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Erratum: Nonequilibrium sum rules for the retarded self-energy of strongly correlated electrons [Phys. Rev. B 77, 205102 (2008)]

V. Turkowski and J. K. Freericks

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We have discovered a subtle error in our derivation of the nonequilibrium moments when the Hamiltonian in the Schrödinger representation has explicit time dependence. The problem arises from the fact that when we take the second or higher time derivatives of an operator in the Heisenberg picture, the operator inherits some additional time dependence from the explicit time dependence of the Schrödinger Hamiltonian and the way in which the operator is evolved as a function of time. This results in terms proportional to derivatives of the Hamiltonian in the Schrödinger representation. We find one missing term in the expressions for the third momentum-dependent spectral moment for the retarded Green's function and for the first momentum-dependent retarded self-energy moment, $\mu_3^R(\mathbf{k},T)$ and $C_1^R(\mathbf{k},T)$, in Eqs. (25) and (60) and three new terms in the expressions for the third momentum-dependent and local spectral moments for the lesser Green's function $\mu_3^<(\mathbf{k},T)$ and $\mu_3^<(T)$, in Eqs. (33) and (37). These terms come from the direct time derivative of the Hamiltonian in the Schrödinger picture in Eq. (13). More specifically, one cannot simply replace high order time derivatives of an operator O_H in the Heisenberg picture $i^n d^n O_H/dT^n$ (which has no explicit time dependence in the Schrödinger picture) by the multiple commutator operator $L^n O_H=[\cdots[[O_H,\mathcal{H}_H(T)],\mathcal{H}_H(T)]\cdots\mathcal{H}_H(T)]$ [defined after Eq. (21)], because the expression for the moments (beginning with $n=2$) will have additional terms proportional to time derivatives of the Hamiltonian (in the Schrödinger representation) with respect to T. Namely, the first derivative of an operator that has no time dependence in the Schrödinger picture can be substituted by a commutator with the Hamiltonian $idO_H/dT=[O_H,\mathcal{H}_H(T)]=L^1O_H$. However, already the second derivative acquires an additional term: $i^2dO_H/dT^2=[idO_H/dT,\mathcal{H}_H(T)]+[O_H,i\partial\mathcal{H}_H(T)/\partial T]=L^2O_H+[O_H,i\partial\mathcal{H}_H(T)/\partial T]$, where $\partial\mathcal{H}_H(T)/\partial T=\mathcal{U}^\dagger(T)[\partial\mathcal{H}_S(T)/\partial T]\mathcal{U}(T)$ is the additional time dependence, with $\mathcal{U}(T)$ the time evolution operator from the initial time to time T. These results can be easily generalized to the case of higher derivatives. While these additional terms do not contribute to the lowest Green's function moments, they can be nonzero for higher order Green's function moments (i.e., for $n\geqslant 3$). In the case of local moments, many of these extra terms end up vanishing, namely, the local retarded Green's function moments have no extra terms (through third order), nor do the local retarded self-energy moments (through first order), but the local lesser Green's function moments do have extra terms starting at third order. To evaluate the corrections to the spectral moments we simply need to determine the form of these extra terms which involve derivatives of the Peierls' substituted band structure with respect to time. For example, the commutator relations in Eqs. (16), (17), (20), and (21) are modified as follows:

$$\mu_2^R(\mathbf{k},T)=\frac{1}{4}[\langle\{L^2c_k(T),c_k^\dagger(T)\}\rangle-2\langle\{L^1c_k(T),L^1c_k^\dagger(T)\}\rangle+\langle\{c_k(T),L^2c_k^\dagger(T)\}\rangle]+\frac{i}{4}(\langle\{[c_k(T),\mathcal{H}_H'(T)],c_k^\dagger(T)\}\rangle+\langle\{c_k(T),[c_k^\dagger(T),\mathcal{H}_H'(T)]\}\rangle), \tag{16}$$

$$\begin{aligned}\mu_3^R(\mathbf{k},T)=&\frac{1}{8}[\langle\{L^3c_k(T),c_k^\dagger(T)\}\rangle-3\langle\{L^2c_k(T),L^1c_k^\dagger(T)\}\rangle+3\langle\{L^1c_k(T),L^2c_k^\dagger(T)\}\rangle-\langle\{c_k(T),L^3c_k^\dagger(T)\}\rangle]\\&+\frac{i}{8}(\langle\{[[c_k(T),\mathcal{H}_H'(T)],\mathcal{H}_H(T)],c_k^\dagger(T)\}\rangle+3\langle[[c_k(T),\mathcal{H}_H(T)],\mathcal{H}_H'(T)],c_k^\dagger(T)\}\rangle-4\langle\{[c_k(T),\mathcal{H}_H'(T)],[c_k^\dagger(T),\mathcal{H}_H(T)]\}\rangle\\&+4\langle\{[c_k(T),\mathcal{H}_H(T)],[c_k^\dagger(T),\mathcal{H}_H'(T)]\}\rangle-3\langle\{c_k(T),[[c_k^\dagger(T),\mathcal{H}_H(T)],\mathcal{H}_H'(T)]\}\rangle-\langle\{c_k(T),[[c_k(T),\mathcal{H}_H'(T)],\mathcal{H}_H(T)]\}\rangle)\\&-\frac{1}{4}(\langle\{[c_k(T),\mathcal{H}_H''(T)],c_k^\dagger(T)]\}\rangle-\langle\{c_k(T),[c_k^\dagger(T),\mathcal{H}_H''(T)]\}\rangle),\end{aligned} \tag{17}$$

$$\mu_2^<(\mathbf{k},T)=\frac{1}{2}[\langle c_k^\dagger(T)L^2c_k(T)\rangle-2\langle(L^1c_k^\dagger(T))(L^1c_k(T))\rangle+\langle(L^2c_k^\dagger(T))c_k(T)\rangle],$$

$$+\frac{i}{2}(\langle c_k^\dagger(T)[c_k(T),\mathcal{H}_H'(T)]\rangle+\langle[c_k^\dagger(T),\mathcal{H}_H'(T)]c_k(T)\rangle), \tag{20}$$

$$\mu_3^<(\mathbf{k},T)=\frac{1}{4}[\langle c_k^\dagger(T)L^3c_k(T)\rangle-3\langle(L^1c_k^\dagger(T))(L^2c_k(T))\rangle+3\langle(L^2c_k^\dagger(T))(L^1c_k(T))\rangle-\langle(L^3c_k^\dagger(T))c_k(T)\rangle],$$

$$+\frac{i}{4}[\langle c_k^\dagger(T)[[c_k(T),\mathcal{H}_H'(T)],\mathcal{H}_H(T)]\rangle + 2\langle c_k^\dagger(T)[[c_k(T),\mathcal{H}_H(T)],\mathcal{H}_H'(T)]\rangle - 3\langle\{[c_k^\dagger(T),\mathcal{H}_H(T)],[c_k(T),\mathcal{H}_H'(T)]\}\rangle$$
$$+3\langle[c_k^\dagger(T),\mathcal{H}_H'(T)][c_k(T),\mathcal{H}_H(T)]\rangle - \langle[[c_k^\dagger(T),\mathcal{H}_H'(T)],\mathcal{H}_H(T)]c_k(T)\rangle - 2\langle[[c_k(T),\mathcal{H}_H(T)],\mathcal{H}_H'(T)]c_k(T)\rangle]$$
$$-\frac{1}{4}(\langle c_k^\dagger(T)[c_k(T),\mathcal{H}_H''(T)]\rangle - \langle[c_k^\dagger(T),\mathcal{H}_H''(T)]c_k(T)\rangle), \tag{21}$$

where $\mathcal{H}_H'(T)=\partial\mathcal{H}_H(T)/\partial T$ and $\mathcal{H}_H''(T)=\partial^2\mathcal{H}_H(T)/\partial T^2$ are the first and the second direct time derivatives of the Hamiltonian inherited from the time dependence in the Schrödinger representation, as described above. While it may appear that the moments should be modified already at second order, the contributions proportional to the derivative of the Hamiltonian cancel at second order for the case considered here. For the retarded second moment in Eq. (16), one can show that the sum of the derivative terms can be rewritten as $i\langle[\{c_{\mathbf{k}}^\dagger(T),c_{\mathbf{k}}(T)\},\mathcal{H}'(T)]\rangle/4=0$ because the anticommutator is a number which commutes with all other operators. Hence, the extra terms always vanish for $\mu_2^R(\mathbf{k},T)$ regardless of the specific form of the derivative of the Hamiltonian. Similarly, the extra terms vanish for $\mu_2^<(\mathbf{k},T)$ whenever the derivative of the Hamiltonian can be expressed as sums of (possibly momentum-dependent) functions of time that multiply the number operator in momentum space. Hence the corrections start at the third moment for nonequilibrium problems described by the Peierls' substitution with respect to a spatially uniform vector potential since this Hamiltonian satisfies the required form for the derivative of the Hamiltonian.

The corrected formula for the momentum-dependent third spectral moment of the retarded Green's function is

$$\mu_3^R(\mathbf{k},T)=[\varepsilon(k-eA(T))-\mu]^3+3U[\varepsilon(k-eA(T))-\mu]^2n_f+3U^2[\varepsilon(k-eA(T))-\mu]n_f+U^2\sum_{p,q}[\varepsilon^f(p+q-eA(T))$$
$$-2\varepsilon^f(p-eA(T))+\varepsilon^f(p-q-eA(T))]\langle f_p^\dagger f_p\rangle(T)-U^2\sum_{p,q,q'}[\varepsilon^f(p+q-eA(T))-\varepsilon^f(p+q+q'-eA(T))-\varepsilon^f(p-eA(T))$$
$$+\varepsilon^f(p+q'-eA(T))]\langle f_{p+q+q'}^\dagger f_p c_{k-q}^\dagger c_{k+q'}\rangle(T)+U^2\sum_{p,p',q}[\varepsilon(k+q-eA(T))-\varepsilon(k-eA(T))+\varepsilon^f(p'-eA(T))$$
$$-\varepsilon^f(p'-q-eA(T))+2\varepsilon^f(p-eA(T))-2\varepsilon^f(p+q-eA(T))]\langle f_{p'-q}^\dagger f_{p'} f_{p+q}^\dagger f_p\rangle(T)+U^3n_f-\frac{1}{4}\frac{d^2}{dT^2}\varepsilon(k-eA(T)), \tag{25}$$

with the last term being the modification. The momentum-dependent third moment of the lesser Green's function becomes

$$\mu_3^<(\mathbf{k},T)=2[\varepsilon(k-eA(T))-\mu]^3\langle c_k^\dagger c_k\rangle(T)+2U(\varepsilon(k-eA(T))-\mu)^2\sum_{p,q}\langle c_k^\dagger c_{k+q} f_{p+q}^\dagger f_p\rangle(T)$$
$$+2U\sum_{p',p}[\varepsilon(k-eA(T))+\varepsilon(p-eA(T))-2\mu+\varepsilon^f(p'-eA(T))$$
$$-\varepsilon^f(p'+p-k-eA(T))](\varepsilon(p-eA(T))-\mu)\langle c_k^\dagger c_p f_{p'+p-k}^\dagger f_{p'}\rangle(T)+2U\sum_{q',p}[\varepsilon(k-eA(T))$$
$$+\varepsilon(k+q'-eA(T))-2\mu+\varepsilon^f(p-eA(T))-\varepsilon^f(p+q'-eA(T))](\varepsilon^f(p-eA(T))$$
$$-\varepsilon^f(p+q'-eA(T)))\langle c_k^\dagger c_{k+q'} f_{p+q'}^\dagger f_p\rangle(T)+2U^2\sum_{p',q',p,q}[\varepsilon(k-eA(T))+\varepsilon(k+q'-eA(T))-2\mu+\varepsilon^f(p'-eA(T))$$
$$-\varepsilon^f(p'+q'-eA(T))]\langle f_{p+q}^\dagger f_p f_{p'+q'}^\dagger f_{p'} c_k^\dagger c_{k+q'+q}\rangle(T)+2U^2\sum_{q',p,q,k'}[\varepsilon^f(p+q-eA(T))$$
$$-\varepsilon^f(p+q+q'-eA(T))-\varepsilon^f(p-eA(T))+\varepsilon^f(p+q'-eA(T))]\langle f_{p+q+q'}^\dagger f_p c_k^\dagger c_{k+q'} c_{k'-q}^\dagger c_{k'}\rangle(T)$$
$$+2U^2\sum_{p',q',p,q}[\varepsilon(k+q+q'-eA(T))-\mu-\varepsilon^f(p'+q'-eA(T))+\varepsilon^f(p'-eA(T))-\varepsilon^f(p+q-eA(T))$$
$$+\varepsilon^f(p-eA(T))]\langle f_{p'+q'}^\dagger f_{p'} f_{p+q}^\dagger f_p c_k^\dagger c_{k+q+q'}\rangle(T)+2U^3\sum_{p',q',p,q,P,Q}\langle f_{P+Q}^\dagger f_P f_{p'+q'}^\dagger f_{p'} f_{p+q}^\dagger f_p c_k^\dagger c_{Q+k+q+q'}\rangle(T)$$
$$-\frac{1}{2}\frac{d^2\varepsilon(k-eA(T))}{dT^2}\langle c_k^\dagger c_k\rangle(T)+\mathrm{Re}\,\frac{i}{2}U\sum_{p,q}\langle f_{p+q}^\dagger f_p c_k^\dagger c_{k+q}\rangle\frac{d}{dT}[\varepsilon(k+q-eA(T))-\varepsilon(k-eA(T))+\varepsilon^f(p-eA(T))$$
$$-\varepsilon^f(p+q-eA(T))]-\mathrm{Re}\,\frac{i}{2}U\sum_{p,q}\langle f_{p+q}^\dagger f_p c_{k-q}^\dagger c_k\rangle\frac{d}{dT}[\varepsilon(k-q-eA(T))-\varepsilon(k-eA(T))+\varepsilon^f(p+q-eA(T))$$
$$-\varepsilon^f(p-eA(T))], \tag{33}$$

with the changes in the last three terms and Re denotes the real part. And the first moment of the momentum-dependent retarded self-energy becomes

$$
\begin{aligned}
C_1^R(\mathbf{k},T) = {} & U^2 n_f(1-n_f)[U(1-n_f)-\mu] + U^2\sum_{p,q}[\varepsilon^f(p+q-eA(T)) - 2\varepsilon^f(p-eA(T)) + \varepsilon^f(p-q-eA(T))]\langle f_p^\dagger f_p\rangle(T) \\
& - U^2\sum_{p,q,q'}[\varepsilon^f(p+q-eA(T)) - \varepsilon^f(p+q+q'-eA(T)) - \varepsilon^f(p-eA(T)) + \varepsilon^f(p+q'-eA(T))]\langle f^\dagger_{p+q+q'} f_p c^\dagger_{k-q} c_{k+q'}\rangle(T) \\
& + U^2\sum_{p,p',q}[\varepsilon(k+q-eA(T)) - \varepsilon(k-eA(T)) + \varepsilon^f(p'-eA(T)) - \varepsilon^f(p'-q-eA(T)) + 2\varepsilon^f(p-eA(T)) \\
& - 2\varepsilon^f(p+q-eA(T))]\langle f^\dagger_{p'-q} f_{p'} f^\dagger_{p+q} f_p\rangle(T) - \frac{1}{4}\frac{d^2}{dT^2}\varepsilon(k-eA(T)),
\end{aligned} \tag{60}
$$

with the last term being the correction. Note that all of the extra terms in the retarded Green's function and retarded self-energy moments cancel when summed over momentum, so the local-moment expressions in Eqs. (29) and (62) are unchanged. Equation (37) must be modified, however, by these new terms, which give additional contributions to the local third moment of the lesser Green's function and can be straightforwardly evaluated as

$$
\begin{aligned}
\mu_3^<(T) = {} & -2\sum_{i,j,l,m}\tilde{t}_{il}\tilde{t}_{lm}\tilde{t}_{mj}\langle c_i^\dagger c_j\rangle(T) - 6\mu\sum_{i,j,l}\tilde{t}_{il}\tilde{t}_{lj}\langle c_i^\dagger c_j\rangle(T) - 6\mu^2\sum_{i,j}\tilde{t}_{ij}\langle c_i^\dagger c_j\rangle(T) - 2\mu^3\sum_i\langle c_i^\dagger c_i\rangle(T) + 2U\sum_{i,l,j}\tilde{t}_{il}\tilde{t}_{lj}\langle c_i^\dagger c_j f_j^\dagger f_j\rangle(T) \\
& + 2(3U\mu^2 - 3U^2\mu + U^3)\sum_i\langle f_i^\dagger f_i c_i^\dagger c_i\rangle(T) + 6U\mu\sum_{i,j}\tilde{t}_{ij}\langle c_i^\dagger c_j f_j^\dagger f_j\rangle(T) + 6U\mu\sum_{i,j}\tilde{t}_{ij}\langle c_i^\dagger c_j f_i^\dagger f_i\rangle(T) \\
& - 2U^2\sum_{i,j}\tilde{t}_{ij}\langle f_j^\dagger f_j c_i^\dagger c_j\rangle(T) - 2U^2\sum_{i,j}\tilde{t}_{ij}\langle f_i^\dagger f_i c_i^\dagger c_j\rangle(T) + 2U\sum_{i,l,j}\tilde{t}_{ij}\tilde{t}_{jl}\langle c_i^\dagger c_l f_j^\dagger f_j\rangle(T) + 2U\sum_{i,l,j}\tilde{t}_{il}\tilde{t}_{lj}\langle c_i^\dagger c_j f_i^\dagger f_i\rangle(T) \\
& - 2U^2\sum_{i,j}\tilde{t}_{ij}\langle f_j^\dagger f_j f_i^\dagger f_i c_i^\dagger c_j\rangle(T) + 2U\sum_{i,j,l}\tilde{t}_{ij}\tilde{t}^f_{il}\langle c_i^\dagger c_j f_i^\dagger f_l\rangle(T) - 2U\sum_{i,j,l}\tilde{t}_{ij}\tilde{t}^f_{li}\langle c_i^\dagger c_j f_l^\dagger f_i\rangle(T) + 2U\mu\sum_{i,j}\tilde{t}^f_{ij}\langle c_i^\dagger c_i f_i^\dagger f_j\rangle(T) \\
& - 2U\mu\sum_{i,j}\tilde{t}^f_{ji}\langle c_i^\dagger c_i f_j^\dagger f_i\rangle(T) + 2U\sum_{i,j,l}\tilde{t}^f_{il}\tilde{t}^f_{lj}\langle c_i^\dagger c_i f_i^\dagger f_j\rangle(T) + 2U\sum_{i,j,l}\tilde{t}^f_{il}\tilde{t}^f_{lj}\langle c_j^\dagger c_j f_i^\dagger f_j\rangle(T) - 4U\sum_{i,j,l}\tilde{t}^f_{ji}\tilde{t}^f_{il}\langle c_i^\dagger c_i f_j^\dagger f_l\rangle(T) \\
& - 2U^2\sum_{i,j}\tilde{t}^f_{ij}[\langle f_i^\dagger f_i f_i^\dagger f_j c_i^\dagger c_i\rangle(T) - \langle f_j^\dagger f_j f_i^\dagger f_j c_j^\dagger c_j\rangle(T)] - 4U^2\sum_{i,j}\tilde{t}^f_{ij}\langle f_i^\dagger f_j c_i^\dagger c_i c_j^\dagger c_j\rangle(T) + 4U^2\sum_{i,j}\tilde{t}^f_{ij}\langle f_i^\dagger f_j c_j^\dagger c_j\rangle(T) \\
& + \frac{1}{2}\sum_{i,j}\frac{d^2\tilde{t}_{ij}(T)}{dT^2}\langle c_i^\dagger c_j\rangle(T) + \mathrm{Re}\, iU\sum_{i,j}\frac{d\tilde{t}_{ij}(T)}{dT}(\langle f_j^\dagger f_j c_i^\dagger c_j\rangle(T) - \langle f_i^\dagger f_i c_i^\dagger c_j\rangle(T)) \\
& + \mathrm{Re}\, iU\sum_{i,j}\frac{d\tilde{t}^f_{ij}(T)}{dT}(\langle f_i^\dagger f_j c_j^\dagger c_j\rangle(T) - \langle f_i^\dagger f_j c_i^\dagger c_i\rangle(T)),
\end{aligned} \tag{37}
$$

with the terms with derivatives with respect to time being the new terms.

These corrections do not affect the main results of the paper, namely the analytical expressions for the local retarded Green's function and self-energy moments and their numerical tests (due to cancellations of the extra terms when summed over momentum). But they do modify the formal expressions for these moments, especially for highest-order momentum-dependent moments.