Erratum: Inhomogeneous spectral moment sum rules for the retarded Green function and selfenergy of strongly correlated electrons or ultracold fermionic atoms in optical lattices [Phys. Rev. B 80, 115119 (2009)]

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We have found a mistake in derivation of the nonequilibrium generalization of the expressions for the nonhomogeneous moments for the Green's function and the self-energy. Namely, in the derivation of these moments for the nonequilibrium case when there is explicit time dependence of the Hamiltonian in the Schrödinger representation, $\mathcal{H}_s = \mathcal{H}_s(T)$, the second and higher time derivatives of an operator in the Heisenberg representation $i^n d^n O_H / dT^n$ cannot be simply substituted by the corresponding multiple commutator of the operator with the Hamiltonian $L^n O_H = [\cdots [[O_H, \mathcal{H}_H(T)], \mathcal{H}_H(T)], \mathcal{H}_H(T)]$. In this case, additional terms proportional to explicit time derivatives of $\mathcal{H}_{S}(T)$ have to be added. Indeed, while the first derivative of an operator can be substituted by a commutator with $\mathcal{H}_H(T)$: $idO_H/dT = [O_H, \mathcal{H}_H(T)]$, beginning with the second time derivative, one finds additional terms. For instance, the second derivative satisfies $i^2 dO_H/dT^2 = [i dO_H/dT, \mathcal{H}_H(T)]$ $+[O_H, i\partial \mathcal{H}_H(T)/\partial T] = L^2 O_H + [O_H, i\partial \mathcal{H}_H(T)/\partial T]$, where the partial time derivative in the last term is equal to $\mathcal{U}^{\dagger}(T)[\partial \mathcal{H}_{S}(T)/\partial T]\mathcal{U}(T)$, and $\mathcal{U}(T)$ is the time evolution operator from the initial time to time T (all partial derivatives of the Hamiltonian are written as a unitary transformation with respect to the evolution operator of the corresponding partial derivative of the Hamiltonian in the Schrödinger representation). Following this procedure, it is easy to obtain the expressions for the higher time derivatives of the operators, which will also contain additional terms. These additional terms will result in additional terms in the expressions for the nonequilibrium spectral moments for the retarded Green's function and the selfenergy, beginning from the third and the first order, respectively. It is possible to show that the sum of the additional terms equals zero in the case of the second Green's function moment, independent of the form of the Hamiltonian.¹

Thus, the expression for the third nonequilibrium retarded Green's function moment (not presented in the original paper) now acquires additional terms when compared to the equilibrium case:

$$\mu_{3}^{R}(\mathbf{R}_{i},\mathbf{R}_{j},T) = \operatorname{Re}\langle\{L^{3}c_{i}(T),c_{j}^{\dagger}(T)\}\rangle + \operatorname{Re}\frac{\iota}{4}[\langle\{[[c_{i}(T),\mathcal{H}_{H}'(T)],\mathcal{H}_{H}(T)],c_{j}^{\dagger}(T)\}\rangle - \langle\{[[c_{i}(T),\mathcal{H}_{H}'(T)],\mathcal{H}_{H}'(T)],c_{j}^{\dagger}(T)\}\rangle] - \operatorname{Re}\frac{1}{4}[\langle\{[c_{i}(T),\mathcal{H}_{H}''(T)],c_{j}^{\dagger}(T)\}\rangle - \langle\{c_{i}(T),[c_{i}^{\dagger}(T),\mathcal{H}_{H}''(T)]\}\rangle],$$
(1)

where $\mathcal{H}'_{H}(T) = \partial \mathcal{H}_{H}(T) / \partial T = \mathcal{U}^{\dagger}(T) [\partial \mathcal{H}_{S}(T) / \partial t] \mathcal{U}(T)$, $\mathcal{H}''_{H}(T) = \partial^{2} \mathcal{H}_{H}(T) / \partial T^{2} = \mathcal{U}^{\dagger}(T) [\partial^{2} \mathcal{H}_{S}(T) / \partial T^{2}] \mathcal{U}(T)$ are explicit partial time derivatives of the Hamiltonian. The correction, which consists of the last two terms in Eq. (1), results in the following nonequilibrium generalization of Eq. (11) for the third moment of the retarded Green's function:

$$\begin{split} \mu_{3}^{R}(\mathbf{R}_{i},\mathbf{R}_{j},T) &= -\sum_{kl} t_{ik}(T)t_{kl}(T)t_{lj}(T) - [\mu_{i}(T) - U_{i}(T)n_{fi}(T)]\sum_{l} t_{il}(T)t_{lj}(T) - \sum_{l} t_{il}(T)[\mu_{l}(T) - U_{l}(T)n_{fl}(T)]t_{lj}(T) \\ &- \sum_{l} t_{il}(T)t_{lj}(T)[\mu_{j}(T) - U_{j}(T)n_{fj}(T)] - [\mu_{i}(T) - U_{i}(T)n_{fi}(T)]^{2}t_{ij}(T) - [\mu_{i}(T) - U_{i}(T)n_{fi}(T)]t_{ij}(T)]t_{ij}(T) \\ &- U_{j}(T)n_{fj}(T)] - t_{ij}(T)[\mu_{j}(T) - U_{j}(T)n_{fj}(T)]^{2} - U_{i}^{2}(T)n_{fi}(T)[1 - n_{fi}(T)]t_{ij}(T) \\ &- U_{i}(T)t_{ij}(T)U_{j}(T)[\langle f_{i}^{\dagger}(T)f_{i}(T)f_{j}^{\dagger}(T)f_{j}(T) - n_{fi}(T)n_{fj}(T)] - t_{ij}(T)U_{j}^{2}(T)n_{fj}(T)[1 - n_{fj}(T)] \\ &- U_{i}(T)t_{ij}(T)U_{j}(T)[\langle f_{i}^{\dagger}(T)f_{i}(T)f_{j}^{\dagger}(T)f_{j}(T) - n_{fi}(T)n_{fj}(T)] - t_{ij}(T)U_{j}^{2}(T)n_{fj}(T)[1 - n_{fj}(T)] \\ &- \delta_{ij}[(\mu_{i}(T) - U_{i}(T)n_{fi}(T))^{3} + 3U_{i}^{2}(T)\mu_{i}(T)n_{fi}(T)(1 - n_{fi}(T)) - U_{i}^{3}(T)n_{fi}(T)(1 - n_{fi}(T))(1 + n_{fi}(T))] \\ &+ \delta_{ij}U_{i}(T)\sum_{l,m} [t_{mi}^{f}(T)t_{m}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T) + t_{mi}^{f}(T)f_{mi}^{f}(T)f_{i}(T) - 2t_{mi}^{f}(T)t_{i}^{f}(T)f_{i}^{f}(T)f_{m}(T)\rangle] \\ &+ \delta_{ij}U_{i}(T)\sum_{l} [\mu_{i}^{f}(T) - \mu_{i}^{f}(T)][t_{i}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T) + t_{mi}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T)\rangle] \\ &+ \delta_{ij}U_{i}(T)\sum_{l} U_{l}(T)[t_{i}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T)c_{i}^{\dagger}(T)c_{i}(T)\rangle] \\ &+ \delta_{ij}U_{i}(T)\sum_{l} U_{l}(T)[t_{i}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T)c_{i}^{\dagger}(T)c_{i}(T)\rangle] \\ &+ U_{i}(T)U_{j}(T)[t_{i}^{f}(T)\langle f_{i}^{\dagger}(T)f_{i}(T)c_{i}^{\dagger}(T)c_{i}(T)\rangle] \\ &+ U_{i}(T)U_{j}(T)[t_{i}^{f}(T)\langle f_{i}^{\dagger}(T)c_{i}^{\dagger}(T)c_{i}(T)\rangle] \\ &+ \frac{1}{4}\operatorname{Re}i\sum_{l} \left[\frac{dt_{il}(T)}{dT}t_{lj}(T) - t_{il}(T)\frac{dt_{lj}(T)}{dT} \right] \\ &+ \frac{1}{4}\operatorname{Re}i\sum_{l} \left[\frac{dt_{il}(T)}{dT}t_{lj}(T) - t_{il}(T)\frac{dt_{lj}(T)}{dT} \right] \\ &+ \frac{1}{4}\operatorname{Re}it_{ij}(T) \left[\frac{d\mu_{i}(T)}{dT} - \frac{d\mu_{i}(T)}{dT} \right] \\ &+ \frac{1}{4}\operatorname{Re}it_{ij}(T) \left[\frac{d\mu_{i}(T)}{dT} - \frac{d\mu_{i}(T)}{dT} \right] \\ &+ \frac{1}{4}\operatorname{Re}it_{ij}(T) \left[\frac{d\mu_{i}(T)}{dT} \right] \\$$

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$$+ \frac{1}{4} \operatorname{Re} i \frac{dt_{ij}(T)}{dT} [U_i(T)n_i(T) - U_j(T)n_j(T)] - \frac{1}{4} \operatorname{Re} it_{ij}(T) \left[\frac{dU_i(T)}{dT}n_i(T) - \frac{dU_j(T)}{dT}n_j(T) \right] + \frac{1}{2} \operatorname{Re} \frac{d^2 t_{ij}(T)}{dT^2} \\ + \frac{1}{2} \delta_{ij} \left(\frac{d^2 \mu_i(T)}{dT^2} - n_i(T) \frac{d^2 U_i(T)}{dT^2} \right),$$

where Re stands for the real part. We also find the corrected formula for the first moment of the retarded self-energy [Eq. (28)] is

$$\begin{split} C_{1}^{R}(\mathbf{R}_{1},\mathbf{R}_{2},T) &= \delta_{ij}U_{i}^{2}(T)n_{fi}(T)(1-n_{fi}(T))[U_{i}(T)\{1-n_{fi}(T)\} - \mu_{i}(T)] \\ &+ \delta_{ij}U_{i}(T)\sum_{m,l} [t_{ml}^{f}(T)t_{lm}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)\rangle + t_{lm}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)\rangle - 2t_{lm}^{f}(T)t_{ll}^{f}(T)\langle f_{l}^{\dagger}(T)f_{m}(T)\rangle] \\ &+ \delta_{ij}U_{i}(T)\sum_{l} (\mu_{l}(T) - \mu_{i}(T))[t_{li}^{f}(T)\langle f_{l}^{\dagger}(T)f_{i}(T)\rangle + t_{ll}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)\rangle] + \delta_{ij}U_{i}^{2}(T)\sum_{l} t_{ll}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)\rangle \\ &+ \delta_{ij}\frac{1}{4}\frac{d^{2}[U_{i}(T)n_{fi}(T)]}{dT^{2}} - \delta_{ij}U_{i}(T)\sum_{l} U_{l}(T)[t_{l}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle + t_{ll}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle \\ &+ \delta_{ij}\frac{1}{4}\frac{d^{2}[U_{i}(T)n_{fi}(T)]}{dT^{2}} - \delta_{ij}U_{i}(T)\sum_{l} U_{l}(T)[t_{l}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle + t_{ll}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle] \\ &- U_{i}(T)t_{ij}(T)U_{j}(T)[\langle f_{l}^{\dagger}(T)f_{l}(T)f_{l}^{\dagger}(T)f_{j}(T)\rangle - \langle n_{fi}^{\dagger}(T)n_{fj}(T)\rangle] \\ &+ U_{i}(T)U_{j}(T)[t_{j}^{f}(T)f_{i}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle + t_{lj}^{f}(T)\langle f_{l}^{\dagger}(T)f_{l}(T)c_{l}^{\dagger}(T)c_{l}(T)\rangle] \\ &+ \frac{1}{4}\operatorname{Re}i\sum_{l} \left[\frac{dt_{il}(T)}{dT}t_{ij}(T) - t_{il}(T)\frac{dt_{ij}(T)}{dT} \right] + \frac{1}{4}\operatorname{Re}it_{ij}(T) \left[\frac{d\mu_{i}(T)}{dT} - \frac{d\mu_{j}(T)}{dT} \right] - \frac{1}{4}\operatorname{Re}i\frac{dt_{ij}(T)}{dT}[\mu_{i}(T) - \mu_{j}(T)] \\ &+ \frac{1}{2}\operatorname{Re}\frac{d^{2}t_{ij}(T)}{dT^{2}} + \frac{1}{2}\delta_{ij} \left(\frac{d^{2}\mu_{i}(T)}{dT^{2}} - n_{i}(T)\frac{d^{2}U_{i}(T)}{dT^{2}} \right). \end{split}$$

In both cases, the additional terms can be identified as depending on derivatives of the parameters of the Hamiltonian with respect to time.

These corrections do not affect the main analytical and numerical results of the paper—the expressions for the local equilibrium Green's function and self-energy moments. This is because the only inhomogeneous nonequilibrium problem we considered was that of a charge density wave in a spatially uniform electric field, where the inhomogeneity is in the interaction term, and the time dependence is in the hopping. That case can be shown to have all extra terms vanish, so the results given in the paper are correct.

¹V. Turkowski and J. K. Freericks, Phys. Rev. B 82, 119904(E) (2010).