Multi-Band Quantum Monte Carlo

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I. RECOMMENDATIONS AND HAMILTONIANS

To understand physics of Quantum Monte Carlo (QMC) I would recommend to read in the first turn paper of R. Blankenbecler, D.J. Scalapino and R.L. Sugar (BSS) "Monte Carlo calculation of coupled boson-fermion systems. I", *Phys. Rev. D*, **24 (1981) 2278** . The next step would be to understand difference between Monte Carlo scheme of BSS and the scheme based on Hirsch-Fye algorithm developed for treatment of the Anderson impurity model. A very good description one can find in Review of A. Georges, G. Kotliar, W. Krauth and M.J. Rozenberg (GKKR), "Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions", *Rev. Mod. Phys.* **68 (1996) 13.** Generalization of the scheme described in the Review for degenerate (multiorbital) case one can find in paper of K. Takegahara, "Quantum Monte Carlo of the Degenerate Anderson Model with Cubic Crystal Field", *J. Phys. Soc. Jpn.* **62 (1993) 1736.** A little modification of formulas presented in this paper for the case of Bethe lattice is given below along with program explanation.

N-band degenerate Hubbard model reads

$$H = \sum_{\langle i,i'\rangle\alpha,\alpha'} t_{i\alpha,i'\alpha'} c^{\dagger}_{i\alpha\sigma} c_{i'\alpha'\sigma} + \frac{1}{2}\sum_{i\alpha\alpha'\sigma} U^{i}_{\alpha,\alpha'} n_{i\alpha\sigma} n_{i\alpha-\sigma} + \frac{1}{2}\sum_{i\alpha\neq\alpha'\sigma} (U^{i}_{\alpha,\alpha'} - J^{i}_{\alpha,\alpha'}) n_{i\alpha\sigma} n_{i\alpha'\sigma}, \tag{1}$$

where $U_{\alpha,\alpha'} = \langle\alpha,\alpha'|V(r-r')|\alpha,\alpha'\rangle$, $J_{\alpha,\alpha'} = \langle\alpha,\alpha'|V(r-r')|\alpha',\alpha\rangle$, $V(r-r')$ is Coulomb repulsion, α is the orbital index. When the model above is considered in the limit of infinite dimensions $d \to \infty$ the lattice model is exactly mapped onto the degenerate impurity model which effective action S:

With self-consistency condition : The self-consistency condition is reduced to: The Anderson impurity Hamiltonian reads as

$$H_{AM} = H_0 + H_I \tag{2}$$

$$H_0 = \sum_{p\geq 2,m} \varepsilon_{p,m} c^{\dagger}_{p,m} c_{p,m} + \sum_{p,m} V_{p,m}(c^{\dagger}_{p,m} f_{p,m} + h.c.) + \sum_{m} (E_m + \frac{(2l_{max}-1)}{2}\tilde{U}_{mm}) n_m \tag{3}$$

$$H_I = \sum_{m}\sum_{m<m'} \tilde{U}_{mm'}\{n_m n_{m'} - \frac{1}{2}(n_m + n_{m'})\}, \tag{4}$$

where conduction bath orbitals have index $p = 2, ..., N$ and impurity corresponds $p = 1$. E_m is the f level energy. $m = \{l, \sigma\}$ includes both orbital, $l = -j, ..., j$ and spin σ indices,
$n_m = f^{\dagger}_m f_m$
$\tilde{\mu} = \mu - \frac{(2l_{max}-1)}{2} U$.

For two bands, $l = 1, 2$

$$\begin{aligned} m = 1 &\implies l = 1,\ \sigma =\uparrow \\ m = 2 &\implies l = 1,\ \sigma =\downarrow \\ m = 3 &\implies l = 2,\ \sigma =\uparrow \\ m = 4 &\implies l = 2,\ \sigma =\downarrow \end{aligned}$$

To solve impurity model we use the Hirsch-Fye Quantum Monte Carlo algorithm. As an input we give $\mathcal{G}_0(\tau)$ into QMC and we get $G(\tau)$ as an output from QMC. Fourier transformation gives us $G(i\omega_n)$ from $G(\tau)$. Then $G(i\omega_n)$ is used in the self-consistency condition to obtain $\mathcal{G}_0(\tau)$. Below we describe the Hirsch-Fye QMC Algorithm.

II. HIRSCH-FYE QMC ALGORITHM: THEORY.

To calculate any physical functions we need to know the partition function in the first turn. To do so, let us discretize time interval (imaginary time) $[0, \beta]$ into L slices of length $\Delta\tau$ so that $\Delta\tau_l = l\Delta\tau$, $l = 1, 2, ..., L$, $\beta = L\Delta\tau$.

Then the partition function reads

$$Z = Tr\exp\{-\beta H\} = Tr\prod\exp\{-\Delta\tau(H_0 + H_I)\} \tag{5}$$

To treat it we need some approximation.

A. The Trotter approximation

We can approximate the partition function using the Trotter formula as

$$Z \approx Z^{\Delta\tau} = Tr\prod\exp\{-\Delta\tau H_0\}\exp\{-\Delta\tau H_I\} \tag{6}$$

The discretized GF is written as

$$G^{\Delta\tau}_{p_1 p_2}(\tau_{l_1}, \tau_{l_2}) = \langle T\{c_{p_1}(\tau_{l_1})c^{\dagger}_{p_2}(\tau_{l_2})\}\rangle = \tag{7}$$

$$\frac{1}{Z^{\Delta\tau}}Tre^{-\beta H}c_{p_1}(\tau_{l_1})c^{\dagger}_{p_2}(\tau_{l_2}), \tag{8}$$

for $l_1 > l_2$.

B. The Hubbard - Stratonovich transformation

In the following we use the Hubbard - Stratonovich transformation to decouple the quadratic interaction H_I:

$$\exp\{-\Delta\tau U_{mm'}\{n_m n_{m'} - \frac{1}{2}(n_m + n_{m'})\}\} = \tag{9}$$

$$\frac{1}{2}\sum_{Smm'=\pm1}\exp\{\lambda_{mm'}S_{mm'}(n_m - n_{m'})\}$$

where $\cosh\lambda_{mm'} = \exp(\frac{\Delta\tau U_{mm'}}{2})$, $S_{mm'}(\tau_l)$ are auxiliary Ising fields at each time slice.

$$\lambda_{mm'} = \mathrm{ArcCosh}(\exp(\frac{\Delta\tau U_{mm'}}{2})) \tag{10}$$

In the non-degenerate Anderson impurity model we have only one auxiliary Ising field $S(\tau_l) = \pm1$ at *each time slice*, whereas in the degenerate case the number of auxiliary fields is equal to the number of m, m' pairs, i.e. ${}^mC_2$.

Using the Hubbard - Stratonovich transformation we can rewrite the partition function as

$$Z = Tr_{\{S_{mm'}(\tau_l)\}}\prod_m \det O_m[\{S_{mm'}(\tau_l)\}], \tag{11}$$

where $NL \times NL$ matrix O_m reads as

$$(O_m)_{l,l} = I, \tag{12}$$

$$(O_m)_{l,l-1} = -\exp(-\Delta\tau H_0)\exp(V^m_{l-1})(1 - 2\delta_{l,1}). \tag{13}$$

$$V^m_l = \sum_{m'(\neq m)}\lambda_{mm'}S_{mm'}(\tau_l)\sigma_{m'}, \tag{14}$$

where
$\sigma_{mm'} = +1$ for $m < m'$
$\sigma_{mm'} = -1$ for $m > m'$.

V^m_l has $N \times N$ size and diagonal.

C. The Greens function

Let us define configuration dependent Greens functions as, $G_m \equiv G_m^{\Delta\tau}[\{S_{mm'}\}]$. One can express G_m through O_m matrix as :

$$G_m = O_m^{-1} \tag{15}$$

The relation between two GFs for two different configurations $\{V^m\}$ and $\{V^{m'}\}$ looks as

$$G_m^{'} = G_m + (G_m - I)[\exp\{(V^m)' - V^m\} - I]G_m^{'} \tag{16}$$

i.e.

$$G_m^{'} = A^{-1}G_m, \tag{17}$$

where

$$A = 1 + (1 - G)[\exp(V' - V) - 1], \tag{18}$$

The ratio,R, of the Boltzmann factor for different configurations is given by

$$R = \prod_m R_m, \tag{19}$$

$$R_m = \frac{\det(O_m^{'})}{\det(O_m)} = \det[I - (G_m - I)[\exp\{(V^m)' - V^m\} - I]]. \tag{20}$$

If we make a local change in the field $S_{mm'} \rightarrow S_{mm'}^{'} = -S_{mm'}$ for $\mathbf{m} < \mathbf{m'}$ at time slice l, then the matrix $[\exp\{(V^m)' - V^m\} - I]$ has only one non-zero diagonal element, at the f-location of the $l-th$ submatrix. In this case the determinant is obtained easily.

$$R = R_m R_{m'}, \tag{21}$$

$$R_m = 1 - \{g_m(l,l) - 1\}\{\exp(-2\lambda_{mm'}S_{mm'}) - 1\}, \tag{22}$$

$$R_{m'} = 1 - \{g_{m'}(l,l) - 1\}\{\exp(+2\lambda_{mm'}S_{mm'}) - 1\}, \tag{23}$$

where g_m is $L \times L$ matrix of the f-Greens function. If R/(1+R) (the heat bath condition) is greater that a random number between 0 and 1, then the flip is accepted, otherwise it is rejected. If the flip is accepted then all time components of the f-GF for the new configuration are obtained from the old one through the relation:

$$g_m^{'}(l_1,l_2) = g_m(l_1,l_2) + \{g_m(l_1,l) - \delta_{l_1,l}\}(\mathrm{e}^{-2\lambda_{mm'}S_{mm'}} - 1)\frac{1}{R_m}g_m(l,l_2), \tag{24}$$

$$g_{m'}^{'}(l_1,l_2) = g_{m'}(l_1,l_2) + \{g_{m'}(l_1,l) - \delta_{l_1,l}\}(\mathrm{e}^{-2\lambda_{mm'}S_{mm'}} - 1)\frac{1}{R_{m'}}g_{m'}(l,l_2), \tag{25}$$

which follows from the Dyson equation (16)

D. The physical Greens function

$$G_m^{physical}(\tau_l,\tau_{l'}) = \frac{1}{Z}Tr_{\{S_{mm'}\}}g_m(\tau_l,\tau_{l'})\det O_m[\{S_{mm'}\}]. \tag{26}$$