Comment on "Green's Function of a Dressed Particle"

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The momentum averaging (MA) approach to the evaluation of the single-electron Green's Function (GF) was proposed in a recent Letter [1], as a new and accurate approximation for the Holstein polaron problem. However, as shown here, the MA suffers from two serious limitations. The contributions to the incoherent continuum are oversimplified to the point of introducing nonphysical behaviors. Similarly, the adiabatic correlations involving different lattice sites are entirely ignored. Therefore, the quantitatively good behavior of some polaron properties reported in Ref. [1] does not establish the accuracy of the MA. Rather it shows that in the considered range of parameters the analyzed quantities are weakly affected by such an approximation.

The MA can be easily set in the context of dynamical mean field theory (DMFT), a point not recognized in Ref. [1]. The DMFT GF in the k space is given by $G_k^{DMFT}(\omega) = [\omega - \varepsilon_k - \Sigma^{DMFT}(\omega)]^{-1}$, with ε_k the free-electron energy characterized by the electron hopping energy t. The (local) self-energy $\Sigma^{DMFT}(\omega)$ is given by [2]

$$\Sigma^{DMFT}(\omega) = \frac{g^2}{\mathcal{G}_{ii}^{-1}(\omega-\omega_0) - \frac{2g^2}{\mathcal{G}_{ii}^{-1}(\omega-2\omega_0)-\ldots}} \ , \qquad (1)$$

where g is the coupling constant, ω_0 is the phonon energy, and $\mathcal{G}_{ii}(\omega)$ is a local GF. $G_k^{DMFT}(\omega)$ is solved iteratively, until the self-consistency condition $1/N\sum_k G_k^{DMFT}(\omega) = [\mathcal{G}_{ii}^{-1}(\omega) - \Sigma^{DMFT}(\omega)]^{-1}$ is reached. The MA corresponds to the first step of this procedure, when the local free-electron GF $\mathcal{G}_{ii}^{(0)}(\omega)$ is used in Eq. (1) as the initial guess.

The MA can be also viewed from the diagrammatic theory [3] side. In the site representation it can easily be verified that $\Sigma^{MA}(\omega)$ is obtained from the exact $\Sigma_{i,i}(\omega)$ by replacing in all diagrams $\mathcal{G}_{i,j}^{(0)}(\omega)$ by $\delta_{i,j}\,\mathcal{G}_{ii}^{(0)}(\omega)$,

$$G_{i,j}^{MA}(\omega) = \mathcal{G}_{i,j}^{(0)}(\omega) + \Sigma^{MA}(\omega)\sum_n \mathcal{G}_{i,n}^{(0)}(\omega) G_{n,j}^{MA}(\omega) \ . \qquad (2)$$

Thus, in the MA case, the electron is supposed to interact with phonons at some lattice site only if all the other sites are unoccupied by phonons.

The MA limitations become quite transparent when this approach is reformulated in terms of eigenstate calculations. Equation (2) is equivalent to the treatment of the Holstein polaron problem within the Hilbert subspace spanned by the states $c_j^\dagger\,|n_{j+m}\rangle$, where $c_j^\dagger$ creates an electron at site j and n_m is the number of phonons at a given neighbor m of the electron. In this respect, the MA is more restrictive than either the self-consistent Born approximation (SCBA) [4] or DMFT, as the latter two include processes involving phonons at different sites at the same instant of time.

In terms of the diagrammatic expansion, Eq. (1) correctly reproduces the leading g^2 diagram for any t/ω_0. In the weak-coupling limit, this diagram defines the low-frequency properties, in particular the ground-state energy E_{GS}. The corrections in g^2 small beyond the leading order describe the incoherent continuum starting at $\omega_c = E_{GS} + \omega_0$ and, for $4t > \omega_0$, the flattening near ω_c of the lowest coherent polaron band. While such results for $\omega \approx \omega_c$ are also derived from the SCBA [4] and DMFT, within the MA both the continuum and the band flattening occur around $\omega_{MA} = -2t + \omega_0$, as for the noninteracting case. This latter result can be easily explained by noting that for $\omega \approx \omega_c$ the system is described by the polaron (dressed electron) in the ground state and a phonon almost uncorrelated with the electron. Such excitations involving electron dressing effects and weakly correlated phonons, which contribute to the incoherent continuum for $\omega \geq \omega_c$, cannot obviously be described within the subspace $c_j^\dagger\,|n_{j+m}\rangle$. This restriction, discussed here from the weak-coupling side, persists for all couplings.

As $\Sigma^{MA}(\omega)$ is exact in the atomic $t = 0$ limit [2], it is appropriate to analyze the adiabatic contributions from the strong-coupling side $g^2/\omega_0 \gg t$, by treating t perturbatively [5]. To the second-order in t one obtains the polaron ground-state wave function involving states $c_j^\dagger|n_j, n_{j\pm\delta}\rangle$ with phonons also at the nearest neighboring sites δ, describing the adiabatic spreading of the small polaron [6] Since these states are not considered within the MA, one finds that the adiabatic corrections to the atomic limit (involving multiple lattice sites) are beyond the MA. In particular, it is known that for $t/\omega_0 \gg 1$ large adiabatic polarons can form in the 1D system. For such polarons, it is essential to retain the k-dependence of the self-energy [3], which is apparently beyond the MA, or any other approach that treats $\Sigma_k(\omega)$ as a local quantity.

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