Linear response formula for current-like observables[1]

Hal Tasaki, Feb. 5, 2012

For any f_x, we have seen in the lecture that

$$\langle f\rangle_{\bar{\boldsymbol{p}}} = \langle f\rangle_{\boldsymbol{p}^{\rm eq}} + \sum_{t=0}^{N-1} \langle \psi(t)\, f(N)\rangle^{\rm eq} + O(\varepsilon^2)$$
$$= \langle f\rangle_{\boldsymbol{p}^{\rm eq}} + \sum_{t=-\infty}^{-1} \langle \psi(t)\, f(0)\rangle^{\rm eq} + O(\varepsilon^2), \tag{1}$$

where the second formula is obtained by shifting and extending the time interval. This is OK.

Now let us consider an arbitrary "current-like" observable $g_{x\to y}$, which satisfies $g_{x\to y} = -g_{y\to x}$. As in the lecture the corresponding observable with a single x is defined as

$$\tilde{g}_x := \sum_{y\in\mathcal{S}} \tau_{x\to y}\, g_{x\to y}. \tag{2}$$

By substituting this into (1), we have[2]

$$\langle \tilde{g}\rangle_{\bar{\boldsymbol{p}}} = \langle \tilde{g}\rangle_{\boldsymbol{p}^{\rm eq}} + \sum_{t=-\infty}^{-1} \langle \psi(t)\, g(0)\rangle^{\rm eq} + O(\varepsilon^2), \tag{3}$$

where $g(t)[\hat{x}] := g_{x(t)\to x(t+1)}$ is the quantity g viewed as a function of path $\hat{x}$. When I was preparing the lecture, I thought (carelessly) that the first term $\langle \tilde{g}\rangle_{\boldsymbol{p}^{\rm eq}}$ was negligible, as its counterpart in continuous time formulation is indeed vanishing. But (as you know) I realized that something was wrong here when I was explaining this part in the lecture. I did not have enough time to think it back during the short lunch break, and had forgot about this. I apologize you for the mistake and for having left it unexplained.

The truth is that $\langle \tilde{g}\rangle_{\boldsymbol{p}^{\rm eq}}$ has a nonvanishing contribution, and it makes the final expression neat. Let me explain this.

From the definitions, we have

$$\langle \tilde{g}\rangle_{\boldsymbol{p}^{\rm eq}} = \sum_{x,y\in\mathcal{S}} \frac{e^{-\beta H_x}}{Z}\, \tau_{x\to y}\, g_{x\to y}. \tag{4}$$

Noting that the definition of $\psi_{x\to y}$ implies[3]

$$e^{-\beta H_x}\, \tau_{x\to y} = e^{-\beta H_y - \psi_{y\to x}}\, \tau_{y\to x}, \tag{5}$$

[1] This is a supplement to a series of lectures that I gave in U. Osaka recently, and does not make quite sense by itself.

[2] For simplicity I assume $g = O(1)$.

[3] This is nothing but the detailed balance condition if $\psi_{x\to y} = 0$.

and recalling that $g_{x\to y} = -g_{y\to x}$, one has

$$\langle \tilde{g} \rangle_{\boldsymbol{p}^{\text{eq}}} = -\sum_{x,y\in\mathcal{S}} \frac{e^{-\beta H_y - \psi_{y\to x}}}{Z} \tau_{y\to x}\, g_{y\to x} = -\sum_{x,y\in\mathcal{S}} \frac{e^{-\beta H_x - \psi_{x\to y}}}{Z} \tau_{x\to y}\, g_{x\to y}, \tag{6}$$

where we have simply switched the two dummy variables x and y to get the final expression. By averaging (4) and (6), we see

$$\langle \tilde{g} \rangle_{\boldsymbol{p}^{\text{eq}}} = \frac{1}{2} \sum_{x,y\in\mathcal{S}} \frac{e^{-\beta H_x}}{Z} \tau_{x\to y}\, g_{x\to y}\, \psi_{x\to y} + O(\varepsilon^2) = \frac{1}{2} \langle \widetilde{g\,\psi} \rangle_{\boldsymbol{p}^{\text{eq}}} + O(\varepsilon^2), \tag{7}$$

where $(\widetilde{g\,\psi})_x := \sum_{y\in\mathcal{S}} \tau_{x\to y}\, g_{x\to y}\, \psi_{x\to y}$. Going to the path-space formalism, one finds that

$$\langle \widetilde{g\,\psi} \rangle_{\boldsymbol{p}^{\text{eq}}} = \langle g(t)\, \psi(t) \rangle^{\text{eq}} \tag{8}$$

with an arbitrary t in the interval[4]. Thus the expression (7) becomes

$$\begin{aligned} \langle \tilde{g} \rangle_{\bar{\boldsymbol{p}}} &= \sum_{t=-\infty}^{-1} \langle \psi(t)\, g(0) \rangle^{\text{eq}} + \frac{1}{2} \langle \psi(0)\, g(0) \rangle^{\text{eq}} + O(\varepsilon^2) \\ &= \frac{1}{2} \sum_{t=-\infty}^{\infty} \langle g(0)\, \psi(t) \rangle^{\text{eq}} + O(\varepsilon^2), \end{aligned} \tag{9}$$

where we have used the time reversal symmetry to get the final expression. As you see the demonstration of the reciprocal relation becomes automatic with this neat form.

[4]To be precise the whole time interval must at least contain t and $t+1$.