Moments of the Hubbard and t-J models

B Sriram Shastry.....
Physics Department, University of California, Santa Cruz, Ca 95064
(Dated: July 22, 2013)

For Hubbard model, write $H = H - \mu \hat{N}$ the Grand canonical Hamiltonian

$$H = \sum_{k\sigma} \xi_k c^\dagger_\sigma(k) c_\sigma(k) + \frac{U}{N_s} \sum_{k,p,Q} c^\dagger_\uparrow(k+Q) c_\uparrow(k) c^\dagger_\downarrow(p-Q) c_\downarrow(p),$$

with $\xi(k) = \varepsilon_k - \mu$, and the time dependent operators

$$c_\sigma(k,\tau) = e^{\tau H} c_\sigma(k) e^{-\tau H},$$

so that the Greens function is

$$G(k,\tau) = -\theta(\tau) Tr\ e^{-\beta H}\ c_\sigma(k,\tau) c^\dagger_\sigma(k) + \theta(-\tau) Tr\ e^{-\beta H}\ c^\dagger_\sigma(k) c_\sigma(k,\tau). \tag{1}$$

The Kubo Martin Schwinger Matsubara (KMSM) boundary condition reads with $-\beta \le \tau \le 0$ and $0 \le \tau + \beta$ as

$$\boxed{G(k,\tau) = -G(k,\tau+\beta),} \tag{2}$$

and using this we write the Fourier series for G as

$$G(k, i\omega_n) = \int_0^\beta d\tau\ e^{i\omega_n \tau}\ G(k,\tau) \tag{3}$$

where $\omega_n = \pi(2n+1) k_B T$ is the odd Matsubara frequency, and the inverse transform

$$G(k,\tau) = k_B T \sum_{\omega_n} e^{-i\omega_n \tau} G(k, i\omega_n). \tag{4}$$

We now study Eq 3 for large ω_n, integrating by parts

$$G(k, i\omega_n) = \frac{1}{i\omega_n} [e^{i\omega_n \tau}\ G(k,\tau)]_{0^+}^{\beta^-} - \frac{1}{i\omega_n} \int_0^\beta d\tau\ e^{i\omega_n \tau}\ \partial_\tau G(k,\tau), \tag{5}$$

and using the KMSM condition Eq 2 we get

$$\begin{aligned} G(k, i\omega_n) &= \frac{1}{i\omega_n} [\ G(k, 0^-) - G(k, 0^+)] - \frac{1}{i\omega_n} \int_0^\beta d\tau\ e^{i\omega_n \tau}\ \partial_\tau G(k,\tau), \\ &= \frac{1}{i\omega_n} \langle \{ c_\sigma(k), c^\dagger_\sigma(k) \} \rangle - \frac{1}{i\omega_n} \int_0^\beta d\tau\ e^{i\omega_n \tau}\ \partial_\tau G(k,\tau) \\ &= \frac{1}{i\omega_n} - \frac{1}{i\omega_n} \int_0^\beta d\tau\ e^{i\omega_n \tau}\ \partial_\tau G(k,\tau). \end{aligned} \tag{6}$$

We used the standard anticommutator here. We next define

$$G^{(p)}(k,\tau) = \frac{d^p}{d\tau^p} G(k,\tau),$$

and

$$c^{(p)}_\sigma(k,\tau) = \frac{d^p}{d\tau^p} c_\sigma(k,\tau) = [K, [K, \ldots [K, c_\sigma(k)] \ldots],$$

and hence by repeating the trick, we obtain an iterative equation

$$G^{(p)}(k, i\omega_n) = \frac{1}{i\omega_n} \langle \{ c^{(p)}_\sigma(k), c^\dagger_\sigma(k) \} \rangle - \frac{1}{i\omega_n} \int_0^\beta d\tau\ e^{i\omega_n \tau}\ G^{(p+1)}(k,\tau). \tag{7}$$

Therefore we obtain a high frequency expansion

$$G(k,i\omega_n) = \sum_{p=0}^{\infty}(\frac{1}{i\omega_n})^{p+1}\ \mu_G^{(p)}(k),$$
$$\mu_G^{(p)}(k) \equiv (-1)^p\langle\{c_\sigma^{(p)}(k), c_\sigma^\dagger(k)\}\rangle \tag{8}$$

this is also called the moment expansion.

Next we discuss the spectral representation

$$\boxed{G(k,i\omega_n) = \int_{-\infty}^{\infty} d\nu\ \frac{\rho_G(k,\nu)}{i\omega_n - \nu}} \tag{9}$$

where

$$\boxed{\rho_G(k,\nu) = \sum_{n,m}(\ p_n + p_m)\ \langle n|c_\sigma(k)|m\rangle\ \langle m|c_\sigma^\dagger(k)|n\rangle\ \delta(\nu - \varepsilon_m + \varepsilon_n).} \tag{9}$$

We may expand this at high frequencies as

$$G(k,i\omega_n) = \sum_{p=0}^{\infty}(\frac{1}{i\omega_n})^{p+1}\int_{-\infty}^{\infty} d\nu\ \rho_G(k,\nu)\ \nu^p \tag{10}$$

and conclude that the moments are given by

$$\mu_G^{(p)}(k) = \int_{-\infty}^{\infty} d\nu\ \rho_G(k,\nu)\ \nu^p = (-1)^p\langle\{c_\sigma^{(p)}(k), c_\sigma^\dagger(k)\}\rangle \tag{11}$$

For the Hubbard model, the Greens function is also decomposed as

$$(G(k,i\omega_n))^{-1} = i\omega_n - \xi(k) - Un/2 - \int_{-\infty}^{\infty}\frac{\rho_\Sigma(k,\nu)}{i\omega_n - \nu}\ d\nu, \tag{12}$$

and hence we may expand this for high frequencies and thereby find the moments of $\rho_\Sigma(k,\nu)$ in terms of those for $\rho_G(k,\nu)$, as a simple exercise. Calling $a_p(k) = \int_{-\infty}^{\infty} d\nu\rho_G(k,\nu)\ \nu^p$, we get: (suppressing the k dependence)

$$a_0 = \mu_G^{(2)} - (\mu_G^{(1)})^2$$
$$a_1 = \mu_G^{(3)} - 2\mu_G^{(2)}\mu_G^{(1)} + (\mu_G^{(3)})^3 \tag{13}$$

We may then write two alternative expressions

$$\boxed{\begin{aligned}(1 - f(\nu))\ \rho_G(k,\nu) &= \rho_G^{>}(k,\nu)\\ f(\nu)\ \rho_G(k,\nu) &= \rho_G^{<}(k,\nu).\end{aligned}} \tag{14}$$

(14)

where

$$\boxed{\begin{aligned}\rho_G^{>}(k,\nu) &= \sum_{n,m} p_n\ \langle n|c_\sigma(k)|m\rangle\ \langle m|c_\sigma^\dagger(k)|n\rangle\ \delta(\nu - \varepsilon_m + \varepsilon_n), \quad \text{or}\\ \rho_G^{<}(k,\nu) &= \sum_{n,m} p_n\ \langle n|c_\sigma^\dagger(k)|m\rangle\ \langle m|c_\sigma(k)|n\rangle\ \delta(\nu - \varepsilon_n + \varepsilon_m)\end{aligned}} \tag{14}$$

We note the relation

$$\boxed{\rho_G^{>}(k,\nu) = e^{\beta\nu}\rho_G^{<}(k,\nu).} \tag{15}$$

In time domain:

$$\boxed{G(k,\tau) = \int_{-\infty}^{\infty} d\nu \ \rho_G(k,\nu) \ e^{-\nu\tau} \left[\theta(-\tau) f(\nu) - \theta(\tau)(1 - f(\nu))\right]} \tag{16}$$

or

$$\boxed{G(k,\tau) = \int_{-\infty}^{\infty} d\nu \ \ e^{-\nu\tau} \left[\theta(-\tau)\rho_G^{<}(k,\nu) - \theta(\tau)\rho_G^{>}(k,\nu)\right].} \tag{17}$$

which is automactically satisfied with the above representation Eq. (17) upon using Eq. (15).

Real time propagators

We will also be interested in

$$i\ G(k,t) = -\theta(t)\ \langle e^{iHt} c_\sigma(k) e^{-iHt} c_\sigma^\dagger(k)\rangle + \theta(-t)\ \langle c_\sigma^\dagger(k) e^{iHt} c_\sigma(k) e^{-iHt}\rangle \tag{18}$$

We see that

$$i\ G(k,t)\ = -\theta(t)\ \int_{-\infty}^{\infty} d\nu \ \ e^{-i\nu t} \rho_G(k,\nu)\ \overline{f}(\nu) + \theta(-t)\ \int_{-\infty}^{\infty} d\nu \ \ e^{-i\nu t} \rho_G(k,\nu) f(\nu) \tag{19}$$