The use of unitary operator to solve eigenvalue problem

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It is sometimes useful to use the unitary operators such as the translation operator and rotation operator in solving the eigenvalue problems. Some examples are presented here.

1. Introduction of New Hamiltonian by unitary operator

Suppose that

$$|\psi'\rangle = \hat{U}|\psi\rangle, \qquad \langle\psi_1|\hat{H}|\psi_2\rangle$$

$\hat{U}$ is the unitary operator. Under that basis of $|\psi'\rangle$, the operator $\hat{H}$ can be changed into

$$\langle\psi_1|\hat{H}|\psi_2\rangle = \langle\psi_1'|\hat{U}\hat{H}\hat{U}^{+}|\psi_2\rangle$$

We now consider the eigenvalue problem of the new Hamiltonian

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^{+}$$

where $\hat{U}$ is the rotation operator or translation operator

(a) Translation operator $\hat{T}_{\boldsymbol{a}}$

We use the formula

$$\hat{T}_{\boldsymbol{a}}^{+}\hat{\boldsymbol{r}}\hat{T}_{\boldsymbol{a}} = \hat{\boldsymbol{r}} + \boldsymbol{a}\hat{1}, \qquad \hat{T}_{\boldsymbol{a}}\hat{\boldsymbol{r}}\hat{T}_{\boldsymbol{a}}^{+} = \hat{\boldsymbol{r}} - \boldsymbol{a}\hat{1}, \qquad \hat{T}_{\boldsymbol{a}}\hat{\boldsymbol{p}}\hat{T}_{\boldsymbol{a}}^{+} = \hat{\boldsymbol{p}}$$

(b) Rotation operator $\hat{R}_z$

We use the formula

$$\hat{R}_z^{+}\hat{\boldsymbol{r}}\hat{R}_z = \Re\hat{\boldsymbol{r}} \qquad \hat{R}_z\hat{\boldsymbol{r}}\hat{R}_z^{+} = \Re^{-1}\hat{\boldsymbol{r}}$$

or

$$\hat{R}_z\hat{x}\hat{R}_z^{+} = \cos\phi\,\hat{x} + \sin\phi\,\hat{y}, \qquad \hat{R}_z\hat{y}\hat{R}_z^{+} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}$$

2. Example-1 (Problem Sakurai 5-4)

Consider an isotropic harmonic oscillator in *two* dimensions. The Hamiltonian is given by

$$H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2).$$

(a) What are the energies of the three lowest-lying states? Is there any degeneracy?

(b) We now apply a perturbation

$$V = \delta m\omega^2 xy,$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenket and the corresponding energy to first order [that is, the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.

(c) Solve the $H_0 + V$ problem *exactly*. Compare with the perturbation results obtained in (b). [You may use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$.]

((**Solution**))

$$\hat{H}_0 = \frac{1}{2m}(\hat{p}_x{}^2 + \hat{p}_y{}^2) + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2), \qquad \hat{V} = \delta m\omega^2 \hat{x}\,\hat{y}$$

The Hamiltonian is invariant under the rotation around the z axis, we have

$$[\hat{H}_0, \hat{R}_z] = 0$$

Suppose that $\hat{U} = \hat{R}_z$ (rotation operator)

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^+ = \hat{R}_z\hat{H}\hat{R}_z{}^+ = \hat{R}_z\hat{H}_0\hat{R}_z{}^+ + \hat{R}_z\hat{V}\hat{R}_z{}^+ = \hat{H}_0 + \hat{R}_z\hat{V}\hat{R}_z{}^+$$

When $\hat{V} = \delta m\omega^2 \hat{x}\,\hat{y}$

$$\begin{aligned}\hat{R}_z\hat{V}\hat{R}_z{}^+ &= \delta m\omega^2(\hat{R}_z\hat{x}\hat{R}_z{}^+)(\hat{R}_z\hat{y}\hat{R}_z{}^+) \\ &= \delta m\omega^2(\cos\phi\,\hat{x} + \sin\phi\,\hat{y})(-\sin\phi\,\hat{x} + \cos\phi\,\hat{y}) \\ &= \delta m\omega^2[-\frac{1}{2}\sin(2\phi)(\hat{x}^2 - \hat{y}^2) + \cos(2\phi)\hat{x}\hat{y}]\end{aligned}$$

when we choose $\phi = \pi / 4$,

$$\hat{R}_z \hat{V} \hat{R}_z^{+} = -\frac{1}{2}\alpha(\hat{x}^2 - \hat{y}^2)$$

Then we have

$$\begin{aligned}\hat{H}' &= \hat{R}_z \hat{H} \hat{R}_z^{+} \\ &= \hat{H}_0 + \hat{R}_z \hat{V} \hat{R}_z^{+} \\ &= \frac{1}{2m}\hat{p}_x^{\ 2} + \frac{1}{2}m\omega^2(1-\delta)\hat{x}^2 + \frac{1}{2m}\hat{p}_y^{\ 2} + \frac{1}{2}m\omega^2(1+\delta)\hat{y}^2\end{aligned}$$

Energy eigenvalue of this Hamiltonian is obtained as

$$\begin{aligned}E'(n_x, n_y) &= (n_x + \frac{1}{2})\hbar\omega\sqrt{1-\delta} + (n_y + \frac{1}{2})\hbar\omega\sqrt{1+\delta} \\ &= (n_x + \frac{1}{2})\hbar\omega(1 - \frac{\delta}{2} - \frac{\delta^2}{8} + ...) + (n_y + \frac{1}{2})\hbar\omega(1 + \frac{\delta}{2} - \frac{\delta^2}{8} + ...) + \\ &= (n_x + n_y + 1)\hbar\omega - \frac{\delta}{2}\hbar\omega(n_x - n_y) + ...\end{aligned}$$

$$\hat{H}'\left|n_x, n_y\right\rangle = \hat{R}_z \hat{H} \hat{R}_z^{+}\left|n_x, n_y\right\rangle = E'(n_x, n_y)\left|n_x, n_y\right\rangle$$

or

$$\hat{H}\hat{R}_z^{+}\left|n_x, n_y\right\rangle = E'(n_x, n_y)\hat{R}_z^{+}\left|n_x, n_y\right\rangle$$

$\hat{R}_z^{+}\left|n_x, n_y\right\rangle$ is the eigenstate of the Hamiltonian $\hat{H}$ with the eigenvalue $E'(n_x, n_y)$.

3. Example-2 Translation operator
Simple harmonics of charged particle in the presence of an electric field

Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics volume I and volume II* (John Wiley & Sons, New York, 1977).

The one-dimensional harmonic oscillator consists of a particle of mass *m* having a potential energy. Assume, in addition, that this particle has a charge *q* that it is placed in a uniform electric field ε parallel to the *x* axis. What are its new stationary states and the corresponding energies.

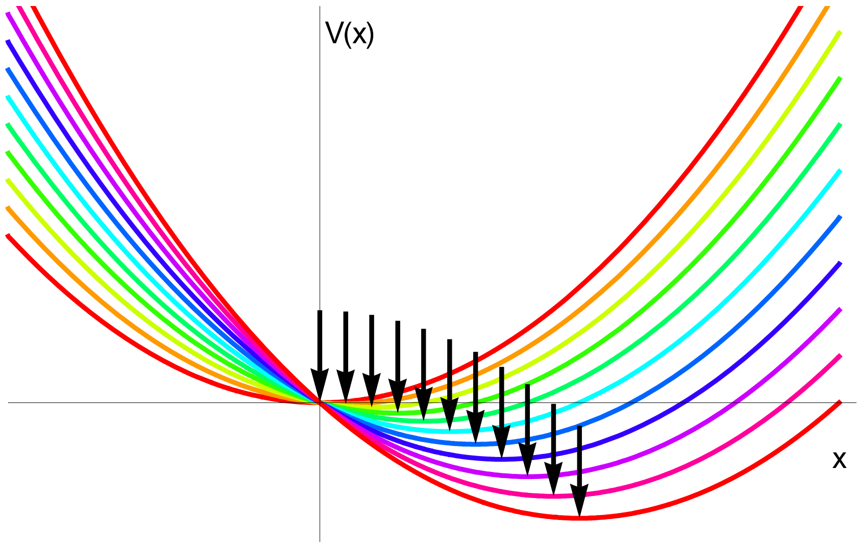

Fig. The potential energy $V(x) = \frac{1}{2} m\omega^2 x^2 - q\varepsilon x$. The potential takes a minimum at $x_0 = \mu = \frac{q\varepsilon}{m\omega_0^{\ 2}}$. The minimum position of the potential energy shifts to the larger x as the electric field increases.

The Hamiltonian of a particle placed in a uniform electric field ε is given by

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - q\varepsilon\hat{x}$$

The new Hamiltonian under the translation operator can be rewritten as

$$\begin{aligned}\hat{H}' &= \hat{T}_\mu \hat{H} \hat{T}_\mu^{\ +} \\ &= \hat{T}_\mu (\frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - q\varepsilon\hat{x})\hat{T}_\mu^{\ +} \\ &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{T}_\mu\hat{x}^2\hat{T}_\mu^{\ +} - q\varepsilon\hat{T}_\mu\hat{x}\hat{T}_\mu^{\ +} \\ &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2(\hat{x}-\mu\hat{1})^2 - q\varepsilon(\hat{x}-\mu\hat{1}) \\ &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - (q\varepsilon + m\omega^2\mu)\hat{x} \\ &\quad + \frac{1}{2}m\omega^2\mu^2 + q\varepsilon\mu\end{aligned}$$

where

$$\hat{T}_\mu\hat{p}^2\hat{T}_\mu^{\ +} = \hat{p}^2, \qquad \hat{T}_\mu\hat{p}\hat{T}_\mu^{\ +} = \hat{p}$$

$$\hat{T}_\mu\hat{x}^2\hat{T}_\mu^{\ +} = (\hat{x}-\mu\hat{1})^2, \qquad \hat{T}_\mu\hat{x}\hat{T}_\mu^{\ +} = (\hat{x}-\mu\hat{1})$$

We choose μ as follows.

$$q\varepsilon + m\omega^2\mu = 0, \qquad \mu = -\frac{q\varepsilon}{m\omega^2}$$

Then we have

$$\hat{H}' = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1} = \hat{H}_0 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1}$$

Suppose that $|n\rangle$ is the eigenket of $\hat{H}_0$ with the eigenvalue $E_n = \hbar\omega_0(n+\frac{1}{2})$,

$$\hat{H}_0|n\rangle = \hbar\omega_0(n+\frac{1}{2})|n\rangle,$$

Then we have

$$\hat{H}'|n\rangle = (\hat{H}_0 - \frac{q^2\varepsilon^2}{2m\omega^2}\hat{1})|n\rangle = [\hbar\omega_0(n+\frac{1}{2}) - \frac{q^2\varepsilon^2}{2m\omega^2}]|n\rangle$$

$|n\rangle$ is the eigenket of $\hat{H}'$ with the energy eigenvalue of $\hat{H}'$ given by

$$E_n' = [\hbar\omega_0(n + \frac{1}{2}) - \frac{q^2\varepsilon^2}{2m\omega^2}$$

Since

$$\hat{T}_\mu \hat{H} \hat{T}_\mu^{\ +} |n\rangle = E_n' |n\rangle$$

or

$$\hat{H} \hat{T}_\mu^{\ +} |n\rangle = E_n' \hat{T}_\mu^{\ +} |n\rangle$$

$\hat{T}_\mu^{\ +}|n\rangle$ is the eigenket of $\hat{H}$ with the energy eigenvalue E_n'

The $|x\rangle$ representation of the eigenket $\hat{T}_\mu^{\ +}|n\rangle$ is

$$\langle x|\hat{T}_\mu^{\ +}|n\rangle = \langle x+\mu|n\rangle = \left\langle x - \frac{q\varepsilon}{m\omega^2}\middle|n\right\rangle$$

with

$$\mu = -\frac{q\varepsilon}{m\omega^2}$$

((Note))

$$\hat{T}_\mu|x\rangle = |x+\mu\rangle, \qquad \langle x+\mu| = \langle x|\hat{T}_\mu^{\ +}$$

4. Example

Find the change of energy eigenvalue for a three dimensional isotropic harmonics oscillator with a charge *q*, when the electric field ***E*** is applied along the *z* axis.

$$\Delta E = -\frac{1}{2}\alpha \boldsymbol{E}^2$$

What is the expression for the polarizability α?

$$\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2\hat{\boldsymbol{r}}^2 - qE_z\hat{z}$$

$$\begin{aligned}
\hat{H}' &= \hat{T}_z(\mu)\hat{H}\hat{T}_z^{\,+}(\mu) \\
&= \hat{T}_z(\mu)(\frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2\hat{\boldsymbol{r}}^2 - qE_z\hat{z})\hat{T}_z^{\,+}(\mu) \\
&= \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2) + \frac{1}{2}m\omega^2\hat{T}_z(\mu)\hat{z}^2\hat{T}_z^{\,+}(\mu) - qE_z\hat{T}_z(\mu)\hat{z}\hat{T}_z^{\,+}(\mu) \\
&= \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2) + \frac{1}{2}m\omega^2(\hat{z} - \mu\hat{1})^2 - qE_z(\hat{z} - \mu\hat{1}) \\
&= \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2) + \frac{1}{2}m\omega^2(\hat{z}^2 - 2\mu\hat{z} + \mu^2\hat{1}) - qE_z\hat{z} + qE_z\mu\hat{1}
\end{aligned}$$

We choose

$$\mu = -\frac{qE_z}{m\omega^2}$$

Then we get

$$\hat{H}' = \frac{1}{2m}\hat{\boldsymbol{p}}^2 + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2 + \hat{z}^2) - \frac{q^2E_z^{\,2}}{2m\omega^2}\hat{1}$$

$$\hat{H}'\left|n_x, n_y, n_z\right\rangle = E'(n_x, n_y, n_z)\left|n_x, n_y, n_z\right\rangle$$

where

$$E'(n_x, n_y, n_z) = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega - \frac{q^2E_z^{\,2}}{2m\omega^2}$$

$\left|n_x, n_y, n_z\right\rangle$ is the eigenket of $\hat{H}'$ with the energy eigenvalue $E'(n_x, n_y, n_z)$.

$$\hat{H}'\left|n_x, n_y, n_z\right\rangle = \hat{T}_z(\mu)\hat{H}\hat{T}_z^{\,+}(\mu)\left|n_x, n_y, n_z\right\rangle = E'(n_x, n_y, n_z)\left|n_x, n_y, n_z\right\rangle$$

or

$$\hat{H}\hat{T}_z^{\,+}(\mu)\left|n_x,n_y,n_z\right\rangle = E'(n_x,n_y,n_z)\hat{T}^{+}{}_z(\mu)\left|n_x,n_y,n_z\right\rangle$$

$\hat{T}_z^{\,+}(\mu)\left|n_x,n_y,n_z\right\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue $E'(n_x,n_y,n_z)$ with

$$\mu = -\frac{qE_z}{m\omega^2}$$

The $\left|\boldsymbol{r}\right\rangle$ representation of $\hat{T}_z^{\,+}(\mu)\left|n_x,n_y,n_z\right\rangle$ is

$$\begin{aligned}\left\langle \boldsymbol{r}\right|\hat{T}_z^{\,+}(\mu)\left|n_x,n_y,n_z\right\rangle &= \left\langle x|n_x\right\rangle\left\langle y|n_y\right\rangle\left\langle z\right|\hat{T}_z^{\,+}(\mu)\left|n_z\right\rangle \\ &= \left\langle x|n_x\right\rangle\left\langle y|n_y\right\rangle\left\langle z+\mu|n_z\right\rangle \\ &= \left\langle x|n_x\right\rangle\left\langle y|n_y\right\rangle\left\langle z-\frac{qE_z}{m\omega^2}\middle|n_z\right\rangle\end{aligned}$$

We note that

$$\Delta E = E'(n_x,n_y,n_z) - E(n_x,n_y,n_z) = -\frac{q^2E_z{}^2}{2m\omega^2} = -\frac{\alpha E_z{}^2}{2}$$

leading to the electric polarizability

$$\alpha = \frac{q^2}{m\omega^2}$$