a point on the Fermi surface of a Fermi liquid, $D_k(T)$ tends to $\partial \text{Re} \Sigma(k_F,\varepsilon)/\partial \varepsilon|_{\varepsilon=0}$ as $T \to 0$. For the one band Hubbard model at 1/4 filling, we found that $D_k(T)$ is weakly temperature dependent and approaches $\partial \text{Re} \Sigma(k,\varepsilon)/\partial \varepsilon|_{\varepsilon=0}$. For the asymmetric Anderson lattice model, we found that the magnitude of $D_k(T)$ increases strongly with decreasing temperature (as did our measure of the quasiparticle effective mass) down to the lowest temperatures that we studied. Here we observe that for $T > T_x$ the temperature dependence of $D_k(T)$ resembles that of $D_{k_F}(T)$ for the asymmetric model. We plot $D_k(T)$ for the symmetric model and for $k$ at the $\Gamma$ point in Fig. 6, in which a distinctive feature at $T = T_x$ is apparent. For $T > T_x$, the system is metallic and the magnitude of $D_\Gamma(T)$ increases with decreasing temperature. As the temperature is further decreased, the opening of the pseudogap acts to reduce con-
tributions from low energy excitations to the fluctuation propagators, leading to a sharp reduction in the magnitude of $D_\Gamma(T)$, which is reflected in the widening of the renormalized gap shown in Fig. 5b. In the limit $T \to 0$, $\text{Im} \Sigma(k, i\varepsilon_n)$ tends to a finite value at low $T$. This is not inconsistent with the formation of the pseudogap; the $U = 0$ Green’s function already contains information on the bare hybridization gap, so $\Sigma(k, \varepsilon_0)$ need not show a divergence as observed, e.g. in the Hubbard model [19].

Effects of strong correlations are also apparent in the quasiparticle band structure determined from the poles of the single particle Green’s function, as shown in Fig. 7. At sufficiently high temperatures, the quasiparticle band structure does not differ significantly from the bare band structure and $\Sigma(k, \varepsilon)$ is to a good approximation independent of $k$. As the temperature is lowered toward $T_x$, a pronounced flattening of the bands around the $\Gamma$ and $M$ points occurs and the self-energy becomes increasingly $k$ dependent. In Fig. 7b we compare the band structure obtained by taking $\Sigma(k, \varepsilon) = \Sigma(\Gamma, \varepsilon)$ for all $k$ with that obtained from the full $k$-dependent self-energy. The momentum dependence of the self energy clearly provides a substantial contribution to the flattening of the band at low energy. Mean field calculations in the limit $U \to \infty$ find a quasiparticle band structure given by the expression for the bare band structure with a renormalized f-level and hybridization. In Fig. 7b we also show the band structure for a noninteracting system along the $\Gamma - X$ direction for $e_f = 0$ and $V = 0.6t$, which reproduces the particle-hole symmetry and gap of the fully renormalized band structure. It is clear that this approach is unable to describe the band flattening and band width along this direction in the FEA.

We have presented the results of a fully self-consistent calculation of the self-energy and spin susceptibility in the fluctuation exchange approximation for the symmetric Anderson lattice model. From a metallic state at high temperature, a pseudogap forms with decreasing temperature. The pseudogap begins to open at the temperature $T_x$ at which the renormalized band gap and the width of the spectral function at the gap edge are comparable. As $T$ is decreased through $T_x$, the density of states at low energy decreases rapidly. The opening of the pseudogap is observed in results obtained directly from imaginary frequency axis
data and through analytic continuation to the real frequency axis. The large temperature-dependent renormalizations of the band structure above $T_x$ are similar to those we have observed in the asymmetric model and suggest that the evolution of a coherent heavy fermion metallic state with decreasing $T$ is cut off by the loss of low energy excitations as the pseudogap develops.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge useful discussions with M. Jarrell, J.D. Thompson and M.F. Hundley. We are grateful to J. Deisz for a critical reading of this manuscript. We thank the Office of Naval Research for their support and the NRL Connection Machine facility for assistance. This work was supported in part by the Office of Naval Research and by the Army High Performance Computing Center under the auspices of the Army Research Office contract number DAALO3-89-C-0038 with the University of Minnesota.
REFERENCES

* Also at Sachs Freeman Associates, Inc., Landover, MD.

[1] Z. Fisk, D.W. Hess, C.J. Pethick, D. Pines, J.L. Smith, J.D. Thompson, J.O. Willis, Science 239, 33 (1988).

[2] J.D. Thompson, W.P. Beyerman, P.C. Canfield, M.F. Hundley, G.H. Kwei, A. Lacerda, Z. Fisk, R.S. Kwok, J.M. Lawrence and A. Severing, in Transport and Thermal Properties of f Electron Systems, H Fujii, T. Fujita and G. Oomi eds., Plenum, New York, 1992; G. Aeppli and Z. Fisk, Comments Cond. Mat. Phys. 16, 155 (1992).

[3] P.S. Riseborough, Phys. Rev. B. 45, 13984 (1992); C. Sanchez-Castro, K.S. Bedell and B.R. Cooper, Phys. Rev. B. 47, 6879 (1993).

[4] P.G. McQueen, D.W. Hess and J.W. Serene, in proceedings of XXth International Conference on Low Temperature Physics, in press.

[5] M. Jarrell, H. Akhlaghpour, Th. Pruschke, Phys. Rev. Lett. 70, 1670 (1993).

[6] Note that an unfortunate error in the hopping term of the Hamiltonian in Eq. [1] of Ref. 7 is corrected here so that the Hamiltonian in Eq. [1] is consistent with the notation used in our previous papers.

[7] P.G. McQueen, D.W. Hess and J.W. Serene, Phys. Rev. Lett. 70, 129 (1993).

[8] J.M. Luttinger and J.C. Ward, Phys. Rev. 118, 1417 (1960).

[9] G. Baym, Phys. Rev. 127, 1391 (1962).

[10] H. Schweitzer and G. Czycholl, Z. Phys. B 74, 303, (1989); 79, 377 (1990); M.M. Steiner, R.C. Albers, D.J. Scalapino, L.J. Sham, Phys. Rev. B 43, 1637 (1991); V. Zlatic, S.K. Ghatak and K.H. Bennemann, Phys. Rev. Lett. 57, 1263 (1986); K. Okada, K. Yamada and K. Yosida, Prog. Theor. Phys. 77, 1297 (1987); K. Yamada and K. Yosida, in Electronic Correlation and Magnetism in Narrow-Band Systems, ed. T. Moriya, Springer
[11] Sungkit Yip, Phys. Rev. B 38, 8785 (1988).

[12] N.E. Bickers, D.J. Scalapino and S.R. White, Phys. Rev. Lett. 62, 961 (1989).

[13] J.W. Serene and D.W. Hess, in Recent Progress in Many-Body Theories, Vol. 3, edited by T.L. Ainsworth et al. (Plenum, New York, 1992); J.W. Serene and D.W. Hess, Phys. Rev. B 44, 3391 (1991).

[14] L.G. Aslamazov and A.I. Larkin, Fiz. Tverd. Tela 10, 1104 (1968) [Sov. Phys. Solid State 10, 875 (1968)].

[15] H.J. Vidberg and J.W. Serene, J. Low Temp. Phys. 19, 179 (1977).

[16] C.R. Leavens and D.S. Ritchie, Solid State Commun. 53, 137 (1985).

[17] The self-energies reported here have been converged so that the fractional difference in the self-energy between successive iterations is, for all frequencies and \( k \) points, less than \( 1 \times 10^{-5} \), while those presented in Ref. [4] were converged to \( 1 \times 10^{-4} \). We believe that this accounts for the qualitative differences between the densities of states presented in this work and those presented in Ref. [4], for temperatures at which the pseudogap is developing. The main conclusion of Ref. [4], that the temperature dependent reduction of the DOS at low energy correlates with the rapid decrease in \( \chi_s \), is supported by the present work.

[18] D.W. Hess and J.W. Serene, J. Phys. Chem. Solids 52, 1385 (1991); J.W. Serene and D.W. Hess, in High-Temperature Superconductivity, edited by J. Ashkenazi, S.E. Barnes, F. Zuo, G. Vezzoli and B.M. Klein (Plenum, New York, 1991).

[19] M. Vekić and S.R. White, Phys. Rev. B 47, 1160 (1993).
FIGURES

FIG. 1. Comparison of three analytic continuations using N-point Padé approximants for $T = 0.055t$ and $0.035t$ (a) low energies, $0 \leq \varepsilon \leq t$; and (b) high energies, $2t \leq \varepsilon \leq 8t$. For $T = 0.055t$ ($0.035t$), 35, 37 and 39 (57, 59 and 61) Padé coefficients were used. Note that the “high energy” $T = 0.035t$ results were shifted by 0.05 for clarity and that 35 coefficients were used for the dashed $T = 0.055t$ curve.

FIG. 2. The uniform static spin susceptibility $\chi_s$ for 2D and $U = 4t = W/2$ ($\bullet$), 3D and $U = 6t = W/2$ ($\triangle$), and the 3D result with all energies scaled by the ratio of the bare conduction bandwidth in 2D to that in 3D bar($\diamond$).

FIG. 3. (a) The spin susceptibility $\chi_s(T)$ for $U = 0$, (dashed) $t(\square)$, $2t(\circ)$, $3t(+)$ and $4t(\bullet)$. (b) The total density $n$ as a function of $\mu$ for $U = 4t$ and $T = 0.0624t(\triangle)$, $0.055t(+)$, $0.03125t(\circ)$, and $0.015625(\circ)$. Also shown for comparison are $n(\mu)$ for $U = 0$ and $T = 0.24t$ (solid), $0.0625t$ (long dashed), and $0.015625t$ (short dashed).

FIG. 4. (a) The density of states over a wide energy range for $T = 0.125t$ (short-dashed) in the metallic state and for $T = 0.035t$ (long-dashed) where a developed pseudogap is evident. (b) The density of states at low energy for temperatures $T = 0.015625t$ (long-dashed showing gap), $0.035t$ (short-dashed showing gap), $0.0625t$ (long-dashed-short-dashed), $0.125t$ (dashed), and $0.25$ (dotted) showing the formation of a pseudogap from a high temperature metallic state with decreasing $T$.

FIG. 5. (a) The spectral function at the $\Gamma$ point (solid) for $T = 0.25t$, $0.125t$, $0.0625t$, and $0.035t$ in order of decreasing peak width. Also shown is the spectral weight for the $M$ point (dashed) and the sum of the $M$ and $\Gamma$ point spectral weights (long dash) for the temperature $T = 0.0625t$ at which the pseudogap begins to open for $U = 4t$. (b) The width of the spectral function at half maximum on the high energy side $\triangle$ and low energy side $\circ$ as a function of $T$ for $k$ at the zone center, and the position of the peak of the spectral function ($\bullet$) as a function of temperature.
FIG. 6. The function $D_k(T)$ (see text) for $k$ at the $\Gamma$ point and for $U = t \,(\circ), \, 2t \,(\square), \, 3t \,(\triangle)$, and $4t \,(\bullet)$. Note the sharp structure marking the opening of the pseudogap and the shift of this structure to lower temperature with increasing $U$.

FIG. 7. (a) Fully renormalized quasiparticle band structure along high symmetry directions in the zone for $U = 4t$ with $T = 0.0625t$ (solid) and $T = 0.25$ (dashed) compared with the bare band structure (long dash-short dash). (b) Fully renormalized band structure for $T = 0.0625t$ (solid) compared with the band structure assuming a momentum independent self energy $\Sigma(k, \varepsilon) = \Sigma(\Gamma, \varepsilon)$ (dashed), the bare band structure (short-dashed) and a fit to the mean field band structure with a renormalized $V = 0.6t$ and $\epsilon_f = 0$ (long dash-short dash).