

Kehrein Replies: In their Comment, Georges and Kotliar [1] discuss the interchangeability of the limit $U \uparrow U_{c2}$ and the “resummation” of the skeleton expansion. They claim that these limits do not commute and conclude that the analysis in Ref. [2] is wrong.

The question of the uniformity of the limit $U \uparrow U_{c2}$ has already been briefly addressed in [2]: It was mentioned there that (i) under the basic assumption of pointwise convergence of the skeleton expansion for $U < U_{c2}$ (as used in Ref. [2] and the previous Comment) and (ii) for the specific density of states upon approaching the Mott transition under consideration there, the above limits can be interchanged. This will be worked out in more detail below. In order to make the argument transparent, I will first outline what kind of behavior of the skeleton expansion would be required in order for the criticism by Georges and Kotliar to be valid. Then it will be shown why this kind of behavior can be ruled out.

Equation (11) in Ref. [2] follows from the assumption of pointwise convergence of the skeleton expansion: Denote with $J^{(N)}(\epsilon)$ the imaginary part of the self-energy obtained as the partial sum of all skeleton diagrams up to order N . Pointwise convergence is defined by $\forall \epsilon \lim_{N \rightarrow \infty} J^{(N)}(\epsilon) = J(\epsilon)$ for a fixed $U < U_{c2}$. What is then required in order to have “nonuniform” behavior as $U \uparrow U_{c2}$? Since one has to generate the narrow resonance in $J(\epsilon)$ on the energy scale $\sqrt{w}t$, some vertex function of order $n_s = O(1/\sqrt{w})$ must develop a narrow resonance for certain values of its arguments: Though $\rho(\epsilon)$ contributes to the integral (11) in [2] on an energy scale set by wt , one finds $n_s \times wt = O(\sqrt{w})t$, i.e., a possible contribution for ϵ of order $\sqrt{w}t$ as required. Since $n_s \rightarrow \infty$ as $U \uparrow U_{c2}$, this would indeed imply the noninterchangeability of the above limits.

Next it will be demonstrated that the vertex functions $\Gamma^{(n)}$ cannot exhibit this nonuniform behavior, at least for the model under consideration here. Using the arguments from Ref. [3], a Schrieffer-Wolff-like transformation can be applied to the Anderson impurity model describing the large- d Hubbard model close to U_{c2} . This unitary transformation generates an effective low-energy Kondo Hamiltonian and a gapped high-energy Hamiltonian. The Kondo Hamiltonian is (for the notation see [3])

$$H_{\text{low}} = wt \left(\sum_{k,\sigma} \tilde{\epsilon}_k n_{k,\sigma} - \frac{J}{2} \tilde{S} \cdot \tilde{s}_L \right). \quad (1)$$

Here $\tilde{\epsilon}_k$ and J are dimensionless parameters. H_{low} can be made dimensionless by dividing with wt

$$\tilde{H}_{\text{low}} \stackrel{\text{def}}{=} H_{\text{low}}/wt. \quad (2)$$

\tilde{H}_{low} determines the low-energy interactions (meaning for energies smaller than the gap in H_{high}) and therefore also the low-energy behavior of the vertex functions $\Gamma^{(n)}$ ex-

pressed in dimensionless variables $\tilde{\epsilon}_k \stackrel{\text{def}}{=} \epsilon_k/wt$. Since $\rho(\tilde{\epsilon})$ (defined as the density of states corresponding to $\tilde{\epsilon}_k$) and J approach finite noncritical values as $U \uparrow U_{c2}$, the *dimensionless* vertex functions are well behaved in this limit. The critical behavior follows only after reintroducing the overall energy scale wt for the dimensional vertex functions. Except for this overall scale dependence on wt , these low-energy vertex functions, therefore, cannot depend on w explicitly. This excludes a sharp resonance in some $\Gamma^{O(1/\sqrt{w})}$ in the limit $w \rightarrow 0$ as required in the nonuniform scenario discussed above.

Summing up, pointwise convergence implies that the limits $N \rightarrow \infty$ and $U \uparrow U_{c2}$ can be interchanged for the *specific* model under consideration here due to the separation of energy scales and the construction of a *noncritical* low-energy theory. Pointwise convergence is also a sufficient condition for the analytic continuation to the noninteracting system and has therefore been used as an analytic criterion for the transition in [2].

The second point in the Comment quotes from Ref. [2]: “In the skeleton expansion the imaginary part of the self-energy is related to the available phase space for scattering processes.” This precisely expresses in words what can be *directly* deduced from Eq. (11) in Ref. [2]: Fermi liquid properties *follow* by analyzing the IR behavior of (11) [4], but the series itself can also be analyzed at finite energies.

Regarding the understanding of the Mott-Hubbard transition in the limit of large dimensions in general, it should also be mentioned that the most recent numerical simulations [5–8] do not yet provide a coherent picture for both the $T = 0$ and $T > 0$ behavior of the transition.

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