高等量子力学第四次作业

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习题 1 受迫谐振子的哈密顿量为:

$$\hat{H} = \hat{H}_0 + \hat{V}; \qquad \hat{H}_0 = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}), \qquad \hat{V} = \hat{V} = \hbar g(\hat{a} + \hat{a}^\dagger).$$

体系初始时刻处于 $\hat{H}_0$ 的基态 $|0\rangle$。

分别在 Schrödinger 绘景、Heisenberg 绘景和 Interaction 绘景下，计算下列物理量的平均值:

$$\hat{n} = \hat{a}^\dagger\hat{a}, \qquad \hat{x} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger), \qquad \hat{p} = \frac{1}{\sqrt{2}i}(\hat{a} - \hat{a}^\dagger).$$

Schrödinger 绘景:

由于体系哈密顿量不显含时间，则在 t 时刻，体系量子态可以写作:

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|0\rangle .$$

记 $\hat{A} = i\hat{H}t/\hbar = i(\omega t(\hat{n} + 1/2) + \sqrt{2}gt\hat{x})$，可以计算:

$$\begin{aligned}
&[\hat{n}, \hat{x}] = -i\hat{p}; \quad [\hat{n}, \hat{p}] = i\hat{x}; \quad [\hat{x}, \hat{p}] = i; \\
&[\hat{A}, \hat{n}] = i[\omega t(\hat{n} + 1/2) + \sqrt{2}gt\hat{x}, \hat{n}] = -\sqrt{2}gt\hat{p}; \\
&[\hat{A}, \hat{x}] = i[\omega t(\hat{n} + 1/2) + \sqrt{2}gt\hat{x}, \hat{x}] = \omega t\hat{p}; \\
&[\hat{A}, \hat{p}] = i[\omega t(\hat{n} + 1/2) + \sqrt{2}gt\hat{x}, \hat{p}] = -\omega t\hat{x} - \sqrt{2}gt.
\end{aligned}$$

(a) 对于 $\hat{n} = \hat{a}^\dagger\hat{a}$ 的平均值，可以先计算 $e^{\hat{A}}\hat{n}e^{-\hat{A}}$ 如下:

$$\begin{aligned}
e^{\hat{A}}\hat{n}e^{-\hat{A}} =& \hat{n} + \frac{1}{1!}[\hat{A}, \hat{n}] + \frac{1}{2!}[\hat{A}, [\hat{A}, \hat{n}]] + \cdots \\
=& \hat{n} + \frac{1}{1!}(-\sqrt{2}gt\hat{p}) + \frac{1}{2!}(\sqrt{2}\omega gt^2\hat{x} + 2g^2t^2) \\
&+ \frac{1}{3!}(\sqrt{2}\omega^2 gt^3\hat{p}) + \frac{1}{4!}(-\sqrt{2}\omega^3 gt^4\hat{x} - 2\omega^2 g^2t^4) + \cdots \\
=& \hat{n} + \frac{\sqrt{2}g}{\omega}\hat{x}\left(\frac{1}{2!}(\omega t)^2 - \frac{1}{4!}(\omega t)^4 + \cdots\right) \\
&- \frac{\sqrt{2}g}{\omega}\hat{p}\left(\frac{1}{1!}(\omega t) - \frac{1}{3!}(\omega t)^3 + \cdots\right) + \frac{2g^2}{\omega^2}\left(\frac{1}{2!}(\omega t)^2 - \frac{1}{4!}(\omega t)^4 + \cdots\right) \\
=& \hat{n} + \frac{\sqrt{2}g}{\omega}\hat{x}(1 - \cos(\omega t)) - \frac{\sqrt{2}g}{\omega}\hat{p}\sin(\omega t) + \frac{2g^2}{\omega^2}(1 - \cos(\omega t)).
\end{aligned}$$

则有:

$$\langle\psi(t)|\,\hat{n}\,|\psi(t)\rangle = \langle 0|\,e^{\hat{A}}\hat{n}e^{-\hat{A}}\,|0\rangle = \frac{2g^2}{\omega^2}(1 - \cos(\omega t)).$$

(b) 对于 $\hat{x}=\frac{1}{\sqrt{2}}(\hat{a}^\dagger+\hat{a})$，可以先计算 $e^{\hat{A}}\hat{x}e^{-\hat{A}}$ 如下:

$$\begin{aligned}
e^{\hat{A}}\hat{x}e^{-\hat{A}} =&\hat{x}+\frac{1}{1!}[\hat{A},\hat{x}]+\frac{1}{2!}[\hat{A},[\hat{A},\hat{x}]]+\cdots\\
=&\hat{x}+\frac{1}{1!}(\omega t\hat{p})+\frac{1}{2!}(-(\omega t)^2\hat{x}-\sqrt{2}\omega g t^2)\\
&+\frac{1}{3!}(-(\omega t)^3\hat{p})+\frac{1}{4!}((\omega t)^4\hat{x}+\sqrt{2}g\omega^3t^4)+\cdots\\
=&\hat{x}\left(1-\frac{1}{2!}(\omega t)^2+\frac{1}{4!}(\omega t)^4+\cdots\right)+\hat{p}\left(\frac{1}{1!}(\omega t)-\frac{1}{3!}(\omega t)^3+\cdots\right)\\
&+\frac{\sqrt{2}g}{\omega}\left(-\frac{1}{2!}(\omega t)^2+\frac{1}{4!}(\omega t)^4+\cdots\right)\\
=&\hat{x}\cos(\omega t)+\hat{p}(\sin(\omega t))+\frac{\sqrt{2}g}{\omega}(\cos(\omega t)-1).
\end{aligned}$$

则有:

$$\langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle=\langle 0|\,e^{\hat{A}}\hat{x}e^{-\hat{A}}\,|0\rangle=\frac{\sqrt{2}g}{\omega}(\cos(\omega t)-1).$$

(c) 对于 $\hat{p}=\frac{1}{\sqrt{2}i}(\hat{a}-\hat{a}^\dagger)$ 的平均值，可以先计算 $e^{\hat{A}}\hat{p}e^{-\hat{A}}$ 如下:

$$\begin{aligned}
e^{\hat{A}}\hat{p}e^{-\hat{A}} =&\hat{p}+\frac{1}{1!}[\hat{A},\hat{p}]+\frac{1}{2!}[\hat{A},[\hat{A},\hat{p}]]+\cdots\\
=&\hat{p}+\frac{1}{1!}(-\omega t\hat{x}-\sqrt{2}gt)+\frac{1}{2!}(-(\omega t)^2\hat{p})+\frac{1}{3!}((\omega t)^3\hat{x}+\sqrt{2}g\omega^2t^3)+\cdots\\
=&\hat{p}\left(1-\frac{1}{2!}(\omega t)^2+\cdots\right)-\hat{x}\left(-\frac{1}{1!}\omega t+\frac{1}{3!}(\omega t)^3+\cdots\right)-\frac{\sqrt{2}g}{\omega}\left(\omega t-\frac{1}{3!}(\omega t)^3\right)\\
=&\hat{p}\cos(\omega t)-\hat{x}\sin(\omega t)-\frac{\sqrt{2}g}{\omega}\sin(\omega t).
\end{aligned}$$

则有:

$$\langle\psi(t)|\,\hat{p}\,|\psi(t)\rangle=\langle 0|\,e^{\hat{A}}\hat{p}e^{-\hat{A}}\,|0\rangle=-\frac{\sqrt{2}g}{\omega}\sin(\omega t).$$

Heisenberg 绘景:

对于 Heisenberg 绘景下算符 $\hat{A}_H(t)=U^\dagger(t,0)\hat{A}_SU(t,0)$，满足 Heisenberg 方程:

$$i\hbar\frac{d\hat{A}_H(t)}{dt}=[\hat{A}_H(t),\hat{H}].$$

则对于三个算符可以计算:

$$\begin{aligned}
i\hbar\frac{d\hat{n}_H(t)}{dt} =&[\hat{n}_H(t),\hat{H}]=-i\sqrt{2}\hbar g\hat{p}_H(t);\\
i\hbar\frac{d\hat{x}_H(t)}{dt} =&[\hat{x}_H(t),\hat{H}]=i\hbar\omega\hat{p}_H(t);\\
i\hbar\frac{d\hat{p}_H(t)}{dt} =&[\hat{p}_H(t),\hat{H}]=-i\hbar\omega\hat{x}_H(t)-i\sqrt{2}\hbar g.
\end{aligned}$$

将第三个方程两侧对时间求导并取平均可得:

$$i\hbar\frac{d^2p_H(t)}{dt^2}=-i\hbar\omega\frac{dx_H(t)}{dt}=-i\hbar\omega^2p_H(t).$$

则有:

$$p_H(t)=a_1\sin(\omega t)+a_2\cos(\omega t)+a_3.$$

利用 $p_H(0)=0$, $\frac{dp_H(0)}{dt}=-\sqrt{2}g$, $\frac{d^2p_H(0)}{dt^2}=0$ 可得: $a_1=-\frac{\sqrt{2}g}{\omega}$, $a_2=a_3=0$。即有:

$$\langle 0|\,\hat{p}_H(t)\,|0\rangle=-\frac{\sqrt{2}g}{\omega}\sin(\omega t).$$

第一个方程两侧取平均有:

$$\frac{dn_H(t)}{dt}=-\sqrt{2}gp_H(t)=\frac{2g^2}{\omega}\sin(\omega t).$$

则有:

$$n_H(t)=-\frac{2g^2}{\omega^2}\cos(\omega t)+b_1.$$

利用 $n_H(0)=0$, 可得: $b_1=\frac{2g^2}{\omega^2}$, 则有:

$$n_H(t)=\frac{2g^2}{\omega^2}(1-\cos(\omega t)).$$

第二个方程两侧取平均有:

$$\frac{dx_H(t)}{dt}=\omega p_H(t)=-\sqrt{2}g\sin(\omega t).$$

则有:

$$x_H(t)=\frac{\sqrt{2}g}{\omega}\cos(\omega t)+c_1$$

利用 $x_H(0)=0$, 可得: $c_1=-\frac{\sqrt{2}g}{\omega}$, 则有:

$$x_H(t)=\frac{\sqrt{2}g}{\omega}(\cos(\omega t)-1).$$

综上所述, 在 Heisenberg 绘景下, 三个算符平均值分别为:

$$\langle 0|\,\hat{n}_H(t)\,|0\rangle=\frac{2g^2}{\omega^2}(1-\cos(\omega t));$$

$$\langle 0|\,\hat{x}_H(t)\,|0\rangle=\frac{\sqrt{2}g}{\omega}(\cos(\omega t)-1);$$

$$\langle 0|\,\hat{p}_H(t)\,|0\rangle=-\frac{\sqrt{2}g}{\omega}\sin(\omega t).$$

Interaction 绘景:

在 Interaction 绘景下, 算符 $\hat{A}_I=U_0^\dagger(t,0)\hat{A}_SU_0(t,0)$ 满足方程:

$$i\hbar\frac{d\hat{A}_I(t)}{dt}=[\hat{A}_I(t),\hat{H}_0]$$

其中 $U_0(t,0)=e^{-i\hat{H}_0 t/\hbar}$。Interaction 绘景下态矢量满足:

$$i\hbar\frac{d}{dt}\left|\psi_I(t)\right\rangle=\hat{V}_I(t)\left|\psi_I(t)\right\rangle.$$

取一阶近似，有:

$$\left|\psi_I(t)\right\rangle=\hat{U}_I(t,0)\left|\psi_I(t)\right\rangle=\left(1+\frac{1}{i\hbar}\int_0^t\hat{V}_I(t')dt'\right)\left|\psi_I(0)\right\rangle.$$

其中 $\left|\psi_I(0)\right\rangle=\left|\psi(0)\right\rangle=\left|0\right\rangle$。从而可以计算:

$$\begin{aligned}\left|\psi_I(t)\right\rangle&=\left|0\right\rangle+\frac{1}{i\hbar}\int_0^t e^{i\omega t(\hat{n}+1/2)}\sqrt{2}g\hbar\hat{x}e^{-i\omega t(\hat{n}+1/2)}\left|0\right\rangle\\&=\left|0\right\rangle-ig\int_0^t e^{i\omega t'}dt'\left|1\right\rangle\\&=\left|0\right\rangle-\frac{g}{\omega}(e^{i\omega t}-1)\left|1\right\rangle.\end{aligned}$$

对于三个算符可以计算:

$$\begin{aligned}i\hbar\frac{d\hat{n}_I(t)}{dt}=&[\hat{n}_I(t),\hat{H}_0]=0;\\i\hbar\frac{d\hat{x}_I(t)}{dt}=&[\hat{x}_I(t),\hat{H}_0]=i\hbar\omega\hat{p}_I(t);\\i\hbar\frac{d\hat{p}_I(t)}{dt}=&[\hat{p}_I(t),\hat{H}_0]=-i\hbar\omega\hat{x}_I(t).\end{aligned}$$

则有:

$$\begin{aligned}\hat{n}_I(t)=&\hat{n}_I(0)=\hat{n};\\\hat{x}_I(t)=&\hat{A}_1\sin(\omega t)-\hat{A}_2\cos(\omega t);\\\hat{p}_I(t)=&\hat{A}_1\cos(\omega t)+\hat{A}_2\sin(\omega t).\end{aligned}$$

利用 $\hat{x}_I(0)=\hat{x}$, $\hat{p}_I(0)=\hat{p}$，可得: $\hat{A}_1=\hat{p}$, $\hat{A}_2=-\hat{x}$。即:

$$\begin{aligned}\hat{x}_I(t)=&\hat{p}\sin(\omega t)+\hat{x}\cos(\omega t);\\\hat{p}_I(t)=&\hat{p}\cos(\omega t)-\hat{x}\sin(\omega t).\end{aligned}$$

则可以计算三个算符的平均值为:

$$\begin{aligned}\left\langle\psi_I(t)\right|\hat{n}_I(t)\left|\psi_I(t)\right\rangle=&\frac{2g^2}{\omega^2}(1-\cos(\omega t));\\\left\langle\psi_I(t)\right|\hat{x}_I(t)\left|\psi_I(t)\right\rangle=&\frac{\sqrt{2}g}{\omega}(\cos(\omega t)-1);\\\left\langle\psi_I(t)\right|\hat{p}_I(t)\left|\psi_I(t)\right\rangle=&-\frac{\sqrt{2}g}{\omega}\sin(\omega t).\end{aligned}$$

习题 2 利用路径积分推导一维谐振子的传播子表达式

传播子为:

$$
\begin{aligned}
K(x_f,t_f;x_i,t_i) &= \prod_{k=1}^{N-1}\sqrt{\frac{m}{2\pi i\hbar\tau}}\int dx_k \prod_{j=0}^{N-1} e^{\frac{i}{\hbar}\tau\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2-V(x_j)\right]} \\
&= \prod_{k=1}^{N-1}\int dx_k \prod_{j=0}^{N-1} K(x_{j+1},x_j,\tau)
\end{aligned}
$$

其中

$$
K(x_{j+1},x_j,\tau)=K(x_{j+1},t_{j+1},x_j,t_j)=\sqrt{\frac{m}{2\pi i\hbar\tau}}e^{\frac{i}{\hbar}\tau\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2-V(x_j)\right]}
$$

当 $\tau\to 0$ 时，可以做如下近似:

$$
V(x_j)\approx\frac{1}{2}(V(x_{j+1})+V(x_j))
$$

则短时传播子为:

$$
\begin{aligned}
K(x_{j+1},x_j,\tau) =&\sqrt{\frac{m}{2\pi i\hbar\tau}}e^{\frac{i}{\hbar}\tau\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2-\frac{1}{2}(V(x_{j+1})+V(x_j))\right]} \\
=&\sqrt{\frac{m}{2\pi i\hbar\tau}}e^{\frac{im}{2\hbar}\frac{1}{\tau}\left[(\frac{x_{j+1}-x_j}{)}^{2}-\frac{\omega^2\tau^2}{2}(x_{j+1}^2+x_j^2)\right]} \\
=&\sqrt{\frac{m\omega}{2\pi i\hbar}}\sqrt{\frac{1}{\omega\tau}}e^{\frac{im\omega}{2\hbar}\frac{1}{\omega\tau}}\left[\left(1-\frac{\omega^2\tau^2}{2}\right)(x_{j+1}^2+x_j^2)-2x_{j+1}x_j\right]
\end{aligned}
$$

可以做变量替换:

$$
\sin\phi=\omega\tau.
$$

当 $\tau\to 0$ 时，有: $\phi\approx\sin\phi=\omega\tau$, $\cos\phi=\sqrt{1-\omega^2\tau^2}\approx 1-\omega^2\tau^2/2$，则有:

$$
F(\eta,\eta';\phi)=K(\eta,\eta';\frac{\sin\phi}{\omega})=\sqrt{\frac{m\omega}{2\pi i\hbar}}\sqrt{\frac{1}{\sin\phi}}e^{\frac{im\omega}{2\hbar}\frac{1}{\sin\phi}[(\eta^2+\eta'^2)\cos\phi-2\eta\eta']}
$$

可以计算:

$$
\begin{aligned}
\int d\eta F(\eta'',\eta;\phi)F(\eta,\eta';\phi) =&\frac{m\omega}{2\pi i\hbar}\frac{1}{\sin\phi}e^{\frac{im\omega}{2\hbar}\frac{\cos\phi}{\sin\phi}(\eta''^2+\eta'^2)}\int d\eta e^{\frac{im\omega}{\hbar}\frac{1}{\sin\phi}[\eta^2\cos\phi-\eta(\eta''+\eta')]} \\
=&\frac{m\omega}{2\pi i\hbar}\frac{1}{\sin\phi}\sqrt{\frac{\pi i\hbar\sin\phi}{m\omega\cos\phi}}e^{\frac{im\omega}{2\hbar}\frac{1}{\sin\phi}[(\eta''^2+\eta'^2)\cos\phi-\frac{(\eta''+\eta)^2}{2\cos\phi}]} \\
=&\sqrt{\frac{m\omega}{2\pi i\hbar}}\sqrt{\frac{1}{\sin 2\phi}}e^{\frac{im\omega}{2\hbar}\frac{1}{\sin 2\phi}[(\eta''^2+\eta'^2)\cos 2\phi-2\eta''\eta']} \\
=&F(\eta'',\eta';2\phi).
\end{aligned}
$$

利用此性质，可以计算传播子如下:

$$
\begin{aligned}
K(x_f,t_f;x_i,t_i) =& \prod_{k=1}^{N-1}\int dx_k\prod_{j=0}^{N-1}F(x_{j+1},x_j,\phi) \\
=&F(x_f,x_i,T)
\end{aligned}
$$

$$
= \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t_f-t_i)}\right)^{1/2} e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t_f-t_i)}[(x_f^2+x_i^2)\cos\omega(t_f-t_i)-2x_f x_i]}.
$$

习题 3 SSH model 的哈密顿量可以写为:

$$
\hat{H}_{SSH}(k) = (t_1 + t_2\cos k)\hat{\sigma}_x + t_2\hat{\sigma}_y.
$$

计算:

$$
\gamma = \int_{-\pi}^{\pi}\sum_i \langle n_i(k)|\, i\frac{\partial}{\partial k}\, |n_i(k)\rangle\, dk.
$$

系统哈密顿量可以写为:

$$
H = \begin{pmatrix} 0 & t_1 + t_2 e^{-ik} \\ t_1 + t_2 e^{ik} & 0 \end{pmatrix}
$$

将其对角化可得两个本征态分别为:

$$
|u_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\frac{t_1+t_2e^{-ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}} & 1\end{pmatrix}^T; \quad |u_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-\frac{t_1+t_2e^{-ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}} & 1\end{pmatrix}^T.
$$

则可以计算 Berry Phase 为:

$$
\begin{aligned}
\gamma_1 =& \int_{-\pi}^{\pi}\langle u_1(k)|\, i\frac{d}{dk}\, |u_1(k)\rangle\, dk \\
=& \frac{i}{2}\int_{-\pi}^{\pi}\frac{t_1+t_2e^{ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}}\frac{d}{dk}\frac{t_1+t_2e^{-ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}}dk \\
=& \frac{i}{2}\int_{-\pi}^{\pi}\frac{t_1+t_2e^{ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}}\left(\frac{-it_2e^{-ik}}{\sqrt{t_1^2+t_2^2+2t_1t_2\cos k}} + \frac{(t_1+t_2e^{-ik})t_1t_2\sin k}{(t_1^2+t_2^2+2t_1t_2\cos k)^{3/2}}\right)dk \\
=& \frac{1}{2}\int_{-\pi}^{\pi}\frac{t_2^2+t_1t_2e^{-ik}+it_1t_2\sin k}{t_1^2+t_2^2+2t_1t_2\cos k}dk \\
=& \frac{1}{2}\int_{-\pi}^{\pi}\frac{t_2^2+t_1t_2\cos k}{t_1^2+t_2^2+2t_1t_2\cos k}dk \\
=& \frac{1}{4}\int_{-\pi}^{\pi}\left(1+\frac{t_2^2-t_1^2}{t_1^2+t_2^2+2t_1t_2\cos k}\right)dk \\
=& \frac{\pi}{2} + \frac{1}{4}\int_{-\pi}^{\pi}\frac{t_2^2-t_1^2}{t_1^2+t_2^2+2t_1t_2\cos k}\, dk
\end{aligned}
$$

其中，可以利用 Mathematica 计算上述积分，当 $t_2 > t_1$ 时，积分等于 2π，此时 $\gamma_1 = \pi$; 当 $t_2 < t_1$ 时，积分等于 -2π，此时 $\gamma_1 = 0$。

同样地，我们可以计算:

$$
\gamma_2 = \int_{-\pi}^{\pi}\langle u_2(k)|\, i\frac{d}{dk}\, |u_2(k)\rangle = \begin{cases}\pi, & t_2 > t_1; \\ 0, & t_2 < t_1.\end{cases}
$$