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

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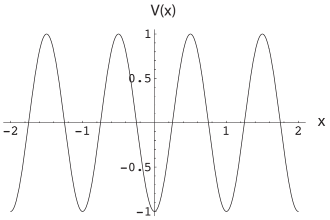
Particle in a periodic potential.

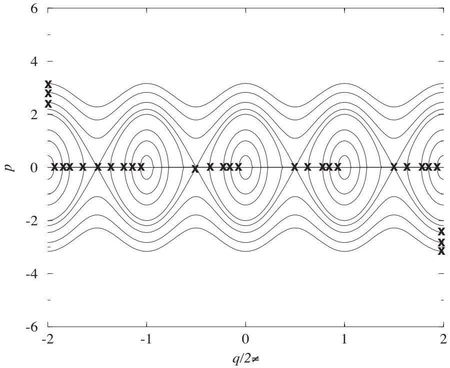
$$V(x) = -V_0 \cos(2\pi x/\lambda)$$

$$H = \frac{p_x^2}{2m} - V_0 \cos(2\pi x/\lambda)$$



Particle in a periodic potential.

Phase space orbits.



Particle in a periodic potential.

for allowed energies,

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

and

$$J(E_n) - J(E_{n-1}) =\approx \left.\frac{dJ(E)}{dE}\right|_{E_n} .\Delta E_n$$

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

Now use

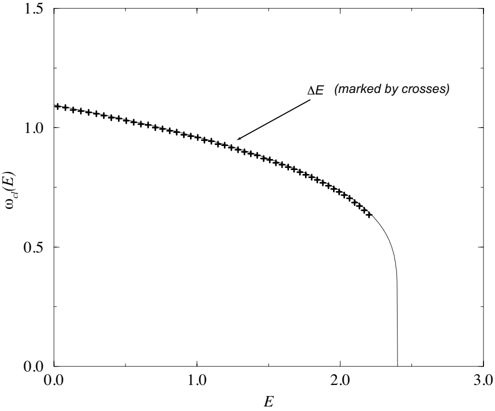
$$\frac{dJ(E)}{dE} = \omega_{cl}(E)$$

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 $Q(q,p)$:

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

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

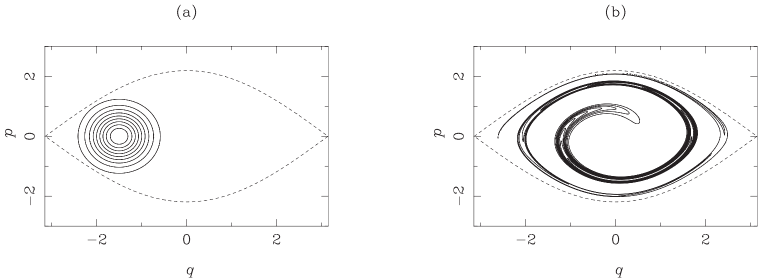


Figure: $\kappa = 1.2$, (a) initially the atom is localized in the region of bounded motion; (b) After just ten classical periods the distribution of the atom is sheered over the trajectories on which it has support.

Particle in a periodic potential.

Classical dynamics of moments of momentum:

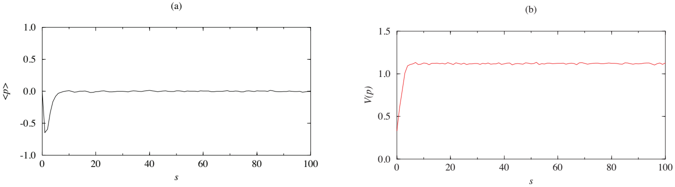


Figure: (a) the mean momentum, $\langle p \rangle$, rapidly collapses to zero due to the sheering action of the nonlinear motion;(b) the momentum variance, $V(p)$

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 ΔE in energy. The difference in the rotational rate is

$$
\begin{aligned}
\delta\omega &= \omega_{cl}(E+\Delta E) - \omega_{cl}(E) \\
&= \frac{d\omega_{cl}(E)}{dE}.\Delta E = \frac{d\omega_{cl}(E)}{dE}.\frac{dE}{dJ}\Delta J \\
&= \frac{d\omega_{cl}(E)}{dE}.\omega_{cl}\Delta J
\end{aligned}
$$

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

$$
T_{col} = \frac{2\pi}{\omega_{cl}}\left(\Delta J \frac{d\omega_{cl}(E)}{dE}\right)^{-1} = T_{cl}\left(\Delta J \frac{d\omega_{cl}(E)}{dE}.\right)^{-1}
$$

Energy eigenstates of a periodic potential.

A periodic potential has a displacement symmetry:

$$V(\hat{q}+d) = V(\hat{q})$$

Displacement is induced by a *unitary operator* $\hat{S}_d$

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

where

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

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:

$$\begin{aligned} \hat{H}\hat{S}_{2\pi}|E\rangle &= \hat{S}_{2\pi}\hat{S}_{2\pi}^{\dagger}\hat{H}\hat{S}_{2\pi}|E\rangle \\ &= \hat{S}_{2\pi}\hat{H}|E\rangle \\ &= E\left(\hat{S}_{2\pi}|E\rangle\right) \end{aligned}$$

We can choose eigenstates of $\hat{H}$ to be eigenstates of $\hat{S}_{2\pi}$

Energy eigenstates of a periodic potential.

The eigenstates of $\hat{S}_{2\pi}$ are clearly momentum eigenstates with eigenvalue $e^{-i2\pi p/\hbar}$.

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 θ, which implies that we must restrict the momentum eigenvalues to $p = m\hbar$.

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 $(q, p) \to (-q, -p)$, 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

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

Mathieu's equation.

Eigenstates differing in quasi-momentum by an amount $\hbar$ 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 $[\hbar/2, -\hbar/2)$, *the first Brillouin zone.*

$u_{n,p}$ are called the *Bloch* functions.

Energy eigenstates of a periodic potential.

Bloch functions.

$$\begin{array}{rcll}
\sum_{n=1}^{\infty}\int_{-\hbar/2}^{\hbar/2} u_{n,p}(q')^* u_{n,p}(q)\,dp & = & 2\pi\hbar\,\delta(q'-q) & \text{(completeness} \\
\int_{-\pi}^{\pi} |u_{n,p}(q)|^2\,dq & = & 1 & \text{(normalization} \\
\int_{-\infty}^{\infty} u_{n',p'}(q)^* u_{n,p}(q)\,dq & = & 2\pi\hbar\,\delta_{n',n}\delta(p'-p) & \text{(orthogonality}
\end{array}$$

Energy eigenstates of a periodic potential.

Bloch functions are not localised. We define a class of localised states *Wannier states.*

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

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

$$|E_n, p\rangle = \sqrt{2\pi} \sum_{m=-\infty}^{\infty} \exp\left(2\pi imp/\bar{k}\right) |W_n, m\rangle \; .$$

Energy eigenstates of a periodic potential.

Position probability amplitude for a Wannier state:

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

$$\begin{array}{lcll} \int_{-\infty}^{\infty} a_{n',m'}(q)^* a_{n,m}(q)\, dq & = & \delta_{n',n}\, \delta_{m',m} & \text{(normalization)}\,, \\ \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} a_{n,m}(q')^* a_{n,m}(q) & = & \delta(q - q') & \text{(completeness)}. \end{array}$$

Energy eigenstates of a periodic potential.

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

$$u_{n,p}(q) = \sum_{m=-\infty}^{\infty} v_n(p + m\hbar) \exp\left[i\left(p + m\hbar\right) q/\hbar\right] \; .$$

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,

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

Now we can prove that

$$v_n(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a_{n,0}(q) \exp\left(-ipq/\hbar\right)\, dq$$

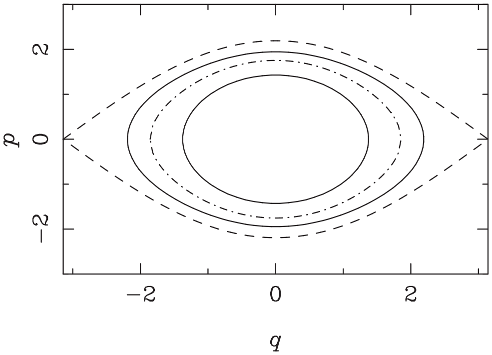
Thus, given the Wannier state $a_{n,0}(q)$ we can find the $v_n(p)$ and thus all the Bloch states.

Energy eigenstates of a periodic potential.

Husimi function for a Wannier state

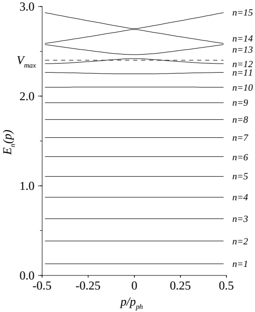
$$Q(q,p) = |\langle \alpha | W_7, 0 \rangle|^2$$

where $\alpha = q + ip$ (choose $\hbar = 0.24$)



Energy eigenstates of a periodic potential.

$\kappa = 1.2$



we can write,

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

Energy eigenstates of a periodic potential.

We can write,

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

where $\bar{E}_n$ is the average energy of the nth band and Δ_n is the *band width*.

The average energy of the nth band satisifes,

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

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,

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

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

Fractional revivals.

Some details

$$J(\bar{E}_n) = \hbar(n + 1/2)$$

$$\begin{aligned}\bar{E}_n &= J^{-1}\left(\hbar(n+1/2)\right)\\ &\approx J^{-1}(\hbar(\bar{n}+1/2)) + \hbar(n-\bar{n})\frac{d}{dE}\,J^{-1}(E)\Big|_{\bar{n}} + \frac{\hbar^2}{2}(n-\bar{n})^2\frac{d^2}{dE^2}\,J^{-1}(E)\Big|_{\bar{n}}\end{aligned}$$

but

$$\frac{d}{dE}\left(J^{-1}(E)\right) = \frac{dE}{dJ} = \omega_{cl}(E)$$

Fractional revivals.

Thus

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

where

$$\chi = \frac{\hbar}{2} \left. \frac{d\omega_{cl}}{dE} \right|_{\bar{n}}$$

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

$$|\psi(t)\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}e^{-i\chi t n^2}|n\rangle$$

Fractional revivals.

Move to a *rotating frame* in complex plane

$$\alpha = \beta e^{i\omega t}$$

in this frame,

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

- 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.*

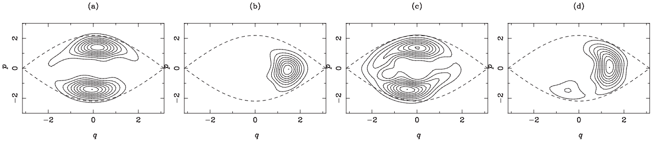
Fractional revivals.

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.



$\hbar = 0.24$,
(a) $t = 13$; (b) $t = 26$; (c) $t = 39$; (d) $t = 52$.

Particle in a periodic potential.

Quantum dynamics of moments of momentum: