Z Appendix B Linear Response and Generating Functionals

B.1 Spin Response Function

自旋响应函数 (spin response function) 描述了自旋的动力学, 具体地说是自旋系统对一个任意弱的时空依赖磁场 (或"源电流(source current") $j_i^\alpha(t)$ 的响应, 其中源电流会在 $t \geq 0$打开. 完整的 source dependent Hamiltonian 为

Ⓝ (AssaB.1)

$$\mathcal{H}[j] = \mathcal{H}_0 - \sum_{i,\alpha} j_i^\alpha(t) S_i^\alpha,$$

- $\alpha = x, y, z$. 这实际上是一个泛函, $\mathcal{H}[\mathbf{j}(t, \mathbf{x})] = \mathcal{H}[j(t)] = \mathcal{H}[j] = \mathcal{H}(t)$, source-dependent 的$\mathcal{H}$依赖于source current的随时间演化函数$j_i^\alpha(t)$, 且这个函数是一个随时变化的矢量场, 即具有时空依赖(space-time dependent).
- $\mathcal{H}_0(\mu)$是巨正则形式下的无相互作用哈密顿量

当 $t > 0$, Hilbert空间中的所有态都在如下薛定谔方程控制下演化,

Ⓝ (AssaB.2)

$$i \frac{\partial}{\partial t} |\psi(t)\rangle = \mathcal{H}[j] |\psi(t)\rangle$$

上式形式上的解可以用时间演化算符表示; 时间演化算符也是 source-dependent 的

Ⓝ (AssaB.3)

$$\begin{aligned} |\psi(t)\rangle &= U[t, j] |\psi(0)\rangle \\ U[t, j] &= T_{t'} \exp\left(-i \int_0^t dt' \mathcal{H}\left[j\left(t'\right)\right]\right), \end{aligned}$$

其中时序指数 (time ordered exponential)定义为如下的离散表达式(无穷小时间演化算符)的极限

Ⓝ (AssaB.4)

$$\begin{aligned} U[t, j] =& T_{t'} \exp\left[-i \int_0^t dt' \mathcal{H}\left(t'\right)\right] \\ =& T_{t'} \exp\left[-i \int_0^\epsilon dt' \mathcal{H}\left(t'\right) - i \int_\epsilon^{2\epsilon} dt' \mathcal{H}\left(t'\right) - \cdots - i \int_{t-\epsilon}^t dt' \mathcal{H}\left(t'\right)\right] \\ =& \lim_{\epsilon \to 0} T_{t'} \exp\left[-i\epsilon \mathcal{H}\left(t' = \epsilon\right) - i\epsilon \mathcal{H}\left(t' = 2\epsilon\right) - \cdots - i\epsilon \mathcal{H}\left(t' = t\right)\right] \\ \approx& \lim_{\epsilon \to 0} T_{t'} \exp\left[-i\epsilon \mathcal{H}\left(t' = \epsilon\right)\right] \exp\left[-i\epsilon \mathcal{H}\left(t' = 2\epsilon\right)\right] \exp\left[-i\epsilon \mathcal{H}\left(t' = t\right)\right] \\ \approx& \lim_{\epsilon \to 0} T_{t'} \left[1 - i\epsilon \mathcal{H}\left(t' = \epsilon\right)\right] \left[1 - i\epsilon \mathcal{H}\left(t' = 2\epsilon\right)\right] \left[1 - i\epsilon \mathcal{H}\left(t' = t\right)\right] \\ =& \lim_{\epsilon \to 0} \underbrace{[1 - i\mathcal{H}(t)\epsilon][1 - i\mathcal{H}(t - \epsilon)\epsilon] \ldots [1 - i\mathcal{H}(\epsilon)\epsilon]}_{N_\epsilon}, \end{aligned}$$

其中 $\epsilon = t / N_\epsilon$ 是无穷小时间步长. 最后一步利用了时序算符, 时间比较晚的项排在前面.

变换到**海森堡绘景**, 一个算符 S_i^α 在 $\mathcal{H}[j]$ 下的演化期望值为

$$
\langle S_i^\alpha(t)\rangle_j = Z^{-1}\operatorname{Tr}\left(\rho U^{-1}[t,j]S_i^\alpha U[t,j]\right)
$$

其中 $Z=\operatorname{Tr}\rho$ 是配分函数, ρ 是密度矩阵, 这些都应该是隐含时间, 显含$j(t)$的. 展开到关于 source current j 的线性阶得到

Ⓝ (AssaB.6)

$$
\langle S_i^\alpha(t)\rangle_j = \langle S_i^\alpha(0)\rangle + i\int_0^t dt' \sum_{i',\alpha'} j_{i'}^{\alpha'} \left\langle \left[S_i^\alpha(t), S_{i'}^{\alpha'}(t')\right]\right\rangle + \mathcal{O}\left(j^2\right),
$$

其中不带下标j的期望值 $\langle\cdot\rangle$ 是 with respect to $\mathcal{H}_0$的期望值. 等号右边中出现的算符$S_i^\alpha(t)$必须得是相互作用绘景的算符, 否则不是关于j一阶的.

> 是否可以从离散定义(AssaB.4)和海森堡绘景出发证明上式? 对j的依赖隐藏在$\mathcal{H}(t-n\epsilon)$之中.
>
> - 保留到关于j的零阶, 则我们要把各个方括号里面的$\mathcal{H}(t-n\epsilon)$里面的j项都扔掉, 最后时间演化算符不需要时序了, 这是一个不含时的哈密顿量$\mathcal{H}_0$给出的时间演化$e^{-iH_0 t}$, 即给出了上式第一项$\langle S_i^\alpha(0)\rangle$.
> - 保留到关于j的一阶, 则把各个方括号里面的$\mathcal{H}(t-n\epsilon)$里面的j项都保留, 但是只考虑这样的项: 从N_ϵ个方括号中, 其中一个取出$i\mathcal{H}_1(t)$, 剩下$N_\epsilon-1$个都只能取出1, 最终有
>
> $$
> \begin{aligned}
> U[t,j] \approx &[1-i\mathcal{H}_0\epsilon - i\mathcal{H}_1(t)\epsilon][1-i\mathcal{H}_0\epsilon]\cdots[1-i\mathcal{H}_0\epsilon]\\
> &+[1-i\mathcal{H}_0\epsilon][1-i\mathcal{H}_0\epsilon - i\mathcal{H}_1(t-\epsilon)\epsilon]\cdots[1-i\mathcal{H}_0\epsilon]\\
> &+\cdots\\
> &+[1-i\mathcal{H}_0\epsilon][1-i\mathcal{H}_0\epsilon]\cdots[1-i\mathcal{H}_0\epsilon - i\mathcal{H}_1(\epsilon)\epsilon]\\
> \approx & e^{-i\mathcal{H}(t)\epsilon}e^{-i\mathcal{H}_0\epsilon}\cdots e^{-i\mathcal{H}_0\epsilon} + e^{-i\mathcal{H}_0\epsilon}e^{-i\mathcal{H}(t-\epsilon)\epsilon}\cdots e^{-i\mathcal{H}_0\epsilon}\\
> &+\cdots + e^{-i\mathcal{H}_0\epsilon}e^{-i\mathcal{H}_0\epsilon}\cdots e^{-i\mathcal{H}(\epsilon)\epsilon}\\
> \overset{?}{=} & e^{-i\mathcal{H}_0 t}\left(1-i\int_0^t dt'\mathcal{H}_1(t)\right)
> \end{aligned}
> $$
>
> 其中将外场项记为了$\mathcal{H}_1(t)=-\sum_{i,\alpha} j_i^\alpha(t)S_i^\alpha$. 如果最后一个等号成立, 则可以得证(AssaB.6), 只不过要注意kernel里面的两个含时S_i^α算符是**相互作用绘景下的含时算符**, $e^{i\mathcal{H}_0 t}S_i^\alpha e^{-i\mathcal{H}_0 t}$.
>
>   - 这个等号必定得是成立的. 这是薛定谔绘景下的演化算符和相互作用绘景下的演化算符之间的关系.
>
> 这不是传统的证明方式. 如Bruus书上6.1 The general Kubo formula是变换到相互作用绘景, 然后将相互作用绘景中的时间演化算符做关于相互作用哈密顿量的一阶截断(Bruus5.19), 自然就能得到Kubo公式(6.6).

推迟关联函数

式(AssaB.6)中积分的kernel就是**响应函数(response function)**

Ⓝ (AssaB.7)

$$
R_{ii'}^{\alpha\alpha'}(t-t') = -i\theta(t-t')\left\langle\left[S_i^\alpha(t), S_{i'}^{\alpha'}(t')\right]\right\rangle.
$$

由于 θ 函数的存在(限制了$t'<t$), R 在数学上被称为**推迟关联函数**. 下面我们会扔掉指标 α,α', 注意区分这个表示方向的上标和Lehmann表象的本征矢标记.

可以使用$\mathcal{H}_0$的本征态和本征能量来计算 R :

Ⓝ (AssaB.8)

$$\mathcal{H}_0(\mu)|\alpha\rangle=E_\alpha|\alpha\rangle.$$

在本征态表象(Lehmann表象)下, (B.7)为 (设$t'=0$)

Ⓝ (AssaB.9)

$$\begin{aligned}R_{ii'}(t)=-i\theta(t)Z^{-1}\sum_{\alpha\beta}e^{-E_\alpha/T}\Big(&e^{i(E_\alpha-E_\beta)t}\left\langle\alpha\left|S_i^\alpha\right|\beta\right\rangle\left\langle\beta\left|S_{i'}^{\alpha'}\right|\alpha\right\rangle\\&-e^{i(E_\beta-E_\alpha)t}\left\langle\alpha\left|S_{i'}^{\alpha'}\right|\beta\right\rangle\left\langle\beta\left|S_i^\alpha\right|\alpha\right\rangle\Big)\end{aligned}$$

考虑自由哈密顿量具有平移不变性, 则 $R_{ii'}=R\left(\mathbf{x}_i-\mathbf{x}_{i'}\right)$, 其中 $\mathbf{x}_i$ 是格点i的空间位置. 对R做时空Fourier变换得到**谱响应函数(spectral response function)**

Ⓝ (AssaB.10)

$$\begin{aligned}R\left(\mathbf{q},\omega+i0^+\right)&=\mathcal{N}^{-1}\sum_{ii'}\int_0^\infty dte^{-i\mathbf{q}(\mathbf{x}_i-\mathbf{x}_{i'})+i\left(\omega+i0^+\right)t}R\left(\mathbf{x}_i-\mathbf{x}_{i'},t\right)\\&=(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\left\langle\alpha\left|S_{\mathbf{q}}^\alpha\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\frac{e^{-E_\alpha/T}-e^{-E_\beta/T}}{E_\alpha-E_\beta+\omega+i0^+}\end{aligned}$$

$$S_{\mathbf{q}}^\alpha=\sum_i e^{-i\mathbf{q}\mathbf{x}_i}S_i^\alpha$$

在做时间Fourier变换时往频率中引入了无穷小正数 0^+, 它保证了长时间时Fourier积分的收敛性.

> 首先注意这本书记号不统一, 式(Assa6.1)中空间Fourier变换乘的是$e^{i\mathbf{q}\cdot\mathbf{x}}$, 这里乘的是$e^{-i\mathbf{q}\cdot\mathbf{x}}$.
>
> 按照这本书的记号, 如果是做$\mathbf{x}_i-\mathbf{x}_{i'}\leftrightarrow\mathbf{q}$的Fourier变换, 是不用乘前置因子$1/\mathcal{N}$的. 这里为什么乘了? 这里涉及到文献中经常出 现的一种susceptibility的写法: 对单个变量做Fourier变换 $\mathbf{x}_i-\mathbf{x}_{i'}\leftrightarrow\mathbf{q}$, 等价于对两个变量分别做Fourier变换 $\mathbf{x}_i\to\mathbf{q},\mathbf{x}_j\to-\mathbf{q}$, 两者至多差一个前置因子. 对于可以分离变量的函数 $R(\mathbf{x},\mathbf{x}')=R(\mathbf{x})R(\mathbf{x}')$, 数学说明如下:
>
> $$\begin{aligned}&\int d\left(\mathbf{x}-\mathbf{x}'\right)e^{-i\mathbf{q}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}R\left(\mathbf{x},\mathbf{x}'\right)\\=&\frac{1}{\mathcal{V}}\int d\mathbf{x}\int d\mathbf{x}'e^{-i\mathbf{q}\cdot\left(\mathbf{x}-\mathbf{x}'\right)}R_1\left(\mathbf{x}\right)R_2\left(\mathbf{x}'\right)\\=&\frac{1}{\mathcal{V}}\int d\mathbf{x}e^{-i\mathbf{q}\cdot\mathbf{x}}R_1\left(\mathbf{x}\right)\int d\mathbf{x}'e^{i\mathbf{q}\cdot\mathbf{x}'}R_2\left(\mathbf{x}'\right)\\=&\frac{1}{\mathcal{V}}R_1\left(\mathbf{q}\right)R_2\left(-\mathbf{q}\right)\end{aligned}$$
>
> 下面是对上式第二个等号一个完整的推导过程

$$
\begin{aligned}
R\left(\mathbf{q},\omega+i0^{+}\right)=&\mathcal{N}^{-1}\sum_{ii'}\int_{0}^{\infty}dte^{-i\mathbf{q}\left(\mathbf{x}_{i}-\mathbf{x}_{i'}\right)+i\left(\omega+i0^{+}\right)t}R\left(\mathbf{x}_{i}-\mathbf{x}_{i'},t\right)\\
=&\mathcal{N}^{-1}Z^{-1}\sum_{\alpha\beta}e^{-E_{\alpha}/T}\sum_{ii'}\int_{0}^{\infty}dt\left(-i\theta(t)\right)e^{-i\mathbf{q}\left(\mathbf{x}_{i}-\mathbf{x}_{i'}\right)+i\left(\omega+i0^{+}\right)t}\\
&\times\left(e^{i\left(E_{\alpha}-E_{\beta}\right)t}\left\langle\alpha\left|S_{i}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{i'}^{\alpha'}\right|\alpha\right\rangle-e^{i\left(E_{\beta}-E_{\alpha}\right)t}\left\langle\alpha\left|S_{i'}^{\alpha'}\right|\beta\right\rangle\left\langle\beta\left|S_{i}^{\alpha}\right|\alpha\right\rangle\right)\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha\beta}e^{-E_{\alpha}/T}\sum_{ii'}e^{-i\mathbf{q}\cdot\mathbf{x}_{i}}e^{i\mathbf{q}\cdot\mathbf{x}_{i'}}(-i)\int_{0}^{\infty}dte^{i\left(\omega+i0^{+}\right)t}\\
&\times\left(e^{i\left(E_{\alpha}-E_{\beta}\right)t}\left\langle\alpha\left|S_{i}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{i'}^{\alpha'}\right|\alpha\right\rangle-e^{i\left(E_{\beta}-E_{\alpha}\right)t}\left\langle\alpha\left|S_{i'}^{\alpha'}\right|\beta\right\rangle\left\langle\beta\left|S_{i}^{\alpha}\right|\alpha\right\rangle\right)\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha\beta}e^{-E_{\alpha}/T}(-i)\\
&\times\left(\int_{0}^{\infty}dte^{i\left(E_{\alpha}-E_{\beta}+\omega+i0^{+}\right)t}\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right.\\
&\left.-\int_{0}^{\infty}dte^{i\left(E_{\beta}-E_{\alpha}+\omega+i0^{+}\right)t}\left\langle\alpha\left|S_{-\mathbf{q}}^{\alpha'}\right|\beta\right\rangle\left\langle\beta\left|S_{\mathbf{q}}^{\alpha}\right|\alpha\right\rangle\right)\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha\beta}e^{-E_{\alpha}/T}(-i)\\
&\times\left(\frac{-1}{i\left(E_{\alpha}-E_{\beta}+\omega+i0^{+}\right)}\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right.\\
&\left.-\frac{-1}{i\left(E_{\beta}-E_{\alpha}+\omega+i0^{+}\right)}\left\langle\alpha\left|S_{-\mathbf{q}}^{\alpha'}\right|\beta\right\rangle\left\langle\beta\left|S_{\mathbf{q}}^{\alpha}\right|\alpha\right\rangle\right)\\
=&(\mathcal{N}Z)^{-1}\left(\sum_{\alpha\beta}\frac{e^{-E_{\alpha}/T}}{\left(E_{\alpha}-E_{\beta}+\omega+i0^{+}\right)}\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right.\\
&\left.-\sum_{\beta\alpha}\frac{e^{-E_{\beta}/T}}{\left(E_{\alpha}-E_{\beta}+\omega+i0^{+}\right)}\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\right)\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\frac{e^{-E_{\alpha}/T}-e^{-E_{\beta}/T}}{E_{\alpha}-E_{\beta}+\omega+i0^{+}}
\end{aligned}
$$

Kramers-Kronig relations

对Fourier空间的 R 取实部和虚部, 需要用到如下恒等式

Ⓝ (AssaB.12)

$$
\frac{1}{x+i0^{+}}=\mathcal{P}\left(\frac{1}{x}\right)-i\pi\delta(x)
$$

其中 $\mathcal{P}$ 会取其argument的主值. 将式(B.12)应用到(B.10), 就证明了 Kramers-Kronig relations

Ⓝ (AssaB.13)

$$
\begin{aligned}
\operatorname{Re}R(\mathbf{q},\omega)&=\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\operatorname{Im}R\left(\mathbf{q},\omega'\right)}{\omega'-\omega}\\
\operatorname{Im}R(\mathbf{q},\omega)&=-\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\operatorname{Re}R\left(\mathbf{q},\omega'\right)}{\omega'-\omega}.
\end{aligned}
$$

$$
\begin{aligned}
&\mathrm{Im}R\left(\mathbf{q},\omega'\right)\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Re}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\mathrm{Im}\left\{\frac{e^{-E_\alpha/T}-e^{-E_\beta/T}}{E_\alpha-E_\beta+\omega+i0^+}\right\}\\
&+(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Im}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\mathrm{Re}\left\{\frac{e^{-E_\alpha/T}-e^{-E_\beta/T}}{E_\alpha-E_\beta+\omega+i0^+}\right\}\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Re}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\left[-\pi\delta\left(E_\alpha-E_\beta+\omega'\right)\right]\left(e^{-E_\alpha/T}-e^{-E_\beta/T}\right)\\
&+(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Im}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\frac{\left(E_\alpha-E_\beta+\omega\right)}{\left(E_\alpha-E_\beta+\omega\right)^2+\eta^2}\left(e^{-E_\alpha/T}-e^{-E_\beta/T}\right)
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\mathrm{Im}R\left(\mathbf{q},\omega'\right)}{\omega'-\omega}\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Re}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\left(e^{-E_\alpha/T}-e^{-E_\beta/T}\right)\\
&\times\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\left(-\pi\delta\left(E_\alpha-E_\beta+\omega'\right)\right)}{\omega'-\omega}\\
&+(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Im}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\left(e^{-E_\alpha/T}-e^{-E_\beta/T}\right)\\
&\times\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega}\frac{\left(E_\alpha-E_\beta+\omega\right)}{\left(E_\alpha-E_\beta+\omega\right)^2+\eta^2}\\
=&(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Re}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\frac{e^{-E_\alpha/T}-e^{-E_\beta/T}}{E_\alpha-E_\beta+\omega}\\
&+(\mathcal{N}Z)^{-1}\sum_{\alpha,\beta}\mathrm{Im}\left\{\left\langle\alpha\left|S_{\mathbf{q}}^{\alpha}\right|\beta\right\rangle\left\langle\beta\left|S_{-\mathbf{q}}^{\alpha'}\right|\alpha\right\rangle\right\}\left(e^{-E_\alpha/T}-e^{-E_\beta/T}\right)\pi\delta\left(\omega+E_\alpha-E_\beta\right)\\
=&\mathrm{Re}R\left(\mathbf{q},\omega\right)
\end{aligned}
$$

$$
\begin{aligned}
&\mathcal{P}\int_{-\infty}^{\infty}d\omega'\frac{1}{\omega'-\omega}\frac{A+\omega'}{\left(A+\omega'\right)^2+\eta^2}\\
=&\mathcal{P}\int_{-\infty}^{\infty}d\omega'\left(\frac{A'}{\omega'-\omega}+\frac{B'\omega'+C'}{\left(A+\omega'\right)^2+\eta^2}\right)\\
=&\int_{-\infty}^{\infty}d\omega'\frac{B'\omega'+C'}{\left(A+\omega'\right)^2+\eta^2}\\
=&\int_{-\infty}^{\infty}dx\frac{B'x-B'A+C'}{x^2+\eta^2},x\equiv A+\omega'\\
=&B'\int_{-\infty}^{\infty}dx\frac{x}{x^2+\eta^2}+\left(-B'A+C'\right)\int_{-\infty}^{\infty}dx\frac{1}{x^2+\eta^2}\\
=&B'\frac{1}{2}\ln\left|x^2+\eta^2\right|\Big|_{-\infty}^{\infty}+\left(-B'A+C'\right)\frac{1}{\eta}\arctan\frac{x}{\eta}\Big|_{-\infty}^{\infty}\\
=&\left(-B'A+C'\right)\frac{\pi}{\eta}
\end{aligned}
$$

> $$\begin{cases} A'+B'=0 \\ 2AA'-B'\omega+C'=1 \\ A^2A'-C'\omega+A'\eta^2=A \end{cases}$$
>
> $$\begin{aligned} A' &= \frac{A+\omega}{(A+\omega)^2+\eta^2} = -B' \\ C' &= 1-(2A+\omega)\frac{A+\omega}{(A+\omega)^2+\eta^2} = \frac{-A^2-A\omega+\eta^2}{(A+\omega)^2+\eta^2} \end{aligned}$$
>
> $$-B'A+C' = \frac{\eta^2}{(A+\omega)^2+\eta^2} = \pi\delta(A+\omega) = \pi\delta(\omega+E_\alpha-E_\beta)$$
>
> $$\frac{A'}{\omega'-\omega}+\frac{B'\omega'+C'}{(A+\omega')^2+\eta^2} = \frac{A'\left((A+\omega')^2+\eta^2\right)}{\omega'-\omega}\frac{(\omega'-\omega)(B'\omega'+C')}{(A+\omega')^2+\eta^2}$$

B.2 Fluctuations and Dissipation

谱响应函数的虚部 $\operatorname{Im} R_{21}(\omega)$ 是耗散部分(为啥下标一定得是21, R^{yx}?), 可以称之为**耗散响应函数(dissipative response function)**. 它描述的是, 由于激发了系统内禀模式, 而引起的频率ω的外加振荡的衰减(damping).

平衡态时两个自旋涨落的关联函数为

Ⓝ (AssaB.14)

$$S^{\alpha\alpha'}_{i,i'}(t-t') = \left\langle S^\alpha_i(t)\cdot S^{\alpha'}_{i'}(t')\right\rangle.$$

其时空Fourier变换被称为**动力学结构因子 (dynamical structure factor)**, 我们之前算过

Ⓝ (AssaB.15)

$$\begin{aligned} S^{\alpha\alpha'}(\mathbf{q},\omega) &= \mathcal{N}^{-1}\sum_{ii'}\int_{-\infty}^{\infty} dt e^{-i\mathbf{q}(\mathbf{x}_i-\mathbf{x}_{i'})+i\omega t} S^{\alpha\alpha'}_{ii'}(t) \\ &= \frac{2\pi}{Z\mathcal{N}}\sum_{\alpha,\beta} e^{-E_\alpha/T}\left\langle\alpha\left|S^\alpha_{\mathbf{q}}\right|\beta\right\rangle\left\langle\beta\left|S^{\alpha'}_{-\mathbf{q}}\right|\alpha\right\rangle\delta(\omega+E_\alpha-E_\beta). \end{aligned}$$

> 我们之前算过$\left\langle\left[S^\alpha_i(t),S^{\alpha'}_{i'}(t')\right]\right\rangle$的时空Fourier变换(见(AssaB.10)), 这里相当于只取对易子的第一项, 过程类似, 同样是在Lehmann表象下进行, 且设$t'=0$. 对时间的积分由于是$-\infty$到$+\infty$, 因此一个指数$e^{i(\omega+E_\alpha-E_\beta)t}$的积分直接得到$\delta$函数.

- 对于厄米可观测量(指的是S^α_i? $S^\alpha_{\mathbf{q}}$不是厄米的.), 结构因子 $S(\mathbf{q},\omega)$ 是实数. #TODO
  - 首先, $\alpha=\alpha'$时则易证. 也可以直接通过涨落耗散定理(AssaB.16)看到它是实数.

- 但对于$\alpha \neq \alpha'$的情况, $\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \neq \langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \rangle^*$, 因此不能直接看出来.

- 动力学结构因子描述了频率 ω 处的自发涨落, 可以通过**涨落实验**来测量. 例如, a polarized inelastic neutron scattering cross section measures the electronic spin structure factor.

通过比较显明表达式(AssaB.10)和(B.15), 可以得到耗散响应函数和结构因子之间的一个简单的关系 (扔掉了关联函数的上标), 被称为**涨落-耗散定理(fluctuation-dissipation theorem)**

✅ TODO Ⓝ (AssaB.16)

$$S(\mathbf{q}, \omega) = -\frac{2}{1 - e^{-\omega/T}} \operatorname{Im} R(\mathbf{q}, \omega).$$

当$\alpha = \alpha'$时, $\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \langle \beta \left| S_{-\mathbf{q}}^{\alpha} \right| \alpha \rangle$是一个实数, 故有如下的简单证明:

$$\begin{aligned} \operatorname{Im} R\left(\mathbf{q}, \omega + i0^+\right) &= \frac{-\pi}{\mathcal{N}Z} \sum_{\alpha,\beta} \langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \left(e^{-E_\alpha/T} - e^{-E_\beta/T} \right) \delta\left(E_\alpha - E_\beta + \omega\right) \\ &= -\frac{\left(1 - e^{-\omega/T}\right)}{2} \frac{2\pi}{\mathcal{N}Z} \sum_{\alpha,\beta} e^{-E_\alpha/T} \langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \delta\left(E_\alpha - E_\beta + \omega\right) \\ &= -\frac{\left(1 - e^{-\omega/T}\right)}{2} S\left(\mathbf{q}, \omega\right) \end{aligned}$$

一般的情况似乎不好证明

$$\begin{aligned} &\operatorname{Im} R\left(\mathbf{q}, \omega + i0^+\right) \\ =&\frac{-\pi}{\mathcal{N}Z} \sum_{\alpha,\beta} \operatorname{Re}\left[\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \right] \left(e^{-E_\alpha/T} - e^{-E_\beta/T} \right) \delta\left(E_\alpha - E_\beta + \omega\right) \\ &\frac{1}{\mathcal{N}Z} \sum_{\alpha,\beta} \operatorname{Im}\left[\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \right] \left(e^{-E_\alpha/T} - e^{-E_\beta/T} \right) \frac{\left(E_\alpha - E_\beta + \omega\right)}{\left(E_\alpha - E_\beta + \omega\right)^2 + \eta^2} \\ =&-\frac{\left(1 - e^{-\omega/T}\right)}{2} \frac{2\pi}{\mathcal{N}Z} \sum_{\alpha,\beta} e^{-E_\alpha/T} \operatorname{Re}\left[\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \right] \delta\left(E_\alpha - E_\beta + \omega\right) \\ &-\frac{\left(1 - e^{-\omega/T}\right)}{2} \frac{2\pi}{\mathcal{N}Z} \sum_{\alpha,\beta} e^{-E_\alpha/T} \operatorname{Im}\left[\langle \alpha \left| S_{\mathbf{q}}^{\alpha} \right| \beta \rangle \left\langle \beta \left| S_{-\mathbf{q}}^{\alpha'} \right| \alpha \right\rangle \right] \frac{-1}{\pi} \frac{\left(E_\alpha - E_\beta + \omega\right)}{\left(E_\alpha - E_\beta + \omega\right)^2 + \eta^2} \end{aligned}$$

- 这是susceptibility(两粒子关联函数)的涨落耗散定理. 利用玻色分布$n_B\left(\omega\right) = 1/(e^{\omega/T} - 1)$, 可以改写为

$$1 + n_B\left(\omega\right) = 1 + \frac{1}{e^{\omega/T} - 1} = \frac{e^{\omega/T}}{e^{\omega/T} - 1} = \frac{1}{1 - e^{-\omega/T}}$$

$$S(\mathbf{q}, \omega) = (1 + n_B(\omega))[-2 \operatorname{Im} R(\mathbf{q}, \omega)]$$

  - 等号右边响应函数的虚部代表体系的耗散, 等号左边动力学结构因子代表涨落, 涨落耗散定理给出了两者的关系.

- $S(\mathbf{q},\omega)$和$R(\mathbf{q},\omega)$其实在定义上就很有关系. 不考虑前置因子, 推迟关联函数$R(\mathbf{q},\omega)$是一个**对易子**$[A,B]$的关联, 结构因子$S(\mathbf{q},\omega)$是**对易子第一项**AB的关联, 其中A,B是单体算符.
  - $A=S_{\mathbf{q}}^{\alpha}, B=S_{-\mathbf{q}}^{\alpha'}$两个算符, 仅当$\alpha=\alpha'$时两个算符互为厄米共轭.
- Bruus书上介绍的是单粒子关联函数的涨落耗散定理, 和这个非常类比.
  - 费米子情形

$$
\begin{aligned}
iG^{>}(\nu,\omega) &= A(\nu,\omega)\left[1-n_F(\omega)\right] \\
-iG^{<}(\nu,\omega) &= A(\nu,\omega)n_F(\omega)
\end{aligned}
$$

  - 玻色子情形: 可以直接对应两粒子关联函数的情形

$$
\begin{aligned}
iG^{>}(\nu,\omega) &= A(\nu,\omega)\left[1+n_B(\omega)\right] \\
iG^{<}(\nu,\omega) &= A(\nu,\omega)n_B(\omega)
\end{aligned}
\tag{1}
$$

  - 谱函数$A(\nu,\omega)=-2\mathrm{Im}G^{R}(\nu,\omega)$, 其中推迟格林函数 $G^{R}(\nu,\omega)$是一个**对易子**$[c,c^{\dagger}]_{\mathrm{B,F}}$的关联; 而趋大格林函数(greater Green's function) $G^{>}(\nu,\omega)$是**对易子第一项**$cc^{\dagger}$的关联.
    - 基于Lehmann 表象的好处, 我们只用考虑对角的格林函数(非对角的一定是零), 即$c=c_{\nu}$, $c^{\dagger}=c_{\nu}^{\dagger}$, 两个算符一定互为厄米共轭.
      - 这样类比的话, 我会怀疑$\alpha\neq\alpha'$时涨落耗散定理是否可以得证. #Question

Z B.3 The Generating Functional

理论学家关心从微观模型出发来计算响应函数或结构因子. 对相互作用多体系统, 一个有用的工具是虚时生成泛函 (imaginary time generating functional). 在正文中, 我们遇到了生成泛函的路径积分表示, 它们易于开展半经典或large-N近似. 这里, 我们证明响应函数 $R(\mathbf{q},\omega)$ 是生成泛函的二阶导.

巨正则生成泛函 (grand canonical generating functional) 定义为

Ⓝ (AssaB.17)

$$
Z[j,\mu]=\mathrm{Tr}\,T_{\tau}\left(\exp\left[-\int_0^{\beta}d\tau\mathcal{H}[j(\tau)]\right]\right)
$$

- 虚时哈密顿量

Ⓝ (AssaB.18)

$$
\mathcal{H}[j(\tau)]=\mathcal{H}_0(\mu)-\sum_{i\alpha}j_i^{\alpha}(\tau)S_i^{\alpha},\quad \tau\in[0,\beta).
$$

- 时序算符 $T(\bullet)$,将算符排序使得τ从左到右递减. 这里是一个虚时演化算符, i 被吸收进了虚时τ里面.

对于旋转对称的 $\mathcal{H}_0$, $\langle S_i^{\alpha}\rangle=0$. 虚时关联函数定义为生成泛函对数的二阶导, 在source current=0处的取值

$$
\begin{aligned}
\tilde{R}_{i,i'}^{\alpha\alpha'}(\tau,\tau') &= \left.\frac{\delta^2 \ln Z}{\delta j_i^\alpha(\tau)\delta j_{i'}^{\alpha'(\tau')}}\right|_{j=0} \\
&= Z^{-1}\,\mathbf{Tr}\left\{e^{-\beta\mathcal{H}_0}T_\tau\left[S_i^\alpha(\tau)S_{i'}^{\alpha'}(\tau')\right]\right\},
\end{aligned}
$$

> 可能需要先把时序展开? 虚时相互作用绘景算符$S_i^\alpha(\tau)$是怎么弄出来的?
>
> $$
> \begin{aligned}
> \tilde{R}_{i,i'}^{\alpha\alpha'}(\tau,\tau') &= \left.\frac{\delta^2 \ln Z}{\delta j_i^\alpha(\tau)\delta j_{i'}^{\alpha'}(\tau')}\right|_{j=0} \\
> &= \frac{1}{Z}\frac{\delta}{\delta j_i^\alpha(\tau)}\mathrm{Tr}\left\{T_\tau\left[\exp\left(\int_0^\beta d\tau\left(\mathcal{H}_0-\sum_{i\alpha}j_i^\alpha(\tau)S_i^\alpha\right)\right)\frac{\delta}{\delta j_{i'}^{\alpha'}(\tau')}\int_0^\beta d\tau\left(\mathcal{H}_0-\sum_{i\alpha}j_i^\alpha(\tau)S_i^\alpha\right)\right]\right\}\Bigg|_{j=0} \\
> &= \frac{1}{Z}\frac{\delta}{\delta j_i^\alpha(\tau)}\mathrm{Tr}\left\{T_\tau\left[\exp\left(\int_0^\beta d\tau\left(\mathcal{H}_0-\sum_{i\alpha}j_i^\alpha(\tau)S_i^\alpha\right)\right)\left(-S_{i'}^{\alpha'}\right)\right]\right\}\Bigg|_{j=0}
> \end{aligned}
> $$

- 虚时相互作用绘景中的算符

Ⓝ (AssaB.20)

$$S_i^\alpha(\tau) \equiv e^{\mathcal{H}_0\tau}S_i^\alpha e^{-\mathcal{H}_0\tau},$$

- 自旋算符的时序: 交换不会变号

Ⓝ (AssaB.21)

$$T_\tau\left[A(\tau)B(\tau')\right] = \begin{cases} A(\tau)B(\tau') & \tau \geq \tau' \\ B(\tau')A(\tau) & \tau < \tau' \end{cases}$$

从式(B.19)出发, 利用求迹的轮换不变性, 可以验证有时间平移不变性

Ⓝ (AssaB.22)

$$\tilde{R}(\tau,\tau') = \tilde{R}(\tau-\tau',0) \equiv \tilde{R}(\tau-\tau'),$$

且 $\tilde{R}(\tau)$ 是区间 $[0,\beta)$上的周期函数:

Ⓝ (AssaB.23)

$$\lim_{\tau\to\beta^-}\tilde{R}(\tau) = \lim_{\tau\to 0^-}\tilde{R}(\tau).$$

对于时空平移不变哈密顿量, 使用$\tilde{R}_{ii'}(\tau)$的Fourier变换是方便的

Ⓝ (AssaB.24)

$$\tilde{R}(\mathbf{q},i\omega_n) = \mathcal{N}^{-1}\sum_{ii'}\int_0^\beta d\tau e^{-i\mathbf{q}(\mathbf{x}_i-\mathbf{x}_{i'})-i\omega_n\tau}\tilde{R}_{ii'}(\tau)$$

Ⓝ (AssaB.25)

$$\omega_n = 2n\pi\beta^{-1}, \quad n = 0,\pm1,\pm2,\ldots$$

这些频率 ω_n 是 Bose-Matsubara 频率. 往(AssaB.19)的算符中插入一组完备本征态, 然后开展式(AssaB.24)中的 $d\tau$ 积分, 我们发现 $\tilde{R}(\mathbf{q},i\omega_n)$ 实际上是谱响应函数(见式(AssaB.10))的解析延拓:

$$\tilde{R}(\mathbf{q},z)\Big|_{z\to\omega+i0^+} = \mathrm{Re}\,R(\mathbf{q},\omega) + i\,\mathrm{Im}\,R(\mathbf{q},\omega).$$

右手边的函数是物理可观测量, 描述系统在频率ω处的响应和耗散. 这些物理量与结构因子通过涨落-耗散定理(AssaB.16)联系. 左手边是从理论如虚时生成泛函得到的.

最后, 我们定义**静态磁化率 (static susceptibility)**, 它是动量$\mathbf{q}$处磁化强度对α方向ordering field的响应, 具有波矢 $\mathbf{q}$:

$$\chi^{\alpha\alpha}(\mathbf{q}) = -\frac{1}{2}\,\mathrm{Re}\,R^{\alpha\alpha}(\mathbf{q},0). \tag{AssaB.27}$$

Bibliography

Some recommended textbooks for this material are:

- P.C. Martin, Measurements and Correlation Functions (Gordon and Breach, 1968);
- G. Rickayzen, Green's Functions and Condensed Matter (Academic Press, 1980).

> See also the bibliographies of Chapters 1 and 2.