Specific heat in QUEST

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We are interested in computing the specific heat of

$$H = \sum_{ij\sigma} h^\sigma_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \tag{1}$$

using $\langle H^2 \rangle - \langle H \rangle^2$. We break H^2 in four pieces $H^2 = TT + TU + UT + UU$ with

$$TT = \sum_{ij\sigma} \sum_{kh\alpha} h^\sigma_{ij} h^\alpha_{kh} c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\alpha} c_{h\alpha} \tag{2}$$

$$TU = \sum_{ij\sigma} \sum_k h^\sigma_{ij} U_k c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{k\uparrow} c_{k\uparrow} c^\dagger_{k\downarrow} c_{k\downarrow} \tag{3}$$

$$UT = \sum_{ij\sigma} \sum_k h^\sigma_{ij} U_k c^\dagger_{k\uparrow} c_{k\uparrow} c^\dagger_{k\downarrow} c_{k\downarrow} c^\dagger_{i\sigma} c_{j\sigma} \tag{4}$$

$$UU = \sum_{ik} U_i U_k c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{k\uparrow} c_{k\uparrow} c^\dagger_{k\downarrow} c_{k\downarrow}. \tag{5}$$

For a given configuration of auxiliary fields, the expectation value can be computed via Wick's theorem. To do so, it is useful to introduce the following quantities

$$G^\sigma_{ji} = \langle c_{j\sigma} c^\dagger_{i\sigma} \rangle \tag{6}$$

$$n_{i\sigma} = \langle c^\dagger_{i\sigma} c_{i\sigma} \rangle \tag{7}$$

$$A^\sigma_{ji} = \sum_k G^\sigma_{ik} h^\sigma_{kj} \tag{8}$$

We then have (the notation closely mirrors the one used in the code)

$$\begin{aligned} \langle TT \rangle &= \sum_{ij\sigma} \sum_{kh\alpha} h^\sigma_{ij} h^\alpha_{kh} \Big[\langle c^\dagger_{i\sigma} c_{j\sigma} \rangle \langle c^\dagger_{k\alpha} c_{h\alpha} \rangle + \langle c^\dagger_{i\sigma} c_{h\alpha} \rangle \langle c_{j\sigma} c^\dagger_{k\alpha} \rangle \Big] \\ &= \Big[\sum_{j\sigma} (h^\sigma_{jj} - A^\sigma_{jj}) \Big]^2 + \sum_{hj\sigma} (h^\sigma_{hj} - A^\sigma_{hj}) A^\sigma_{jh} \end{aligned} \tag{9}$$

$$\begin{aligned} \langle TU \rangle &= \sum_{ij\sigma} \sum_k h^\sigma_{ij} U_k \Big[\langle c^\dagger_{i\sigma} c_{j\sigma} \rangle \langle c^\dagger_{k\uparrow} c_{k\uparrow} \rangle \langle c^\dagger_{k\downarrow} c_{k\downarrow} \rangle + \langle c^\dagger_{i\sigma} c_{k\sigma} \rangle \langle c_{j\sigma} c^\dagger_{k\sigma} \rangle \langle c^\dagger_{k-\sigma} c_{k-\sigma} \rangle \Big] \\ &= \Big[\sum_k U_k n_{k\uparrow} n_{k\downarrow} \Big] \Big[\sum_{j\sigma} h^\sigma_{jj} - A^\sigma_{jj} \Big] + \sum_{jk\sigma} U_k n_{k-\sigma} (h^\sigma_{kj} - A^\sigma_{kj}) G^\sigma_{jk} \end{aligned} \tag{10}$$

$$\begin{aligned} \langle UT \rangle &= \sum_{ij\sigma} \sum_k h^\sigma_{ij} U_k \Big[\langle c^\dagger_{i\sigma} c_{j\sigma} \rangle \langle c^\dagger_{k\uparrow} c_{k\uparrow} \rangle \langle c^\dagger_{k\downarrow} c_{k\downarrow} \rangle + \langle c^\dagger_{k\sigma} c_{j\sigma} \rangle \langle c_{k\sigma} c^\dagger_{i\sigma} \rangle \langle c^\dagger_{k-\sigma} c_{k-\sigma} \rangle \Big] \\ &= \Big[\sum_k U_k n_{k\uparrow} n_{k\downarrow} \Big] \Big[\sum_{j\sigma} h^\sigma_{jj} - A^\sigma_{jj} \Big] - \sum_{jk\sigma} U_k n_{k-\sigma} A^\sigma_{kj} G^\sigma_{jk} + \sum_{k\sigma} U_k n_{k-\sigma} A^\sigma_{kk} \end{aligned} \tag{11}$$

$$\begin{aligned} \langle UU \rangle &= \sum_{ik} U_i U_k \Big[\langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle \langle c^\dagger_{k\uparrow} c_{k\uparrow} \rangle + \langle c^\dagger_{i\uparrow} c_{k\uparrow} \rangle \langle c^\dagger_{i\uparrow} c_{k\uparrow} \rangle \Big] \Big[\langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle \langle c^\dagger_{k\downarrow} c_{k\downarrow} \rangle + \langle c^\dagger_{i\downarrow} c_{k\downarrow} \rangle \langle c^\dagger_{i\downarrow} c_{k\downarrow} \rangle \Big] \\ &= \sum_{ik} U_i U_k \Big[n_{i\uparrow} n_{k\uparrow} + (\delta_{ik} - G^\uparrow_{ki}) G^\uparrow_{ik} \Big] \Big[n_{i\downarrow} n_{k\downarrow} + (\delta_{ik} - G^\downarrow_{ki}) G^\downarrow_{ik} \Big] \end{aligned} \tag{12}$$

What gets computed in QUEST

QUEST works in the grand-canonical ensemble with a specific heat computed as

$$C_\mu = \frac{1}{N_s}\frac{\partial\langle H-\mu N\rangle}{\partial T} = \frac{\langle (H-\mu N)^2\rangle - \langle (H-\mu N)\rangle^2}{N_s T^2} \tag{13}$$

where N_s is the number of unit cell in the cluster. The QUEST Hamiltonian is written as

$$H = \sum_{i\sigma}\epsilon_i^\sigma c_{i\sigma}^\dagger c_{i\sigma} - \sum_\sigma\sum_{i\neq j} t_{ij}^\sigma c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U_i(n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2) \tag{14}$$

with ϵ, t and U read from the `.geom` file. Note the hybrid convention for the sign of the single particle matrix elements that depends on whether the matrix element is diagonal or not (would it be better to homogenize this?). We can write $H-\mu N$ in the form of Eq.1, and use the previous equation for $\langle H^2\rangle$, provided we set

$$h_{ij}^\sigma = -t_{ij}^\sigma + \delta_{ij}(\epsilon_i^\sigma - \mu - U_i/2). \tag{15}$$

Eq.14 also contains a constant energy shift, $\sum_i U_i/4$, whose contributions gest exactly canceled when evaluating the specific heat. At the moment QUEST omits this contribution from the energy as well.

Where things are computted in QUEST

In `DQMC_Phy0_Meas`

- $\frac{\langle U\rangle}{N_s} = \frac{1}{N_s}\sum_i U_i c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow}^\dagger c_{i\uparrow}$ computed and accumulated in `Phy0%meas(P0_NUD,tmp)`.
- $\frac{\langle T\rangle}{N_s} = \frac{1}{N_s}\Big[-\sum_{ij} t_{ij}^\sigma\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle + \sum_{i\sigma}(-\mu_{i\sigma} - U/2)c_{i\sigma}^\dagger c_{i\sigma}\Big]$ with $\mu_{i\sigma} = \mu - \epsilon_{i\sigma}$ computed and accumulated in `Phy0%meas(P0_KE,tmp)`.
- $\frac{\beta^2}{N_s}\langle (T+U)^2\rangle$ computed and accumulated in `Phy0%meas(P0_CV,tmp)`

In `DQMC_Phy0_Avg`

- $\frac{1}{N_s}\langle U\rangle$ is permanently stored in `Phy0%meas(P0_NUD,idx)`
- $\frac{1}{N_s}\langle T\rangle$ is permanently stored in `Phy0%meas(P0_KE,idx)`
- $\frac{1}{N_s}\langle T+U\rangle$ is permanently stored in `Phy0%meas(P0_ENERGY,idx)`
- $\frac{1}{N_s}\beta^2\langle (T+U)^2\rangle$ is permanently stored in `Phy0%meas(P0_CV,idx)`

In `DQMC_Phy0_GetErr`, averages and errors are computed. This is where the value for the specific heat is finally assembled. For instance, the average value is computed as

- $\frac{1}{N_s}\beta^2\langle (T+U)^2\rangle - \frac{1}{N_s}\beta^2\langle (T+U)\rangle^2 =$ `Phy0%meas(P0_CV,avg)` $-N_s\beta^2$`Phy0%meas(P0_ENERGY,avg)`^{2}

Note on definition of specific heat

The definition of specific heat used in QUEST corresponds to

$$\frac{1}{N_s}\left.\frac{\partial S}{\partial T}\right|_\mu = \frac{C_\mu}{T} \tag{16}$$

i.e. C_μ is related to the derivative of S at constant μ, not constant density. One can get to the latter using standard thermodynamic manipulations

$$\left.\frac{dS}{dT}\right|_N - \left.\frac{dS}{dT}\right|_\mu = -\left.\frac{\partial N}{\partial T}\right|_\mu^2 \left.\frac{\partial N}{\partial \mu}\right|_T^{-1} \tag{17}$$

We are often interested in cases where $\partial N/\partial T = 0$ (*i.e.* a particle-hole symmetric Hamiltonian) in which case $C_\mu = C_N$.