介观物理第三次作业

董建宇 202328000807038

Problem I.1 Verify the Kramers-Kronig relation using the explicit solution given in Eq. (12).

$$\bar{\chi}(\omega) = \frac{1}{m}\frac{1}{\omega^2 - \omega_0^2 + i\gamma\omega},$$
$$\bar{\chi}(t-t') = -\frac{1}{m}\int \frac{d\omega}{2\pi}\frac{e^{-i\omega(t-t')}}{\omega^2 - \omega_0^2 + i\gamma\omega}.$$

Proof. $Kramers-Kronig$ 关系为:

$$\chi'(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi''(\omega')P\frac{1}{\omega'-\omega},$$
$$\chi''(\omega) = -\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi'(\omega')P\frac{1}{\omega'-\omega}.$$

其中 $\chi'(\omega)$ 和 $\chi''(\omega)$ 分别为 $\chi(\omega)$ 的实部和虚部。

$$\chi'(\omega) = \frac{1}{m}\frac{\omega_0^2 - \omega^2}{(\omega^2-\omega_0^2)^2 + \gamma^2\omega^2};$$
$$\chi''(\omega) = \frac{1}{m}\frac{\gamma\omega}{(\omega^2-\omega_0^2)^2 + \gamma^2\omega^2}$$

则可以计算:

$$\begin{aligned}
\mathbf{I_1} =& \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{1}{m}\frac{\gamma\omega'}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}P\frac{1}{\omega'-\omega}\\
=&\frac{1}{\pi m}\int_{-\infty}^{\infty}\frac{\gamma\omega'}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\left[-\frac{1}{\omega-\omega'+i0^+} - i\pi\delta(\omega-\omega')\right]d\omega'\\
=&-\frac{1}{\pi m}\int_{-\infty}^{\infty}\frac{\gamma\omega'}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\frac{1}{\omega-\omega'+i0^+}d\omega' - \frac{i}{m}\frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}.
\end{aligned}$$

被积函数记作:

$$\begin{aligned}
f(\omega') =& \frac{\gamma\omega'}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\frac{1}{\omega-\omega'+i0^+}\\
=&\frac{\gamma\omega'}{(\omega+i0^+-\omega')(\omega'-\omega_1)(\omega'-\omega_2)(\omega'-\omega_1^*)(\omega'-\omega_2^*)}.
\end{aligned}$$

其中

$$\omega_1 = \frac{i\gamma+\sqrt{\Delta}}{2};\quad \omega_2 = \frac{i\gamma-\sqrt{\Delta}}{2};\quad \Delta = 4\omega_0^2 - \gamma^2.$$

即被积函数在上半复平面有三个奇点，分别是 $\omega + i0^+$; ω_1; ω_2。分别计算其留数可得:

$$\mathbf{Res}[f(\omega'), \omega+i0^+] = -\frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2};$$
$$\mathbf{Res}[f(\omega'), \omega_1] = \frac{\gamma\omega_1}{(\omega-\omega_1)(\omega_1-\omega_2)(\omega_1-\omega_1^*)(\omega_1-\omega_2^*)}$$

$$
\begin{aligned}
&=\frac{\omega_1}{\omega-\omega_1}\cdot\frac{\gamma}{\sqrt{\Delta}(i\gamma)(i\gamma+\sqrt{\Delta})}\\
&=\frac{1}{2i\sqrt{\Delta}(\omega-\omega_1)};\\
\mathbf{Res}[f(\omega'),\omega_2] &=\frac{\gamma\omega_2}{(\omega-\omega_2)(\omega_2-\omega_1)(\omega_2-\omega_1^*)(\omega_2-\omega_2^*)}\\
&=\frac{\omega_2}{\omega-\omega_2}\cdot\frac{\gamma}{\sqrt{\Delta}(i\gamma)(-i\gamma+\sqrt{\Delta})}\\
&=\frac{1}{2i\sqrt{\Delta}(\omega-\omega_2)}.
\end{aligned}
$$

利用留数定理可得，积分式为:

$$
\begin{aligned}
\int_{-\infty}^{\infty} f(\omega')d\omega' &=2\pi i(\mathbf{Res}[f(\omega'),\omega+i0^+]+\mathbf{Res}[f(\omega'),\omega_1]+\mathbf{Res}[f(\omega'),\omega_2])\\
&=\frac{2\pi i}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\left(-\gamma\omega+\frac{\omega^2-\omega_0^2+i\gamma\omega}{2i}\right)
\end{aligned}
$$

则有:

$$
\begin{aligned}
\mathbf{I_1} =&-\frac{1}{\pi m}\int_{-\infty}^{\infty} f(\omega')d\omega'-\frac{i}{m}\frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\\
=&\frac{1}{m}\frac{\omega_0^2-\omega^2}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\\
=&\chi'(\omega).
\end{aligned}
$$

同样的，考虑

$$
\begin{aligned}
\mathbf{I_2} =&-\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{1}{m}\frac{\omega_0^2-\omega'^2}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}P\frac{1}{\omega'-\omega}\\
=&-\frac{1}{\pi m}\int_{-\infty}^{\infty}\frac{\omega_0^2-\omega'^2}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\left[-\frac{1}{\omega-\omega'+i0^+}-i\pi\delta(\omega-\omega')\right]d\omega'\\
=&\frac{1}{\pi m}\int_{-\infty}^{\infty}\frac{\omega_0^2-\omega'^2}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\frac{1}{\omega-\omega'+i0^+}d\omega'+\frac{i}{m}\frac{\omega_0^2-\omega^2}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}.
\end{aligned}
$$

被积函数记作:

$$
\begin{aligned}
g(\omega') =&\frac{\omega_0^2-\omega'^2}{(\omega'^2-\omega_0^2)^2+\gamma^2\omega'^2}\frac{1}{\omega-\omega'+i0^+}\\
=&\frac{\omega_0^2-\omega'^2}{(\omega+i0^+-\omega')(\omega'-\omega_1)(\omega'-\omega_2)(\omega'-\omega_1^*)(\omega'-\omega_2^*)}.
\end{aligned}
$$

即被积函数在上半复平面有三个奇点，分别是 $\omega+i0^+$; ω_1; ω_2。分别计算其留数可得:

$$
\begin{aligned}
\mathbf{Res}[g(\omega'),\omega+i0^+] &=\frac{\omega^2-\omega_0^2}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2};\\
\mathbf{Res}[g(\omega'),\omega_1] &=\frac{\omega_0^2-\omega_1^2}{(\omega-\omega_1)(\omega_1-\omega_2)(\omega_1-\omega_1^*)(\omega_1-\omega_2^*)}\\
&=\frac{\omega_0^2-\omega_1^2}{\omega-\omega_1}\cdot\frac{1}{\sqrt{\Delta}(i\gamma)(i\gamma+\sqrt{\Delta})}
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{\omega_2(\omega_0^2-\omega_1^2)}{\omega-\omega_1}\frac{-1}{2i\gamma\omega_0^2\sqrt{\Delta}};\\
\mathbf{Res}[g(\omega'),\omega_2] &= \frac{\omega_0^2-\omega_2^2}{(\omega-\omega_2)(\omega_2-\omega_1)(\omega_2-\omega_1^*)(\omega_2-\omega_2^*)}\\
&= \frac{\omega_0^2-\omega_2^2}{\omega-\omega_2}\cdot\frac{1}{\sqrt{\Delta}(i\gamma)(-i\gamma+\sqrt{\Delta})}\\
&= \frac{\omega_1(\omega_0^2-\omega_1^2)}{\omega-\omega_2}\frac{1}{2i\gamma\omega_0^2\sqrt{\Delta}}.
\end{aligned}
$$

利用留数定理可得，积分式为:

$$
\begin{aligned}
\int_{-\infty}^{\infty} g(\omega')d\omega' &= 2\pi i(\mathbf{Res}[g(\omega'),\omega+i0^+]+\mathbf{Res}[g(\omega'),\omega_1]+\mathbf{Res}[g(\omega'),\omega_2])\\
&= \frac{2\pi i}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\left(-\frac{i\gamma\omega}{2}+\frac{\omega^2-\omega_0^2}{2}\right)
\end{aligned}
$$

则有:

$$
\begin{aligned}
\mathbf{I_2} &= \frac{1}{\pi m}\int_{-\infty}^{\infty} g(\omega')d\omega' + \frac{i}{m}\frac{\omega_0^2-\omega^2}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\\
&= \frac{1}{m}\frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\\
&= \chi''(\omega).
\end{aligned}
$$

□

Problem I.2 * Read Kubo's paper entitled "The fluctuation-dissipation theorem".

Problem I.3 Derive the Kubo formula in Eq. (28).

$$
\chi(\mathbf{r},\mathbf{r}';\omega) = \frac{i}{\hbar}\int_{-\infty}^{t} dt' e^{i\omega(t-t')}\langle 0|\,[\hat{X}(\mathbf{r},t),\hat{X}(\mathbf{r}',t')]\,|0\rangle\,.
$$

Proof. 响应函数为:

$$
\chi(\mathbf{r},t;\mathbf{r}',t') = \frac{i}{\hbar}\theta(t-t')\langle 0|\,[\hat{X}(\mathbf{r},t),\hat{X}(\mathbf{r}',t')]\,|0\rangle\,.
$$

对于不显含时的哈密顿量，响应函数只与 $t-t'$ 相关，令 $t''=t-t'$，做傅里叶变换可得:

$$
\begin{aligned}
\chi(\mathbf{r},\mathbf{r}';\omega) &= \int_{-\infty}^{\infty} e^{i\omega t''}\chi(\mathbf{r},\mathbf{r}';t'')\,dt''\\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} e^{i\omega(t-t')}\theta(t'')\langle 0|\,[\hat{X}(\mathbf{r},t),\hat{X}(\mathbf{r}',t')]\,|0\rangle\;dt''\\
&= \frac{i}{\hbar}\int_{0}^{\infty} e^{i\omega t''}\langle 0|\,[\hat{X}(\mathbf{r},t),\hat{X}(\mathbf{r}',t')]\,|0\rangle\;dt''\\
&= \frac{i}{\hbar}\int_{-\infty}^{t} e^{i\omega(t-t')}\langle 0|\,[\hat{X}(\mathbf{r},t),\hat{X}(\mathbf{r}',t')]\,|0\rangle\;dt'.
\end{aligned}
$$

即得到 Kubo 公式。 □