双模坐标耦合谐振子体系的量子力学处理

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[摘要] 为了精确求解双模坐标耦合谐振子体系的动力学问题, 利用动量本征矢在 Fock表象中的表示构造不对称积分, 找到了与经典正则变换对应的量子幺正算符. 借助于动量表象的完备性条件, 证明了该算符的幺正性及其变换特性. 应用此量子幺正算符, 精确求解了双模坐标耦合谐振子体系的动力学问题.

[关键词] 正则变换, 动量本征矢, 幺正算符, 双模坐标耦合谐振子
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Solving Dynamic Problems of Double Coordinate Coupling Harmonic Oscillators With Quantum Mechanics

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Abstract In order to solve exactly the dynamic problems of the double coordinate coupling harmonic oscillators, the quantum unitary operator corresponding with classical canonical transformation is derived using the momentum eigenvector in Fock representation by constructing asymmetric integration. The unitarity and transformation properties of the operator are analyzed by virtue of completeness of momentum representation. The dynamic problems of the double coordinate coupling harmonic oscillators are solved exactly by using the operator.

Key words canonical transformation, momentum eigenvector, unitary operator, double coordinate coupling harmonic oscillator

物理学中存在许多经典变换, 如空间反演、坐标平移、标度变换、经典正则变换和辛变换等, 到了量子力学中, 这些经典变换将与一定的量子力学幺正变换相对应[1,2]. 本文利用动量本征矢在 Fock表象中的表示[3,4], 通过构造不对称积分, 诱导出了与经典正则变换对应的量子幺正算符, 并借助于动量表象的完备性条件证明了其幺正性及变换特性. 应用此量子幺正算符, 精确求解了双模坐标耦合谐振子体系的动力学问题.

1 动量本征矢在 Fock表象中的展开式

设粒子数算符 $\hat{N} = \hat{a}^{\dagger}\hat{a}$ 的本征态 $|n\rangle$, 它的基态 $|0\rangle$ 在动量表象中表示为

$$\langle p|0\rangle = \left(\frac{1}{\pi m\omega\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{1}{2m\omega\hbar}p^2\right), \tag{1}$$

为方便起见以下取自然单位 $\hbar = \omega = m = 1$, 则

$$\langle p|n\rangle = \langle p|\frac{\hat{a}^{\dagger n}}{\sqrt{n!}}|0\rangle = \langle p|\frac{(\hat{q}-i\hat{p})^n}{\sqrt{2^n n!}}|0\rangle = \frac{(-i)^n}{\sqrt{2^n n!}}\left(p-\frac{d}{dp}\right)^n\langle p|0\rangle = \frac{\pi^{-1/4}(-i)^n}{\sqrt{2^n n!}}e^{-\frac{p^2}{2}}H_n(p),\ (i^2=-1). \tag{2}$$

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上式利用了厄米多项式的表达式

$$H_n(p) = \mathrm{e}^{\frac{p^2}{2}}\left(p - \frac{\mathrm{d}}{\mathrm{d}p}\right)^n \mathrm{e}^{-\frac{p^2}{2}},$$

因此动量本征矢在 Fock表象中的表示为

$$|p\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|p\rangle = \pi^{-\frac{1}{4}} \mathrm{e}^{-\frac{p^2}{2}} \sum_{n=0}^{\infty}\left(\frac{\mathrm{i}\hat{a}^{\dagger}}{\sqrt{2}}\right)^n \frac{1}{n!} H_n(p)|0\rangle =$$

$$\pi^{-\frac{1}{4}} \exp(-p^2/2 + \sqrt{2}\mathrm{i}p\hat{a}^{\dagger} + \hat{a}^{\dagger 2}/2)|0\rangle, \tag{3}$$

其中利用了厄米多项式的母函数公式

$$\sum_{n=0}^{\infty} \frac{H_n(p)}{n!} t^n = \exp(2pt - t^2).$$

动量表象是完备的 $\int_{-\infty}^{\infty} \mathrm{d}p\, |p\rangle\langle p| = 1.$

2 与经典正则变换对应的量子幺正算符

在对体系的哈密顿量进行变数变换获取循环坐标时, 必须利用正则变换[5], 否则很难求解哈密顿正则方程. 基于经典正则变换 $(p_1, p_2) \rightarrow (Ap_1 + Bp_2, Cp_1 + Dp_2)$, 构造如下不对称积分型投影算符

$$\hat{U}_p = \iint_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right|, \ (AD - BC = 1), \tag{4}$$

其中 $\left|\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle = |p_1, p_2\rangle$ 是双模动量本征态. 于是

$$\hat{U}_p \hat{U}_p^{\dagger} = \int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \mathrm{d}p'_1 \mathrm{d}p'_2 \left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right|\left|\begin{pmatrix} p'_1 \\ p'_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p'_1 \\ p'_1\end{pmatrix}\right| =$$

$$\int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \mathrm{d}p'_1 \mathrm{d}p'_2 \left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle \delta(p_1 - p'_1)\delta(p_2 - p'_2)\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p'_1 \\ p'_1\end{pmatrix}\right| =$$

$$\int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right| =$$

$$\int_{-\infty}^{\infty} \mathrm{d}p''_1 \mathrm{d}p''_2 \left|\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right| = \int_{-\infty}^{\infty} \mathrm{d}p''_1 \mathrm{d}p''_2 \left|\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right| = 1 = \hat{U}_p^{\dagger}\hat{U}_p,$$

式中已令 $p''_1 = Ap_1 + Bp_2$, $p''_2 = Cp_1 + Dp_2$. 所以 $\hat{U}_p$ 为幺正算符. 在 $\hat{U}_p$ 的作用下

$$\hat{U}_p \hat{q}_1 \hat{U}_p^{\dagger} = \int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \mathrm{d}p'_1 \mathrm{d}p'_2 \left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right| \hat{q}_1 \left|\begin{pmatrix} p'_1 \\ p'_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p'_1 \\ p'_2\end{pmatrix}\right| =$$

$$\int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \mathrm{d}p'_1 \mathrm{d}p'_2 \left[-\mathrm{i}\frac{\partial}{\partial p'_1}\left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle \delta(p_1 - p'_1)\delta(p_2 - p'_2)\right]\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p'_1 \\ p'_2\end{pmatrix}\right| =$$

$$\int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 \left[-\mathrm{i}\frac{\partial}{\partial p_1}\left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\right]\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right| =$$

$$-\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}p_1 \mathrm{d}p_2 [-A(Ap_1 + Bp_2) - C(Cp_1 + Dp_2) + \mathrm{i}\sqrt{2}Aa_1^{\dagger} + \mathrm{i}\sqrt{2}Ca_2^{\dagger}]\left|\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} p_1 \\ p_2\end{pmatrix}\right| =$$

$$-\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}p''_1 \mathrm{d}p''_2 (-Ap''_1 - Cp'' + \mathrm{i}\sqrt{2}Aa_1^{\dagger} + \mathrm{i}\sqrt{2}Ca_2^{\dagger})\left|\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix} p''_1 \\ p''_2\end{pmatrix}\right| =$$

$$-\mathrm{i}\pi^{-1}\int_{-\infty}^{\infty} \mathrm{d}p''_1 \mathrm{d}p''(-Ap''_1 - Cp'' + \mathrm{i}\sqrt{2}Aa_1^{\dagger} + \mathrm{i}\sqrt{2}Ca_2^{\dagger}) : \exp\left[-p''^2_1 - p''^2_2 - \mathrm{i}\sqrt{2}p''_1(\hat{a}_1 - \hat{a}_1^{\dagger}) - \right.$$

$$\left.\mathrm{i}\sqrt{2}p''_2(\hat{a}_2 - \hat{a}_2^{\dagger}) + \frac{(\hat{a}_1 - \hat{a}_1^{\dagger})^2}{2} + \frac{(\hat{a}_2 - \hat{a}_2^{\dagger})^2}{2}\right] : = A\hat{q}_1 + C\hat{q}_2.$$

同理可证 $\hat{U}_p\hat{q}_2\hat{U}_p^{\dagger}=B\hat{q}_1+D\hat{q}_2$, 另一方面

$$\hat{U}_p\hat{p}_1\hat{U}_p^{\dagger}=\iiiint_{-\infty}^{\infty}\mathrm{d}p_1\mathrm{d}p_2\mathrm{d}p'_1\mathrm{d}p'_2\left|\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p_1\\p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}p_1\\p_2\end{pmatrix}\right|\hat{p}_1\left|\begin{pmatrix}p'_1\\p'_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p'_1\\p'_2\end{pmatrix}\right|=$$

$$\iiiint_{-\infty}^{\infty}\mathrm{d}p_1\mathrm{d}p_2\mathrm{d}p'_1\mathrm{d}p'_2\left|\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p_1\\p_2\end{pmatrix}\right\rangle p'_1\delta(p_1-p'_1)\delta(p_2-p'_2)\left\langle\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p'_1\\p'_2\end{pmatrix}\right|=$$

$$\iint_{-\infty}^{\infty}\mathrm{d}p_1\mathrm{d}p_2 p_1\left|\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p_1\\p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}A&B\\C&D\end{pmatrix}\begin{pmatrix}p_1\\p_2\end{pmatrix}\right|=$$

$$\iint_{-\infty}^{\infty}\mathrm{d}p''_1\mathrm{d}p''_2(Dp''_1-Bp''_2)\left|\begin{pmatrix}p''_1\\p''_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}p''_1\\p''_2\end{pmatrix}\right|=$$

$$\iint_{-\infty}^{\infty}\mathrm{d}p''_1\mathrm{d}p''_2(Dp''_1-Bp''_2):\exp\Big[-p''^2_1-p''^2_2-\mathrm{i}\sqrt{2}p''_1(\hat{a}_1-\hat{a}_1^{\dagger})-$$

$$\mathrm{i}\sqrt{2}p''_2(\hat{a}_2-\hat{a}_2^{\dagger})+\frac{(\hat{a}_1-\hat{a}_1^{\dagger})^2}{2}+\frac{(\hat{a}_2-\hat{a}_2^{\dagger})^2}{2}\Big]:=D\hat{p}_1-B\hat{p}_2.$$

亦可证明 $\hat{U}_p\hat{p}_2\hat{U}_p^{\dagger}=A\hat{p}_2-C\hat{p}_1$. 由此可见, 由动量本征矢构造的幺正算符 $\hat{U}_p$ 对坐标算符和动量算符的变换特性.

3　双模坐标耦合谐振子能量本征值的精确解

利用幺正算符 $\hat{U}_p$ 的变换特性可以解决一些动力学问题, 以最简单的 2个坐标耦合谐振子为例, 其哈密顿量为

$$\hat{H}=\frac{1}{2m}(\hat{p}_1^2+\hat{p}_2^2)+\frac{1}{2}m\omega^2(\hat{x}_1^2+\hat{x}_2^2)-\lambda\hat{x}_1\hat{x}_2,\tag{5}$$

要想精确求解体系的能量本征值, 必须设法使体系的哈密顿量对角化从而消除耦合项. 一些文献对耦合谐振子的方法作过大量讨论[6-8], 在此我们利用(4)式所定义量子幺正算符 $\hat{U}_p$ 对哈密顿量施以如下幺正变换

$$\hat{U}_p\hat{H}\hat{U}_p^{\dagger}=\frac{1}{2m}[(D\hat{p}_1-B\hat{p}_2)^2+(A\hat{p}_2-C\hat{p}_1)^2]+\frac{1}{2}m\omega^2[(A\hat{x}_1+C\hat{x}_2)^2+(B\hat{x}_1+D\hat{x}_2)^2]-$$

$$\lambda(A\hat{x}_1+C\hat{x}_2)(B\hat{x}_1+D\hat{x}_2)=\frac{1}{2m}(C^2+D^2)\hat{p}_1^2+\frac{1}{2m}(A^2+B^2)\hat{p}_2^2+\left[\frac{1}{2}m\omega^2(A^2+B^2)-\lambda AB\right]\hat{x}_1^2+$$

$$\left[\frac{1}{2}m\omega^2(C^2+D^2)-\lambda CD\right]\hat{x}_2^2-\frac{AC+BD}{m}\hat{p}_1\hat{p}_2+[m\omega^2(AC+BD)-\lambda(AD+BC)]\hat{x}_1\hat{x}_2,$$

令交叉项 $\hat{p}_1\hat{p}_2$ 和 $\hat{x}_1\hat{x}_2$ 前面的系数等于零, 同时令 $A=1$, 得到方程组:

$$\begin{cases}m\omega^2(AC+BD)=\lambda(AD+BC),\\AC+BD=0,\\AD-BC=1,\\A=1.\end{cases}$$

解之得一组解 $A=1, B=1, C=-1/2, D=1/2$, 所以所用的幺正变换算符为

$$\hat{U}_p=\iint_{-\infty}^{\infty}\mathrm{d}p_1\mathrm{d}p_2\left|\begin{pmatrix}1&1\\-1/2&1/2\end{pmatrix}\begin{pmatrix}p_1\\p_2\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}p_1\\p_2\end{pmatrix}\right|,\tag{6}$$

可以看出 $\hat{U}_p$ 既包含了转动变换又包含了压缩变换. 在 $\hat{U}_p$ 的作用下

$$\hat{U}_p\hat{H}\hat{U}_p^{\dagger}=\frac{\hat{p}_1^2}{4m}+\frac{\hat{p}_2^2}{m}+(m\omega^2-\lambda)\hat{x}_1^2+\frac{1}{4}(m\omega^2+\lambda)\hat{x}_2^2,$$

令 $M_1=2m,\quad M_2=\frac{m}{2},\quad \Omega_1=\left(\frac{m\omega^2-\lambda}{m}\right)^{1/2},\quad \Omega_2=\left(\frac{m\omega^2+\lambda}{m}\right)^{1/2}$, 于是

$$\hat{U}_p \hat{H} \hat{U}_p^{-1} = \frac{\hat{p}_1^2}{2M_1} + \frac{\hat{p}_2^2}{2M_2} + \frac{1}{2}M_1\Omega_1^2 + \frac{1}{2}M_2\Omega_2^2, \tag{7}$$

由于对$\hat{H}$施以的是幺正变换, 并不改变体系的能级分布, 对比一维谐振子的情况[9], 立即可以得到体系的能量本征值为

$$E_{n_1,n_2} = \left(n_1 + \frac{1}{2}\right)\hbar\Omega_1 + \left(n_2 + \frac{1}{2}\right)\hbar\Omega_2 \quad n_1, n_2 = 0, 1, 2\cdots$$

当 $\gamma = 0$时, 即为无耦合的情况

$$E_{n_1,n_2} = (n_1 + n_2 + 1)\hbar\omega \quad n_1, n_2 = 0, 1, 2\cdots$$

4 结论

根据动量本征矢在 Fock表象中的表示, 通过构造不对称积分引入了与经典正则变换对应的量子力学算符, 并借助表象的完备性条件, 证明了其幺正性及变换特性, 并提供了一种由经典变换向量子幺正变换的途径. 应用此量子幺正算符, 精确求解了双模坐标耦合谐振子体系的能量本征值.

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