MATH4104: Quantum nonlinear dynamics. Lecture Seven. Quantum dynamics in a periodic potential.

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Particle in a periodic potential.

\[ V(x) = -V_0 \cos(2\pi x / \lambda) \]

\[ H = \frac{p_x^2}{2m} - V_0 \cos(2\pi x / \lambda) \]
Particle in a periodic potential.

Phase space orbits.
for allowed energies,

\[ J(E_n) - J(E_{n-1}) = \hbar \]

and

\[ J(E_n) - J(E_{n-1}) \approx \frac{dJ(E)}{dE} \bigg|_{E_n} \Delta E_n \]

where \( \Delta E_n = E_n - E_{n-1} \).

Now use

\[ \frac{dJ(E)}{dE} = \omega_{cl}(E) \]

thus

\[ \Delta E_n = \hbar \omega_{cl}(E) \]
Particle in a periodic potential.

Phase space orbits.
Particle in a periodic potential.

Dynamics of a classical distribution $Q(q, p)$:

$$\frac{\partial Q}{\partial t} = - \{H, Q\}_{q,p} = -p \frac{\partial Q}{\partial q} + \kappa \sin q \frac{\partial Q}{\partial p} ,$$

solved by the method of characteristics*.

$$Q_0(q, p) = \frac{1}{2\pi \sqrt{\sigma_q \sigma_p}} \exp \left[ \frac{(p - p_0)^2}{2\sigma_p} \right] \exp \left[ \frac{(q - q_0)^2}{2\sigma_q} \right]$$

$(q_0, p_0) = (-1.5, 0), \sigma_q = 0.18, \sigma_p = 0.33$
Particle in a periodic potential.

Dynamics of a *classical* distribution $Q(q,p)$: Plot contours of $Q$

**Figure:** $\kappa = 1.2$, (a) initially the atom is localized in the region of bounded motion; (b) After just ten classical periods the distribution of the atom is sheered over the trajectories on which it has support.
Particle in a periodic potential.

Classical dynamics of moments of momentum:

Figure: (a) the mean momentum, $\langle p \rangle$, rapidly collapses to zero due to the sheering action of the nonlinear motion; (b) the momentum variance, $V(p)$
Particle in a periodic potential.

The time for *collapse* of the oscillation.

The inner and outer bounds of the distribution rotate at different rates in phase space, resulting in a rotational sheering.

Consider two initial points separated by $\Delta E$ in energy. The difference in the rotational rate is

$$\delta \omega = \omega_{cl}(E + \Delta E) - \omega_{cl}(E)$$

$$= \frac{d\omega_{cl}(E)}{dE} \cdot \Delta E = \frac{d\omega_{cl}(E)}{dE} \cdot \frac{dE}{dJ} \Delta J$$

$$= \frac{d\omega_{cl}(E)}{dE} \cdot \omega_{cl} \Delta J$$

The collapse time is defined by $\delta \omega T_{col} \sim 2\pi$

$$T_{col} = \frac{2\pi}{\omega_{cl}} \left( \Delta J \frac{d\omega_{cl}(E)}{dE} \right)^{-1} = T_{cl} \left( \Delta J \frac{d\omega_{cl}(E)}{dE} \right)^{-1}$$
A periodic potential has a displacement symmetry:

\[ V(\hat{q} + d) = V(\hat{q}) \]

Displacement is induced by a \textit{unitary operator} \( \hat{S}_d \)

\[ \hat{S}_d^{\dagger} \hat{q} \hat{S}_d = \hat{q} + d \]

where

\[ \hat{S}_d = e^{-id\hat{p}/\hbar} \]

\textbf{Prove this.}

For \( V(\hat{q}) = -\kappa \cos \hat{q} \), the unitary symmetry transformation is \( \hat{S}_{2\pi} \)
Energy eigenstates of a periodic potential.

Symmetries have an effect on the energy eigenstates,

$$\hat{S}_{2\pi}^\dagger \hat{H} \hat{S}_{2\pi} = \hat{H}$$

Thus, if $|E\rangle$ is an energy eigenstate,

$$\hat{H} |E\rangle = E |E\rangle$$

so is $\hat{S}_{2\pi} |E\rangle$

Proof:

$$\hat{H} \hat{S}_{2\pi} |E\rangle = \hat{S}_{2\pi} \hat{S}_{2\pi}^\dagger \hat{H} \hat{S}_{2\pi} |E\rangle$$

$$= \hat{S}_{2\pi} \hat{H} |E\rangle$$

$$= E \left( \hat{S}_{2\pi} |E\rangle \right)$$

We can choose eigenstates of $\hat{H}$ to be eigenstates of $\hat{S}_{2\pi}$.
The eigenstates of $\hat{S}_{2\pi}$ are clearly momentum eigenstates with eigenvalue $e^{-i2\pi p/k}$.

In the case of a pendulum, the potential has a similar periodicity. However, the coordinate is an *angle*, $0 \leq \theta < 2\pi$.

The energy eigenstates must be periodic in $\theta$, which implies that we must restrict the momentum eigenvalues to $p = mk$.

But in this problem $\hat{q}$ is the position of a particle on the real line, thus the momentum $p$ can take any value at all.

The topology of the classical phase space matters!
Energy eigenstates of a periodic potential.

Denote the simultaneous eigenstates of \( \hat{H} \) and \( \hat{S}_{2\pi} \) as \( |E_n, p\rangle \) (where \( n \) is an integer and \( p \) is a real number).

\[
\hat{H}|E_n, p\rangle = E_n(p)|E_n, p\rangle
\]

Notice that \( \hat{H} \) is invariant if \((q, p) \rightarrow (-q, -p)\), a parity symmetry.

Let \( \hat{P} \) be the parity operator,

\[
\hat{P}|p\rangle = |-p\rangle
\]

This implies that the momentum operator transforms as \( \hat{P}\hat{p}\hat{P} = -\hat{p} \), and that the translation operator is reversed: \( \hat{P}\hat{S}_{2\pi}\hat{P} = \hat{S}_{-2\pi} \).

This means that the states \( |E_n, p\rangle \) and \( |E_n, -p\rangle \) have the same energy.
Energy eigenstates of a periodic potential.

The position probability amplitudes for energy eigenstates must satisfy

$$- \frac{k^2}{2} \frac{d^2 u_{n,p}}{dq^2} + 2\kappa \sin^2 (q/2) u_{n,p} = E_n(p) u_{n,p}. $$

Mathieu’s equation.

Eigenstates differing in quasi-momentum by an amount $k$ must have the same energy and the same translation eigenvalue.

Hence the energy and the $u_{n,p}$ functions repeat themselves in quasi-momentum space. For uniqueness $p$ is usually restricted to the interval $[\kappa/2, -\kappa/2)$, the first Brillouin zone.

$u_{n,p}$ are called the Bloch functions.
Energy eigenstates of a periodic potential.

Bloch functions.

\[
\sum_{n=1}^{\infty} \int_{-k/2}^{k/2} u_{n,p}(q')^* u_{n,p}(q) \, dp = 2\pi k \delta(q' - q) \quad \text{(completeness)}
\]

\[
\int_{-\pi}^{\pi} |u_{n,p}(q)|^2 \, dq = 1 \quad \text{(normalization)}
\]

\[
\int_{-\infty}^{\infty} u_{n',p'}(q)^* u_{n,p}(q) \, dq = 2\pi k \delta_{n',n} \delta(p' - p) \quad \text{(orthogonality)}
\]
Energy eigenstates of a periodic potential.

Bloch functions are not localised. We define a class of localised states \textit{Wannier states}.

\[ |W_n, m\rangle = \frac{1}{\sqrt{2\pi k}} \int_{-k/2}^{k/2} \exp\left(-\frac{2\pi imp}{k}\right) |E_n, p\rangle \, dp. \]

The Wannier state \( |W_n, m\rangle \) is localized at the point \( q = 2\pi m \) and it is easy to verify that it satisfies the translation identity, \( \hat{S}_{2\pi} |W_n, m\rangle = |W_n, m + 1\rangle. \)

Express the Bloch states in terms of the Wannier states

\[ |E_n, p\rangle = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} \exp\left(2\pi imp/k\right) |W_n, m\rangle. \]
Energy eigenstates of a periodic potential.

Position probability amplitude for a Wannier state:

\[ a_{n,m}(q) = \langle q | W_n, m \rangle \]

\[ \int_{-\infty}^{\infty} a_{n',m'}(q)^* a_{n,m}(q) \, dq = \delta_{n',n} \delta_{m',m} \quad \text{(normalization)} \]

\[ \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} a_{n,m}(q')^* a_{n,m}(q) = \delta(q - q') \quad \text{(completeness)} \]
Energy eigenstates of a periodic potential.

The Bloch states are periodic, thus we can make a Fourier expansion,

\[ u_{n,p}(q) = \sum_{m=-\infty}^{\infty} v_n(p + mk) \exp \left[ i \left( p + mk \right) \frac{q}{\hbar} \right]. \]
Energy eigenstates of a periodic potential.

A useful property of the Wannier states: Using the definition of $|W_n, m\rangle$ in terms of Bloch states,

$$a_{n,m}(q) = \frac{1}{2\pi k} \int_{-k/2}^{k/2} e^{-2\pi i mp/k} u_{n,p}(q)$$

Now we can prove that

$$\nu_n(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a_{n,0}(q) \exp \left(-i\frac{dq}{k}\right) dq$$

Thus, given the Wannier state $a_{n,0}(q)$ we can find the $\nu_n(p)$ and thus all the Bloch states.
Energy eigenstates of a periodic potential.

Husimi function for a Wannier state

\[ Q(q, p) = |\langle \alpha | W_7, 0 \rangle|^2 \]

where \( \alpha = q + ip \) (choose \( \tilde{k} = 0.24 \))
Energy eigenstates of a periodic potential.

\( \kappa = 1.2 \)

we can write,

\[
E_n(p) = \bar{E}_n + k\Delta_n \cos(2\pi p/k)
\]
We can write,

$$ E_n(p) = \bar{E}_n + \hbar \Delta_n \cos\left(\frac{2\pi p}{\hbar}\right) $$

where $\bar{E}_n$ is the average energy of the $n$th band and $\Delta_n$ is the band width.

The average energy of the $n$th band satisfies,

$$ J(\bar{E}_n) = \hbar \left( n + \frac{1}{2} \right) $$
Fractional revivals.

Recall, Wannier state $|W_n, m\rangle$ is centred in the well at $2\pi m$, and is localised on an annulus determined by $n$.

Thus an initial state localised in the well near $q = 0$ can be written as

$$|\psi(0)\rangle = \sum_n a_n |W_n, 0\rangle .$$

will evolve to

$$|\psi(t)\rangle = \sum_n a_n \exp \left(-i\bar{E}_n t/\hbar\right) |W_n, 0\rangle .$$

Assume the energy varies slowly with $n$,

$$\bar{E}_n \approx \bar{E}_{\bar{n}} + \hbar \omega_{cl}(\bar{E}_{\bar{n}})(n - \bar{n}) + \frac{\hbar^2}{2}(n - \bar{n})^2 \frac{\partial \omega_{cl}}{\partial E}\bigg|_{\bar{n}} .$$

The linear term in $n$ is like the SHO, it would make the dynamics perfectly periodic. What does the $n^2$ term do?
Some details

\[ J(\bar{E}_n) = \bar{k}(n + 1/2) \]

\[ \bar{E}_n = J^{-1}(\bar{k}(n + 1/2)) \]

\[ \approx J^{-1}(k(\bar{n} + 1/2)) + k(n - \bar{n}) \frac{d}{dE} J^{-1}(E)|_{\bar{n}} + \frac{k^2}{2} (n - \bar{n})^2 \frac{d^2}{dE^2} J^{-1}(E)|_{\bar{n}} \]

but

\[ \frac{d}{dE} (J^{-1}(E)) = \frac{dE}{dJ} = \omega_{cl}(E) \]
Thus

\[ |\psi(t)\rangle = e^{-i\tilde{E}_n t} \sum_n a_n e^{-i\omega(n-\bar{n}) - i\chi t(n-\bar{n})^2} |W_m, 0\rangle \]

where

\[ \chi = \frac{k}{2} \left. \frac{d\omega_{cl}}{dE} \right|_{\bar{n}} \]

ignore phase pre-factor. Shift sum index

\[ |\psi(t)\rangle = \sum_m a_{m+\bar{n}} e^{-i\omega tm - i\chi tm^2} |W_m, 0\rangle \]
Fractional revivals.

An analogy: anharmonic oscillator

\[ H = \hbar \omega a^\dagger a + \hbar \chi (a^\dagger a)^2 \]

Eigenstates are \(|n\rangle\) with eigenvalues, \(E_n = \hbar \omega n + \hbar \chi n^2\).

Take initial coherent state

\[
|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle
\]

Evolves to

\[
|\psi(t)\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} e^{-i\chi t n^2} |n\rangle
\]
Fractional revivals.

Move to a *rotating frame* in complex plane

\[ \alpha = \beta e^{i\omega t} \]

in this frame,

\[
|\tilde{\psi}(t)\rangle = e^{-|\beta|^2/2} \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{n!}} e^{-i\chi tn^2} |n\rangle
\]

- clearly periodic \( \chi t = 2\pi \)
- if \( \chi t = \pi \), state is \( | - \beta \rangle \) ... a revival.
- if \( \chi t = \pi/2 \) state is

\[
e^{-i\pi/4} |\beta\rangle + e^{i\pi/4} | - \beta\rangle
\]

a fractional revival.
Fractional revivals.

Now return to periodic potential and plot the Husimi function for an initial Gaussian state,

\[ Q(\alpha, t) = |\langle \alpha | \psi(t) \rangle|^2 \]

\[ \alpha = q + ip \]
Fractional revivals.

\( k = 0.24, \)

(a) \( t = 13; \) (b) \( t = 26; \) (c) \( t = 39; \) (d) \( t = 52. \)
Particle in a periodic potential.

Quantum dynamics of moments of momentum: