Berciu Replies: The preceding Comment [1] makes a valuable point about the meaning of the momentum average (MA) approximation in real space: Indeed, it replaces all free propagators appearing in the proper self-energy diagrams $G_0(i, j, \omega - n\Omega) \to \delta_{i,j}\bar{g}_0(\omega - n\Omega)$. In terms of the continued fractions

$$A_n(\omega) = \frac{n\bar{g}_0(\omega - n\Omega)}{1 - g^2\bar{g}_0(\omega - n\Omega)A_{n+1}(\omega)}, \quad (1)$$

the resulting MA self-energy is $\Sigma_{\mathrm{MA}}(\omega) = g^2 A_1(\omega)$. As shown in Refs. [2,3], this simple expression gives results in very good agreement with numerical simulations over most of the parameter space. This was explained in terms of sum rules for the spectral weight, which MA satisfies exactly for orders $n \leq 5$ and with high accuracy for all higher orders. As pointed out in Ref. [3] and in the Comment, there are also some failings: MA does not show the expected continuum at $E_{\mathrm{GS}} + \Omega$, and its accuracy becomes worse as $\Omega \to 0$.

This real-space interpretation [1] offers an alternative way to see why the MA approximation should be accurate at least for low energies. The polaron ground state is below the free-particle continuum $E_{\mathrm{GS}} < -2dt$. If $\omega - n\Omega < -2dt$, the free propagators $G_0(i, j, \omega - n\Omega)$ decrease exponentially with the distance $|i - j|$. The decay is faster the lower ω and the higher n are. Thus, for energies $\omega \sim E_{\mathrm{GS}}$, keeping only the diagonal terms $i = j$ is a good first-order approximation, especially for larger coupling g (lower E_{GS}) and larger phonon frequency Ω.

Clearly, a systematic way to improve the MA approximation is to keep all free propagators with small n exactly. Let us call $\mathrm{MA}^{(n)}$ the approximation where, in all proper self-energy diagrams, all free propagators $G_0(k, \omega - m\Omega)$, with $m > n$, are momentum averaged (because they decay fastest with the distance $|i - j|$), whereas the ones with $m \leq n$ phonons are kept exactly. The resulting self-energies can still be calculated exactly (details will be presented elsewhere [4]). For example, for the Holstein polaron we find

$$\Sigma_{\mathrm{MA}^{(1)}}(\omega) = \frac{g^2\bar{g}_0(\tilde{\omega})}{1 - g^2\bar{g}_0(\tilde{\omega})[A_2(\omega) - A_1(\omega - \Omega)]}, \quad (2)$$

where $\tilde{\omega} = \omega - \Omega - \Sigma_{\mathrm{MA}}(\omega - \Omega)$. Since $\bar{g}_0(\omega)$ is imaginary for $-2dt \leq \omega \leq 2dt$, it follows that $\Sigma_{\mathrm{MA}^{(1)}}(\omega)$ first acquires a finite imaginary part (i.e., it predicts a continuum) when $\tilde{\omega} > -2dt$, i.e., at an energy $E_{\mathrm{GS}}^{\mathrm{MA}} + \Omega$. This is slightly larger than $E_{\mathrm{GS}}^{\mathrm{MA}^{(1)}} + \Omega$, because $\mathrm{MA}^{(1)}$ is more accurate than MA. For the $\mathrm{MA}^{(2)}$ and higher levels, the gap to the first continuum is Ω, as expected. This is shown in Figs. 1(a) and 1(b). As argued in Ref. [3], within MA the discrete states account for the continuum's weight.

For the Holstein Hamiltonian, for $n \geq 2$ the self-energy $\Sigma_{\mathrm{MA}^{(n)}}(k, \omega)$ has *explicit momentum dependence*, since the second-order diagrams, which are momentum-dependent, are now summed exactly. The accuracy is systematically improved with increasing n, as shown in Figs. 1(c) and 1(d)

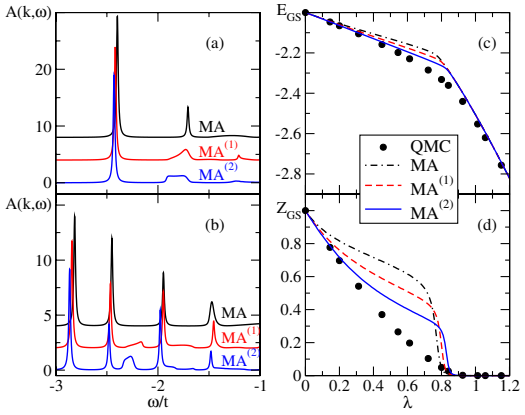

FIG. 1 (color online). (a) Spectral weight $A(0, \omega)$ in 1D, for $t = 1$, $\Omega = 0.5t$, $\eta = 0.01t$, and $\lambda = g^2/(2dt) = 0.6$. The curves have been shifted for clarity. (b) Same as (a), for $\lambda = 1.1$; (c),(d) are polaron ground-state energy and quasiparticle weight vs λ, respectively, for $t = 1$, $\Omega = 0.1t$. Quantum Monte Carlo simulations (QMC) results shown as circles are from Ref. [5].

for one dimension and $\Omega = 0.1t$ (here MA compared worst against available numerics [3]). More results will be shown elsewhere [4]. The improved accuracy is reflected by the sum rules as well. For example, $\mathrm{MA}^{(1)}$ satisfies exactly sum rules up to $n = 7$ and is more accurate than MA for higher order sum rules, since the diagrams are more accurate [3]. On the other hand, the evaluation of these self-energies becomes more involved as n increases, although $\mathrm{MA}^{(2)}$ is still numerically trivial [4] (we do not show the expressions here for lack of space).

Finally, the MA approximations can be generalized to models with a phonon momentum-dependent coupling $g(q)$. In this case, even $\Sigma_{\mathrm{MA}}(k, \omega)$ is momentum-dependent [4]. These results will hopefully end claims that MA is just some "poor version" of dynamical mean-field theory. In fact, the MAs are a hierarchy of simple approximations that allow one to systematically improve accuracy in obtaining dressed particles' Green's functions.

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Received 4 January 2007; published 17 May 2007
DOI: 10.1103/PhysRevLett.98.209702
PACS numbers: 71.38.−k, 63.20.Kr, 72.10.Di

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