Comment on "Dynamical mean field solution of the Bose-Hubbard model"

K. Byczuk[1] and D. Vollhardt[2]

[1] *Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, PL-00-681 Warszawa, Poland*
[2] *Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany*

In their preprint Anders *et al.* [arXiv:1004.0510] propose a crucial modification of the Bosonic Dynamical Mean-Field Theory (B-DMFT) derived by us [Phys. Rev. B **77**, 235106 (2008)]. Here we show that the modification consists of two steps which, in fact, cancel each other. Consequently their self-consistency equations are identical to ours.

According to Anders *et al.* [1] they have modified the Bosonic Dynamical Mean-Field Theory (B-DMFT) [2] "to avoid double counting of kinetic energies" and thereby found stable solutions to the B-DMFT equations. Here we show that the alleged double counting is caused by an improper definition by Anders *et al.* [1] of the condensate wave function. In Ref. [1] the error introduced thereby is subsequently compensated by (mathematically uncontrolled) Bogoliubov shifts of the integration variables.

For simplicity we only consider the non-interacting case ($U = 0$) with nearest-neighbor hopping of the bosons on a lattice with finite coordination number Z since this is sufficient to illustrate our point. The generalization to finite U is straightforward. The B-DMFT maps the lattice problem onto a single site (say, $i = 0$) which is self-consistently coupled to two dynamical baths, one composed of normal and the other of condensed bosons [2]. For all coordination numbers $2 \leq Z < \infty$ the exact partition function may be derived from a path integral with the local action $Z_{\rm exact} = Z^{(0)} \int D[b_0^* b_0] \exp(-S_0[b_0^* b_0])$. Here a superscript (0) refers to a lattice with a cavity, i.e., where the impurity site $i = 0$ is removed, while a subscript 0 refers to the impurity site itself. The local action for $U = 0$ reads

$$\begin{aligned} S_0 = &\int d\tau b_0^*(\tau)(\partial_\tau - \mu) b_0(\tau) \\ &+ \left[\kappa\phi \int d\tau_1 b_0^*(\tau_1) + H.c.\right] \\ - &\int d\tau_1 \int d\tau_2 \Delta(\tau_1 - \tau_2) b_0^*(\tau_1) b_0(\tau_2), \end{aligned} \tag{1}$$

where the condensate wave function

$$\phi = \langle b_j \rangle_{S^{(0)}} \tag{2}$$

and the hybridization function

$$\Delta(\tau_1 - \tau_2) = \sum_{j_1 j_2} t_{0j_1} t_{j_2 0} \langle b_{j_1}(\tau_1) b_{j_2}^*(\tau_2) \rangle_{S^{(0)}} \tag{3}$$

are determined *on the lattice with the cavity*, and $\kappa = \sum_j t_{0j} = Zt$ is a geometric factor; cf. Appendix A of Ref. [2] for a derivation and notation. In particular we note that expectation values $\langle \dots \rangle_{S^{(0)}}$ only contain connected terms.

In Ref. [1] a different approach is taken. Here the expectation value of the boson is calculated *on the impurity site* $i = 0$, $\langle b_0 \rangle_{S_0}$, and this quantity is incorrectly identified with the condensate wave function ϕ. By performing Bogoliubov shifts of the integration variables b_0 and b_0^* the corresponding error in ϕ is compensated, whereby the geometric term κ now acquires an additional, but spurious term linear in the hybridization function, and thus takes the form $\kappa = Zt - \int d\tau_2 \Delta(\tau_1 - \tau_2)$. For this reason the authors of [1] refer to κ as "the coupling between the impurity and the condensate".

It should be noted, however, that on a Bravais lattice with $2 < Z < \infty$ the two averages are *not* the same, i.e., $\langle b_j \rangle_{S^{(0)}} \neq \langle b_0 \rangle_{S_0}$. This fact was already noted in Ref. [3] and was employed by them to solve the B-DMFT equations numerically. In fact, as proved in the Appendix, the two local averages obey the following exact relation in Matsubara representation:

$$\langle b_j \rangle_{S^{(0)}} = \langle b_0 \rangle_{S_0} \left(1 - \frac{G_{j0}}{G_{00}}\right), \tag{4}$$

where G_{ij} are two-site correlation functions on the corresponding translationally invariant lattice. Using the correct definition of ϕ, namely $\phi = \langle b_j \rangle_{S^{(0)}}$, and the identity $\sum_{j_1} t_{0j_1} G_{j_1 0}(\omega_n) = -1 + \omega_n G_{00}(\omega_n)$ [4] it immediately follows that the spurious hybridization term in κ introduced by the Bogoliubov shifts in Ref. [1] disappears again, whereby their self-consistency equations become identical to ours [2]. The claims by Anders *et al.* [1] concerning deficiencies of the original B-DMFT [2] are therefore invalid. In fact, their numerical results [1] are the solution of the B-DMFT equations previously derived by us in Ref. [2].

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Appendix: Proof of eq. (4)

The local correlation functions are determined via a functional derivative with respect to infinitesimally weak $U(1)$ symmetry breaking fields η_i which are added to the action, i.e., $\langle b_j(\tau)\rangle_{S^{(0)}} = \delta \ln Z^{(0)}/\delta\eta_j^*$. The second derivative gives the two-site correlation functions

$$\langle b_{j_1}(\tau_1) b^*_{j_2}(\tau_2)\rangle_{S^{(0)}} = \frac{\delta^2 \ln Z^{(0)}}{\delta\eta^*_{j_1}\delta\eta_{j_2}} = \frac{\delta}{\delta\eta_{j_2}}\langle b_{j_1}(\tau_1)\rangle_{S^{(0)}}. \quad (5)$$

In the linear regime of η_i the solution of (5) reads $\langle b_{j_1}(\tau_1)\rangle_{S^{(0)}} = \sum_{j_2}\langle b_{j_1}(\tau_1) b^*_{j_2}(\tau_2)\rangle_{S^{(0)}}\eta_{j_2}$. Employing the exact relation between two-site correlation functions defined on a lattice with a cavity, $G^{(0)}_{j_1 j_2}$, and on a translationally invariant lattice, $G_{j_1 j_2}$, respectively, namely $G^{(0)}_{j_1 j_2} = G_{j_1 j_2} - G_{j_1 0} G_{00}^{-1} G_{0 j_2}$ [4], we find

$$\begin{aligned}\langle b_{j_1}\rangle_{S^{(0)}} &= \sum_{j_2}(G_{j_1 j_2}\eta_{j_2} - G_{j_1 0}G_{00}^{-1}G_{0 j_2}\eta_{j_2}) \\ &= \phi_{j_1} - G_{j_1 0}G_{00}^{-1}\phi_0, \end{aligned} \quad (6)$$

where ϕ_{j_1} and ϕ_0 are local correlation functions at site j_1 and 0, respectively, on a translationally invariant lattice. In view of the translational invariance these quantities are the same, i.e., $\phi_{j_1} = \phi_0$, which proves Eq. (4).

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