Librations, instantons,tunneling and low bands of 2-D Schrödinger operator for quantum dimers

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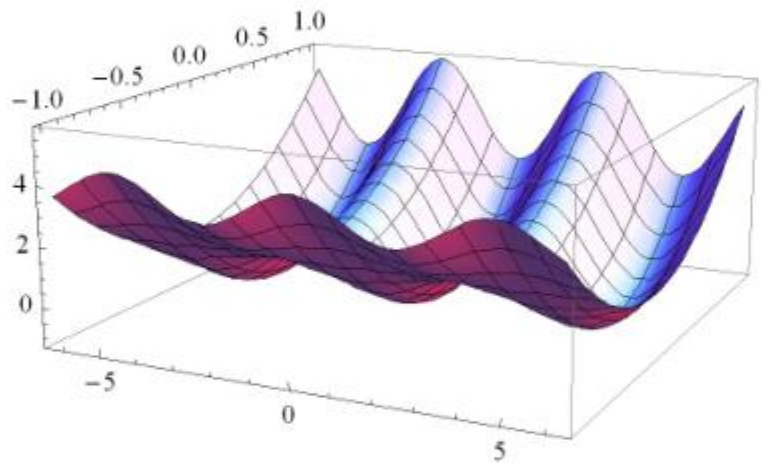
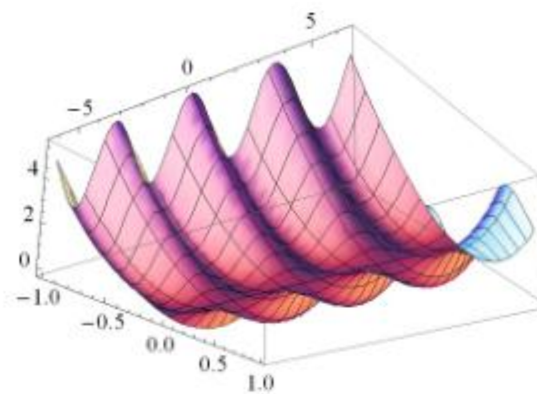
FORMULATION OF THE PROBLEM

$$\widehat{H}\psi = [-\frac{h^2}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{y^2}{2} - \alpha \cos \beta x \cos(y - y_0)]\Psi = E\Psi$$

$$0 < h << 1 \qquad \psi(x + 2\pi/\beta, y) = e^{2\pi i q}\psi(x, y)$$





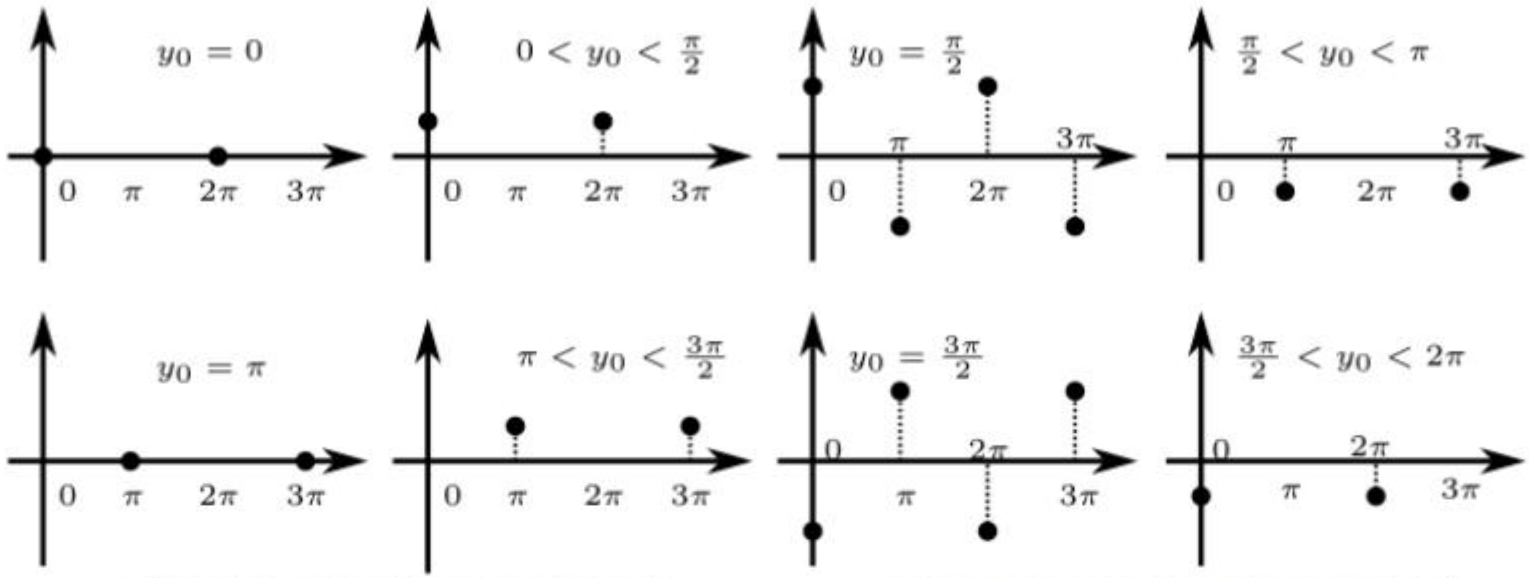
$$\widehat{\mathcal{H}} = -\frac{\hbar^2 \Delta}{2m} + \frac{K^2}{2}(x_2 - x_1 - l)^2 + U_0\Big(2 - \cos(kx_1) - \cos(kx_2)\Big)$$

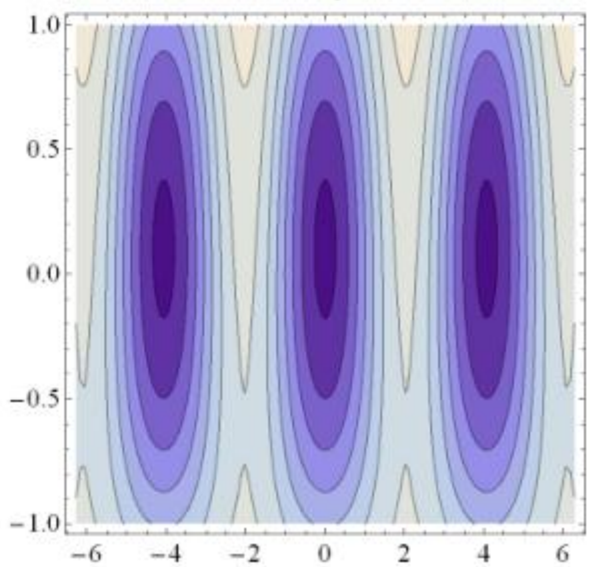
Classical Hamiltonian

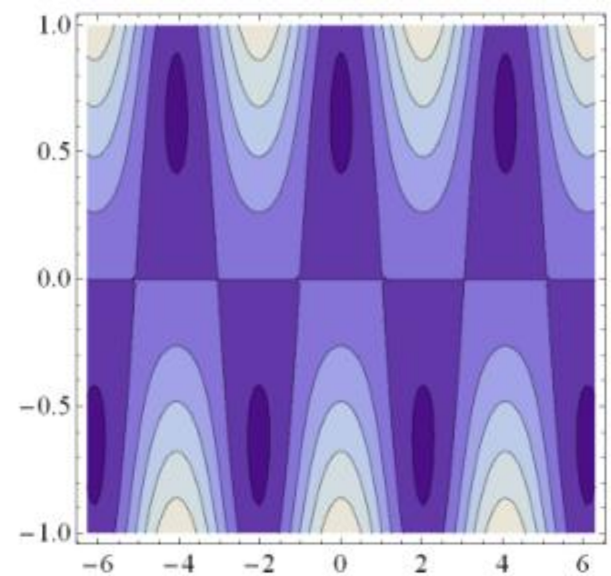
$$H = \frac{1}{2}(p_x^2 + p_y^2) + U(x, y), \qquad U = \frac{y^2}{2} - \alpha \cos \beta x \cos(y - y_0)$$

C. Fusco, A. Fasolino, T. Janssen, Eur. Phys. J. B 31, 95–102 (2003)

Points of global minimum for U. Horisontal is x-axis, vertical is y-axis.







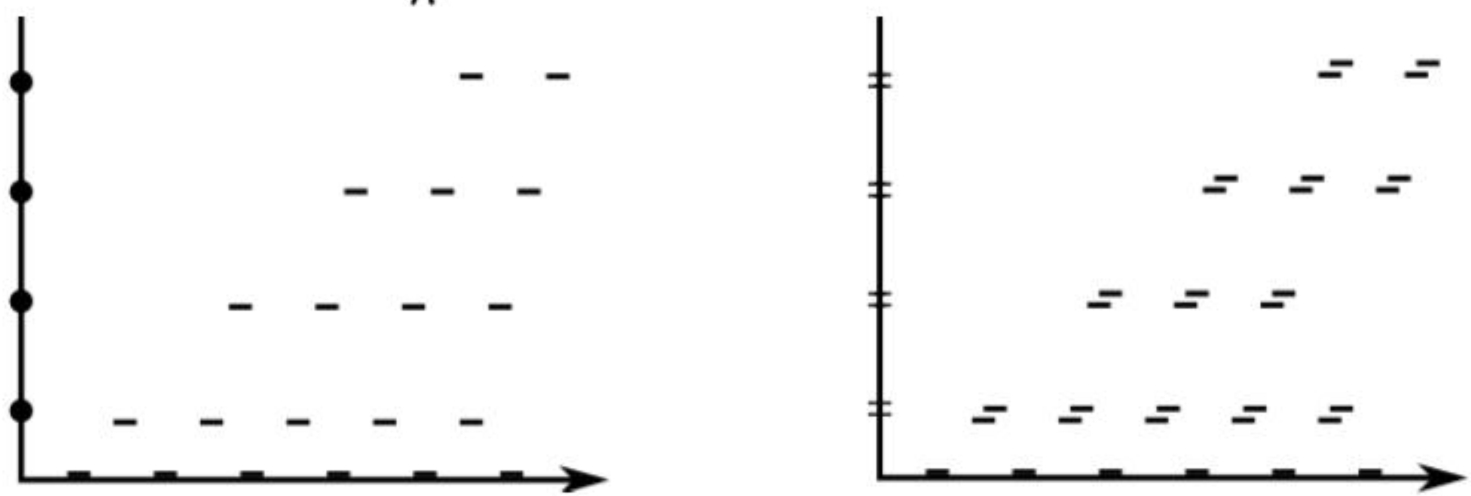
Band spectrum at least near the bottom. The "track" of bands: the Harmonic oscillator approximation

$$E_\nu(q) = \sum_{j=1}^{2} \omega_j(\nu_j + \tfrac{1}{2})h + O(h^2) \qquad \nu \in \mathbb{Z}_+^2$$

$U_{\min} = U(\tilde{x}, \tilde{y})$, and ω_1^2, ω_2^2 are eigenvalues of $\dfrac{\partial^2 U}{\partial x^2}(\tilde{x}, \tilde{y})$

$$E_\nu(q) - E_\nu(0) = 2\mathcal{A}(h)(\cos 2\pi q - 1)(1 + o(1))$$

$$|\mathcal{A}(h)| = b_m \frac{\omega_1 h}{\pi} e^{-\frac{S(\varepsilon(h))}{h}} \big(1 + o(1)\big)$$



Landau-Lifshits, Maslov, Poljakov, Agmon, H arell, Jona-Lazinio, Sent-Justin, Slavjanov, Pankratova, Hellfer, Söstrand, Simon,Wilkinson, Hanney, Mohamed,.....

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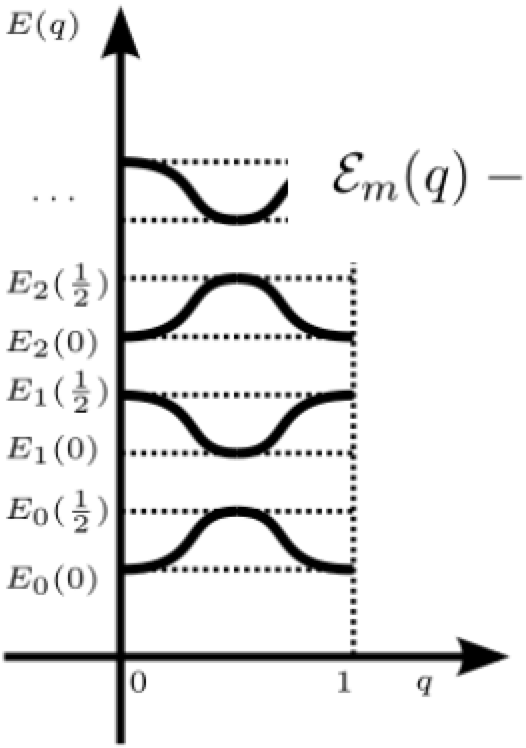
1-D periodic Schrödinger operator

$$\widehat{H}_1\Phi = \mathcal{E}\Phi, \quad \widehat{H}_1 = -\frac{h^2}{2}\frac{\partial^2}{\partial x^2} + v(x) \qquad \text{e.g.} \quad v(x) = \frac{\omega_1^2}{2}(1-\cos x)$$

$$\Phi^m(x+2\pi, q) = e^{2\pi i q}\Phi^m(x,q)$$



$$\mathcal{E}_m(q) - \mathcal{E}_m(0) = (-1)^m b_m \frac{\omega_1 h}{\pi} e^{-\frac{S_m(h)}{h}}(1-\cos 2\pi q)(1+o(1))$$

$$b_m = \frac{2^{-m}\sqrt{\pi}(2m+1)^{\frac{2m+1}{2}}}{m! e^{\frac{1}{2}+m}}$$

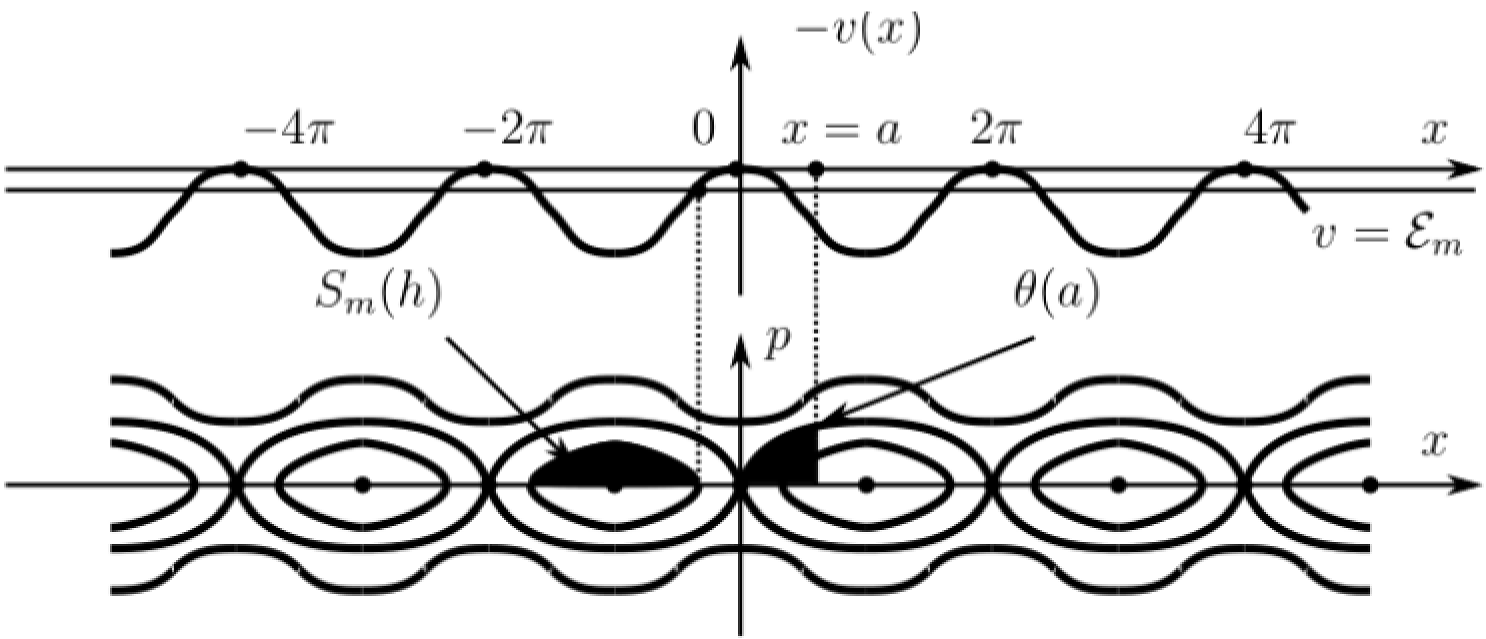
$$\Phi^m(x,q) = \sum_{k=-\infty}^{\infty} w_m(x-2\pi k)e^{2\pi i k q}$$

Wannier functions

$$w_m(x) \approx A_m(x,h)e^{-\frac{\theta(x)}{h}} \approx \mathbf{H}_m\left(\frac{\omega_1 x}{\sqrt{h}}\right)e^{-\frac{\omega_1 x^2}{2h}}, \quad \theta(x) = \left|\int_{x_k}^{x_k+x}\sqrt{2v(z)}dz\right|$$

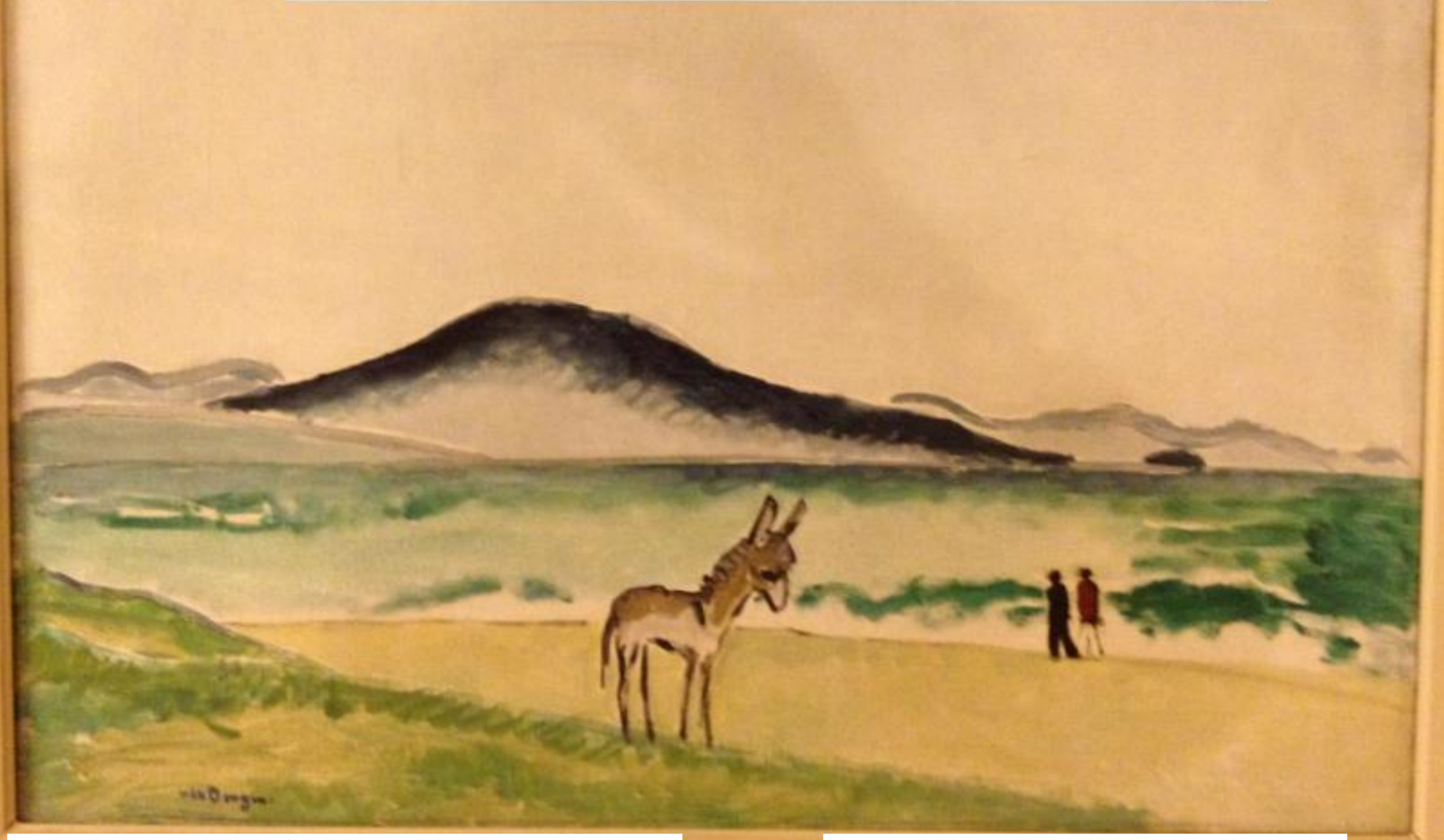
$$S_m(h) = \int_{x_-(h,m)}^{x_+(h,m)} \sqrt{2v(x) - h\omega_1(2m+1)}\, dx = \pi J_m$$

inverted potential



LANDAU-LIFSHITS SPLITTING FORMULAS

$$E_n^+ - E_n^- = b\frac{\omega h}{\pi}e^{-\pi J_n/h}(1 + O(h))$$



Kees van Dongen, Small Donkey on the Beach, Musee de lAnnonciade, Saint-Tropez

DOUBLE WELL IN 1-DCASE

The Schrödinger equation

$$(-\frac{h^2}{2}\frac{d^2}{dx^2} + V(x))\Psi = E\Psi$$

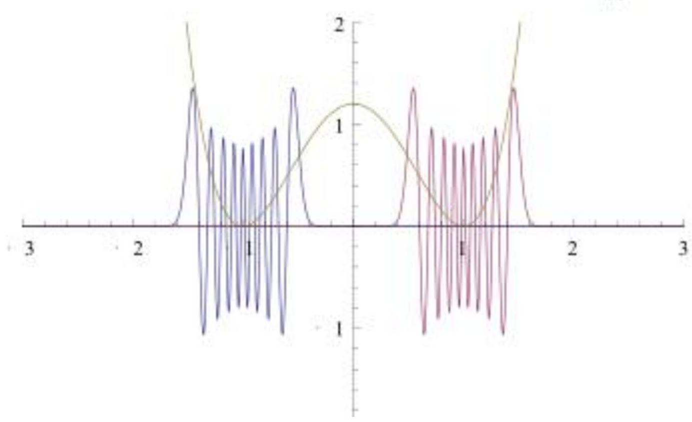
$V(x) = V(-x)$ is a smooth function increasing at infinity with two nondegenerating minimum points $x_\pm$ such that $V(x_\pm) = 0$.

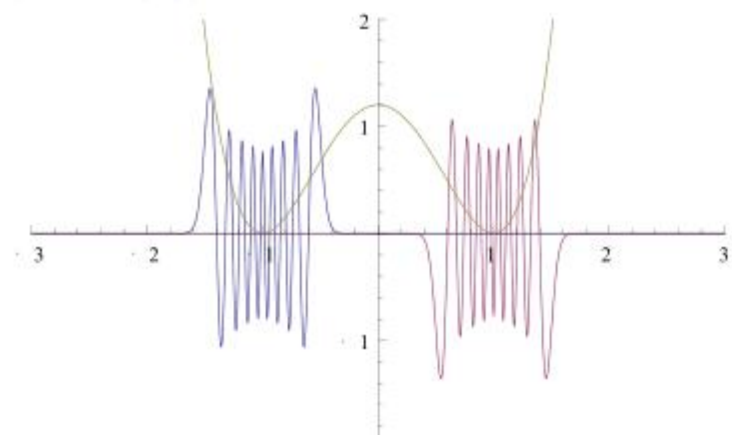
The spectrum under the barrier: $E = E_n^\pm$ **the Bohr–Sommerfeld quantization rule**

$$\frac{1}{2\pi}\oint p\,dx = (n + \frac{1}{2})h,$$

The splitting (Landau-Lifshits)

$$E_n^+ - E_n^- = \frac{\omega h}{\pi} e^{-\pi J/h}(1 + O(h)).$$





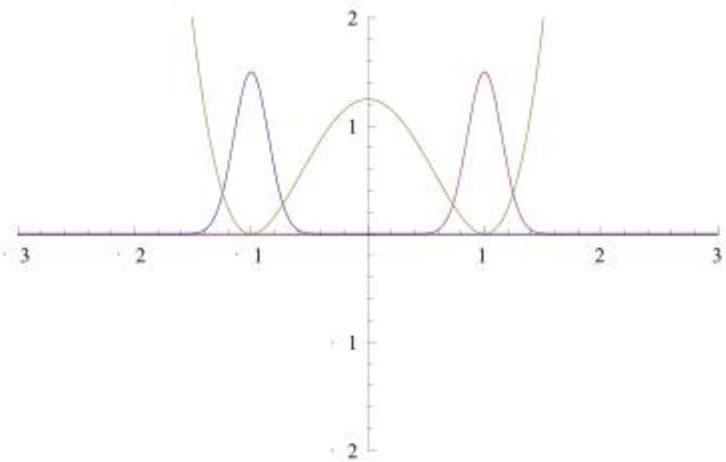
The ground states:

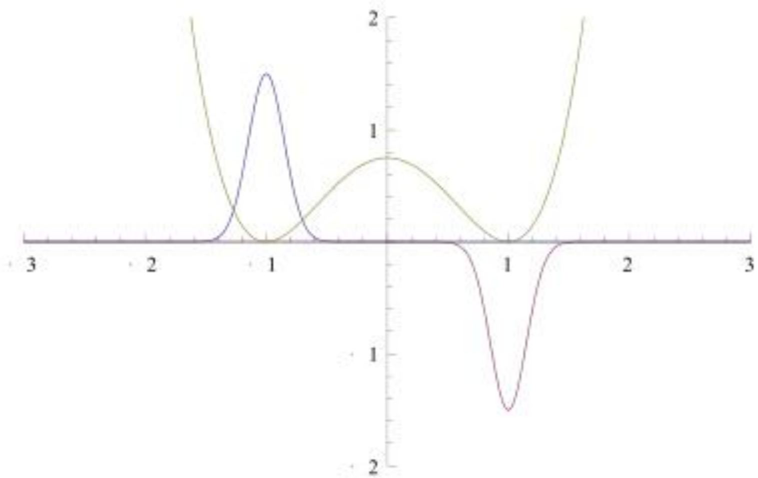
semiclassics $\sim$ the harmonic oscillator approximation

$$E_n = \frac{\omega_0 h}{2}$$

$\omega_0 = V_{xx}(x_\pm)$ is the frequency of the "limit periodic motions"

$$E_0^+ - E_0^- = \sqrt{\frac{\pi}{e}} \frac{\omega_0 h}{\pi} e^{-\pi J_0/h}(1 + O(h)).$$



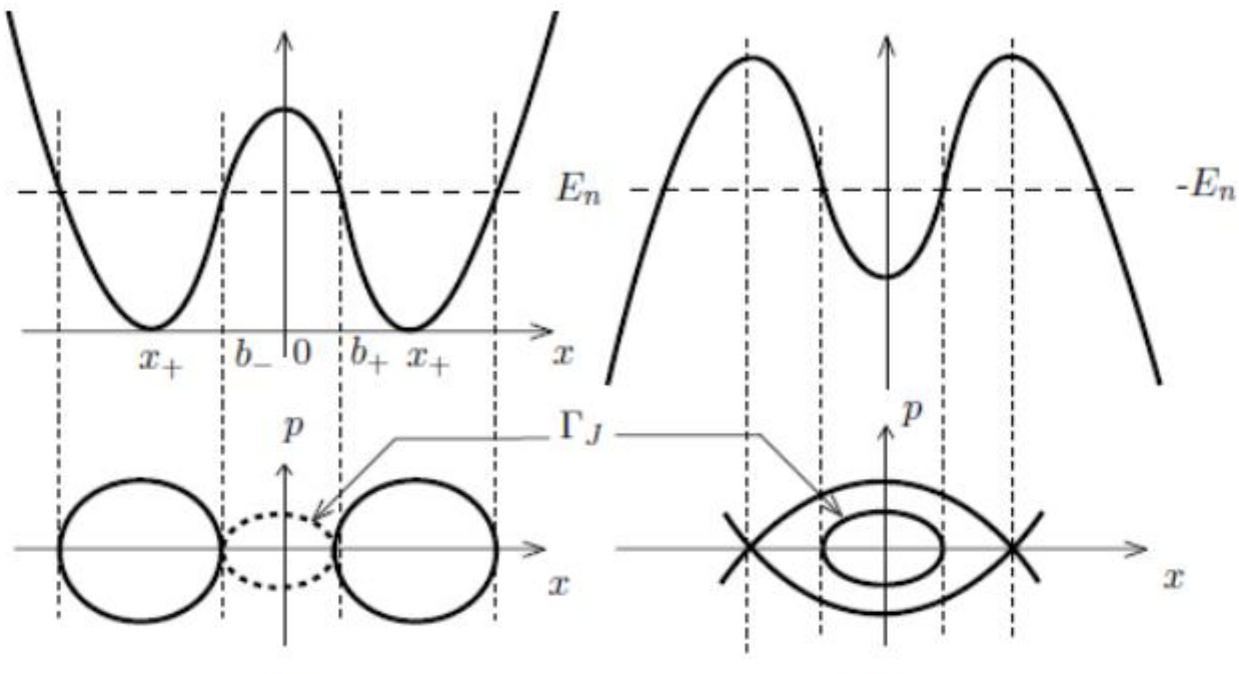


Geometrical interpretation

Two types of asymptotics:

Standard WKB: $\Psi = A(x)e^{\frac{i}{\hbar}S(x)}$,
the Hamiltonian $H(p,x) = \frac{p^2}{2} + V(x)$, S is real

Tunnel WKB: $\Psi = A(x)e^{-\frac{1}{\hbar}S(x)}$,
the Hamiltonian $\mathcal{H}(p,x) = -H(ip,x) = \frac{p^2}{2} - V(x)$, S is real



(a) (b)

Two types of asymptotics:

The Hamiltonian mechanics for Standard WKB:
$\Psi = \sum_j A_j(x) e^{\frac{i}{h} S_j(x)}$,
the Hamiltonian $H(p,x) = \frac{p^2}{2} + V(x)$, $\ddot{x} = -V_x$, S is real
the Hamilton-Jacoby equation+ an invariant structure with respect to the Fourier transform $F(A_j(x) e^{\frac{i}{h} S_j(x)}) = \sum_j \tilde{A}_j(p) e^{\frac{i}{h} \tilde{S}_j(p)}$, $\tilde{S}_j(p)$ is real

Lagrangian Mechanics for tunneling: $\Psi = \sum_j A_j(x) e^{-\frac{1}{h} S_j(x)} = A_j(x) e^{-\frac{1}{h} \mathrm{min_j S_j(x)}} + O(e^{-\rho/h}) \quad \Longrightarrow \quad \Psi = A(x) e^{-\frac{1}{h} S(x)}$,
the Hamiltonian $\mathcal{H}(p,x) = -H(ip,x) = \frac{p^2}{2} - V(x)$, $\ddot{x} = V_x$, S is real

the Hamilton-Jacoby-Bellmann equation for S ("tropical mathematics")+ there is no an invariant structure with respect to the Fourier transform $F(A_j(x) e^{-\frac{1}{h} S_j(x)}) =???? \tilde{A}_j(p) e^{\frac{i}{h} \tilde{S}_j(p)}$,
$\tilde{S}_j(p)$ is **complex-valued**, $A_j(x) e^{-\frac{1}{h} \mathrm{min_j S_j(x)}}$ is the **Agmon metric**

Remark 1: How does the frequency ω_n appear in splitting?
$\Longleftrightarrow$ The jump of action I:

The Bohr-Sommerfeld rule: $I_n^{\pm} = h(\frac{1}{2} + n) + O(h^2)$, $I_n^- - I_n^+ = \Delta_n$

The Lioville theorem: $E = H(I) \implies$

$$E_n^- - E_n^+ = H(I_n^-) - H(I_n^+) = \frac{\partial H}{\partial I}\Delta_n + O(\Delta^2) = \omega_n \Delta_n + O(\Delta^2)$$

Remark 2: How to find $\Delta_n = qe^{-\pi J_n}$?
Assume that $V(x)$ is analytic $\implies$
there exist two integrals $I = I(p, x)$ and $J(p, x) = J(ip, x)$

Due to general properties of Hamiltonian system $J = J(I) \implies$
choosing $I = I_n^{\pm}$ we got

$$\Delta_n = qe^{-\pi J(I_n^{\pm})}$$

The methods:

1) matching various asymptotics (Landau-Lifshits)

2) Complex WKB: passage to the complex plain (Stokes)

3) tunnel WKB: $\Psi = A(x)e^{-\frac{1}{\hbar}S(x)}$

+the Lifshits-Herring formula: $\Psi^{\pm}, E^{\pm}, \Delta E = E^{-}E^{+}$

$$\Delta E = \frac{\int_{\partial\Omega}(\Psi^{+}\nabla\Psi^{-} - \Psi^{-}\nabla\Psi^{+})\, d\sigma}{\int_{\Omega}(\Psi^{+}\Psi^{-}\, dV}$$

+ the Laplace method on the boundary $\partial\Omega \Longrightarrow$ the answer is based on the separatrix $\sim$ instanton in N-D-case.

This method is working for the lower states.

4) The Helffer and Sjöstrand interaction matrix

2-D case

Let $(\omega^1)^2, (\omega^2)^2, \quad 0 < \omega_1 < \omega_2$ are eigenvalues of $||\frac{\partial^2 V}{\partial x_1 \partial x_2}||$ in the minima points $\pm(a, \frac{b}{w_2}a)$

The ground states (the Harmonic oscillator approximation)

$$E_0^{\pm} = \frac{h}{2}(\omega^1 + \omega^2) + O(h^2)$$

The splitting

$$\Delta_0 = E_0^+ - E_0^- = \sqrt{\frac{\pi}{e}}\frac{\omega^1 h}{\pi} e^{-\pi J_0/h}(1 + O(h)).$$

$$J_0 = ??????$$

Geometrical interpretation

Exited states: one should change the trajectories (family) by the so-called 2-D Lagrangian manifolds Λ^2 in 4-D phase space $\mathbb{R}^4_{p_1,p_2,x_1,x_2}$, which are Liouville tori for the spectral problems $\Longrightarrow$ assumption the Hamiltonian system is completely integrable

The Bohr-Sommerfeld quantization rule + Maslov indices:

$$I_j = \frac{1}{2\pi}\oint_{\gamma_j} p\,dx = (n_j + \frac{1}{2})h, \gamma_j, \quad n_j \in \mathbb{Z}^2, j = 1,2$$

γ_1, γ_2 are **cycles** and are not **trajectories** usually, I_1, I_2 are action variables and integrals of classical motion.

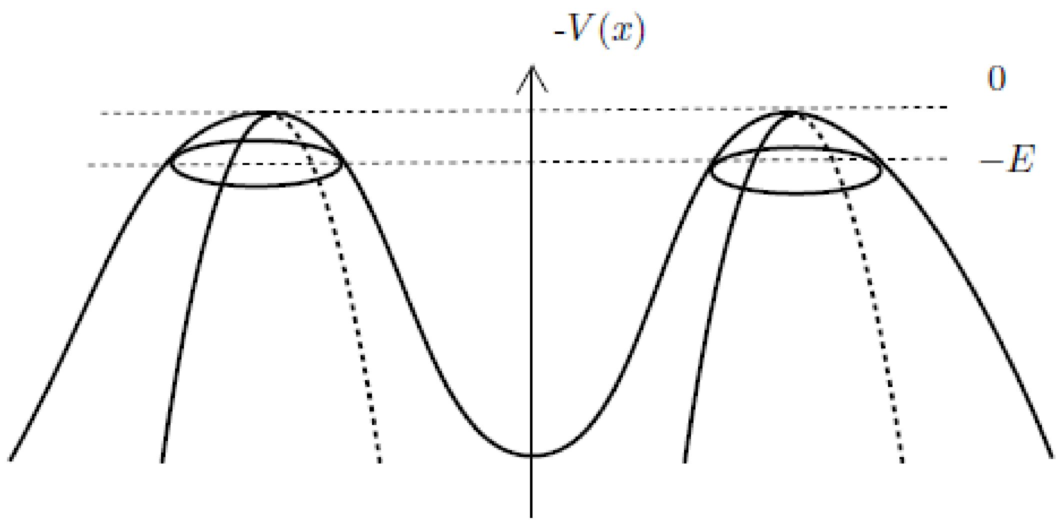
Small I_j (Lower levels) :
Using the Tailor expansion one can change the Hamiltonian H in the neighborhood of minima points by a quadratic polynomial ("normal form"). This gives an **integrable** Hamiltonian system ("almost integrability" of the original hamiltonian) and leads to

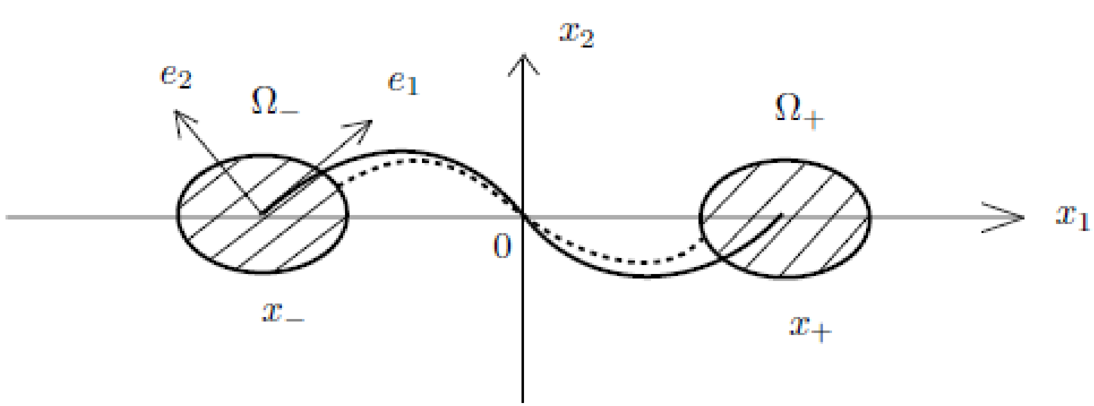
$$H = \omega^1 I_1 + \omega^2 I_2 + O(I^2)$$

and to Harmonic approximation for the Schrödinger operator

2-D-splitting

Libration are **unstable** trajectories of $\ddot{x} = V_x$ coinciding the level cuts of the 2-D potential (final proof of their existence: Kozlov and Bolotin). They give the family of **unstable** trajectories in the 4-D phase space $\mathbb{R}^4_{p_1,p_2,x_1,x_2}$ located near the instanton.





Librations + Birkhoff and Williamson normal forms gives the expansion of tunnel Hamiltonian in the neighborhood of the closed trajectories:

$$\mathcal{H} = \frac{p^2}{2} - V(x) = \mathcal{H}_0(J_1) - \beta(J_1)J_2 + O(J_2^2)$$

Here J_1, J_2 are the action functions near the librations and are "almost" integrals of Hamiltonian system with the Hamiltonian $\mathcal{H}$ and $J_j = J_j(p, x)$.

Under assumption about analyticity one may extend integrals $J_j(p, x)$ to imaginary ip and obtain integrals of the "standard" Hamiltonian system with the Hamiltonian $\mathcal{H} = \frac{p^2}{2} + V(x)$.

Thus $J_1 = J_1(I_1, I_2), J_2 = J_2(I_1, I_2)$

Proposition. $J_2 = I_2 + O(I_2^2)$

$$-E = \mathcal{H}_0(J_1) - \beta(J_1)J_2 + O(J_2^2) = -\omega^1 I_1 - \omega^2 I_2 + O(I^2)$$

We put $I_1 = I_2 = J_2 = h$, and $J_0 = J_1$, $\Longrightarrow$ the equation for J_0

$$\mathcal{H}(J_0) - \frac{1}{2}\beta(J_0)h = -\frac{h}{2}(\omega^1 + \omega^2)$$

and the splitting

$$\Delta_0 = E_0^+ - E_0^- = \sqrt{\frac{\pi}{e}}\frac{\omega^1 h}{\pi}e^{-\pi J_0/h}(1 + O(h)).$$

The splitting in $n-D$ case
(accurate proof is given by A.Anikin, to appear in RJMP):

$$E_0^+ - E_0^- = \sqrt{\frac{\pi}{e}}\frac{\omega^1 h}{\pi}e^{-\pi J_0/h}(1+O(h)).$$

$$\mathcal{H}(J_0) - \frac{1}{2}(\beta^2(J_0)+\ldots+\beta^n(J_0))h = -\frac{h}{2}(\omega^1+\omega^2+\ldots+\omega^n).$$

Assumption (technical ??????) $\quad \omega^1 < \frac{1}{2}\min(\omega^2,\ldots,\omega^n)$

For comparison: the splitting formula based on the **instanton**

$$E_0^+ - E_0^- = \frac{4\sqrt{\omega^1\cdot\ldots\cdot\omega^n h}}{\sqrt{\pi}}\frac{\sqrt{V(0)}}{(\det C)}\left(\lim_{t\to\infty} e^{(\omega^1+\ldots+\omega^n)t}\det Z(t)\right)e^{-\pi J_{ins}/h}(1+O(h)).$$

⇑ ⇑
"determinant problem"

$$\ddot{Z}_{ij}(t) = \sum_{k=1}^{2}\left.\frac{\partial^2 V}{\partial x_i \partial x_k}\right|_{x=X(t)} Z_{kj}(t), \qquad Z(0)=E, \quad Z(\infty)=0,$$

Remark about complex Lagrangian manifold and "tunnel" cycle (some heuristic consideration)

The pair of "Liouville" tori + libration and its neighborhood belong

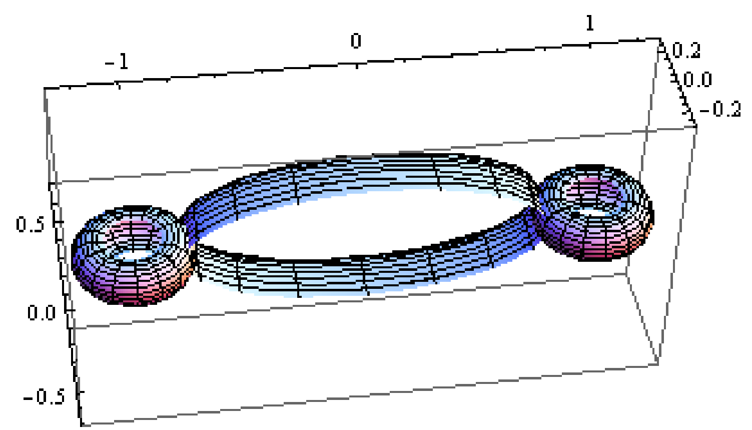
to the 2-complex D complex almost "invariant" Lagrangian manifold Λ

from the surface $\{H(p,x)|_\Lambda \approx \mathcal{E} = \frac{h}{2}(\omega^1 + \omega^1)\}$ in the 4-complex D

complex phase space $\mathbb{C}_{px}$. We emphasize that the libration is

NOT a trajectory for the energy level, it is a **CYCLE** on Λ

and J_0 is the action on this cycle.



2-D case with magnetic field. Simple important observation:

$$\widehat{H}\psi = \Big[\frac{1}{2}\Big(-ih\frac{\partial}{\partial y}\Big)^2 + \frac{1}{2}\Big(-ih\frac{\partial}{\partial z} + by\Big)^2 + V(z,y)\Big]\Psi = E\Psi,$$

Tunnel WKB $\Psi = A(z,y)e^{-\frac{1}{h}S(z,y)} \implies$ the presence of a magnetic field give the ***complex*** Hamiltonian and the ***complex*** phase space etc:

$$\mathcal{H} = \frac{1}{2}(-p_y^2 + (ip_z + by)^2) + v_1(y) + \frac{w_2^2 z^2}{2}, \qquad v_1(y) = w_1^2(y^2 - a^2)^2/(8a^2)$$

The trick: mixed representation $\Longrightarrow$
the standard 2-D double well problem

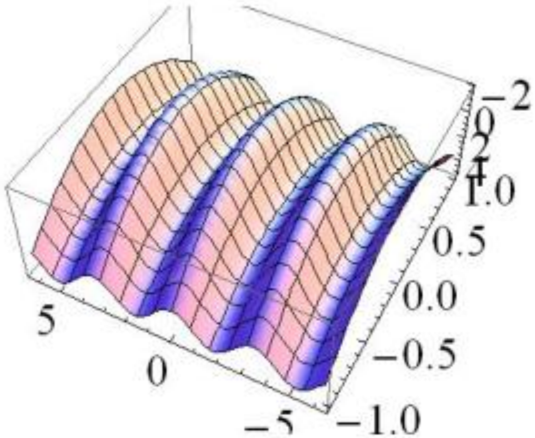
$$\widetilde{\psi}(y, p_z) = \int_{-\infty}^{\infty} \psi(y,z)e^{\frac{i\omega_2 p_z z}{h}}\, dz.$$

We put $x_1 = y \;\; x_2 = p_z$ then

$$\hat{H}' = \frac{1}{2}\Big(-ih\frac{\partial}{\partial x_1}\Big)^2 + \frac{1}{2}\Big(-ih\frac{\partial}{\partial x_2}\Big)^2 + v_1(x_1) + \frac{(w_2 x_2 - bx_1)^2}{2},$$

Symmetry: $x_{1,2} \to -x_{1,2}$.

Minima points $(x_1, x_2) = (a, \frac{b}{w_2}a) \;\; (x_1, x_2) = -(a, \frac{b}{w_2}a)$, here $a > 0$ is the minimum of v_1.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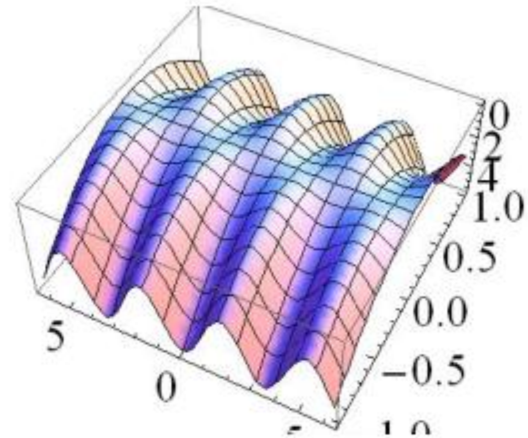
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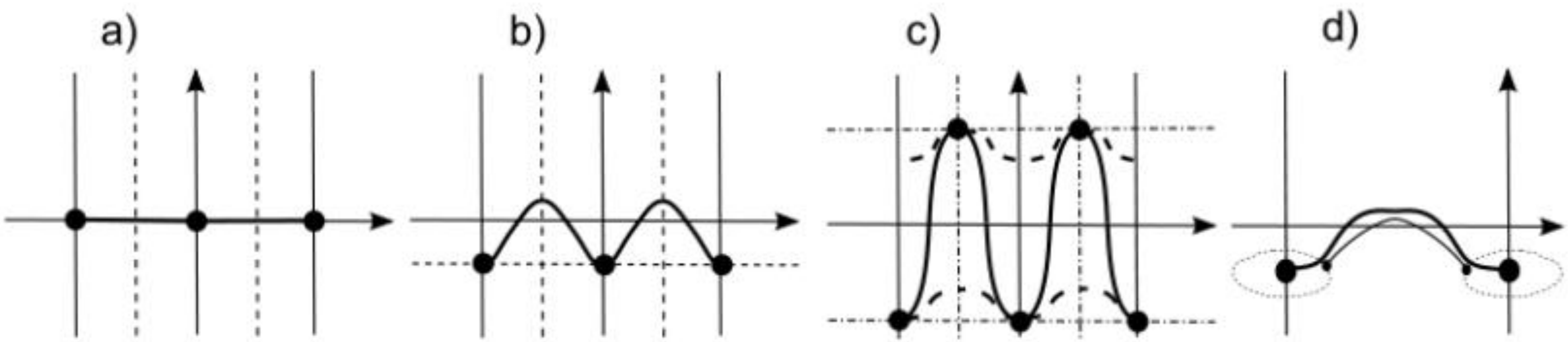
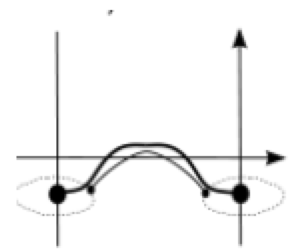
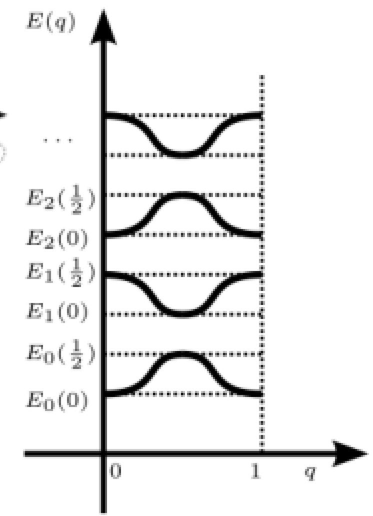

a)
b)
c)
d)

Let $\gamma_{\mathcal{E}}$ be the libration with energies $-\mathcal{E} = \frac{p^2}{2} - U(x,y)$, $\lambda(\mathcal{E}) > 0$ be a non-trivial Floquet exponent of a corresponding libration. Then the equation

$$\mathcal{E} + \frac{h}{2}\lambda(\mathcal{E}) = \frac{h}{2}\Big(\omega_-(2m+1) + \omega_+\Big)$$

has a unique solution $\mathcal{E} = \mathcal{E}_m(h)$ for each m and sufficiently small h and $\mathcal{E}$. This determines a sequence of energies $\mathcal{E} = \mathcal{E}_m(h)$ or a sequence of "tunnel" librations $\gamma_{\mathcal{E}_m(h)}$ with actions $S(\varepsilon_m(h))$.





$$E_\nu(q) = \omega_-\Big(\nu_- + \frac{1}{2}\Big)h + \omega_+\Big(\nu_+ + \frac{1}{2}\Big)h + O(h^2)$$

$$E_\nu(q) - E_\nu(0) = 2\mathcal{A}(h)(\cos 2\pi q - 1)(1 + o(1))$$

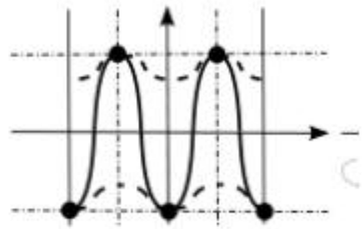
$$C_1 h^{\kappa_1} e^{-\frac{d_0}{h}} \le \Big|\mathcal{A}(h)\Big| \le C_2 h^{\kappa_2} e^{-\frac{d_0}{h}}$$

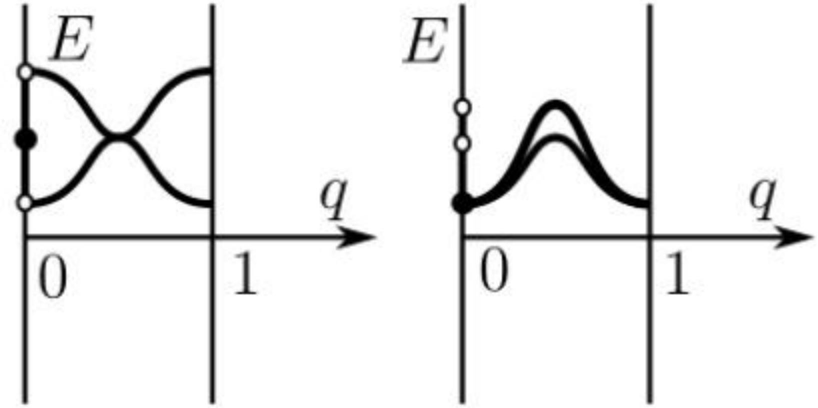
if $\nu_+ = 0$

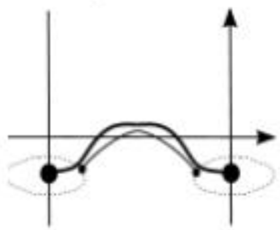
$$|\mathcal{A}(h)| = b_{\nu_-}\frac{\omega_- h}{\pi} e^{-\frac{S(\varepsilon_{\nu_-}(h))}{h}}\big(1 + o(1)\big)$$

$$b_m = \frac{2^{-m}\sqrt{\pi}(2m+1)^{\frac{2m+1}{2}}}{m! e^{\frac{1}{2}+m}}$$

c)







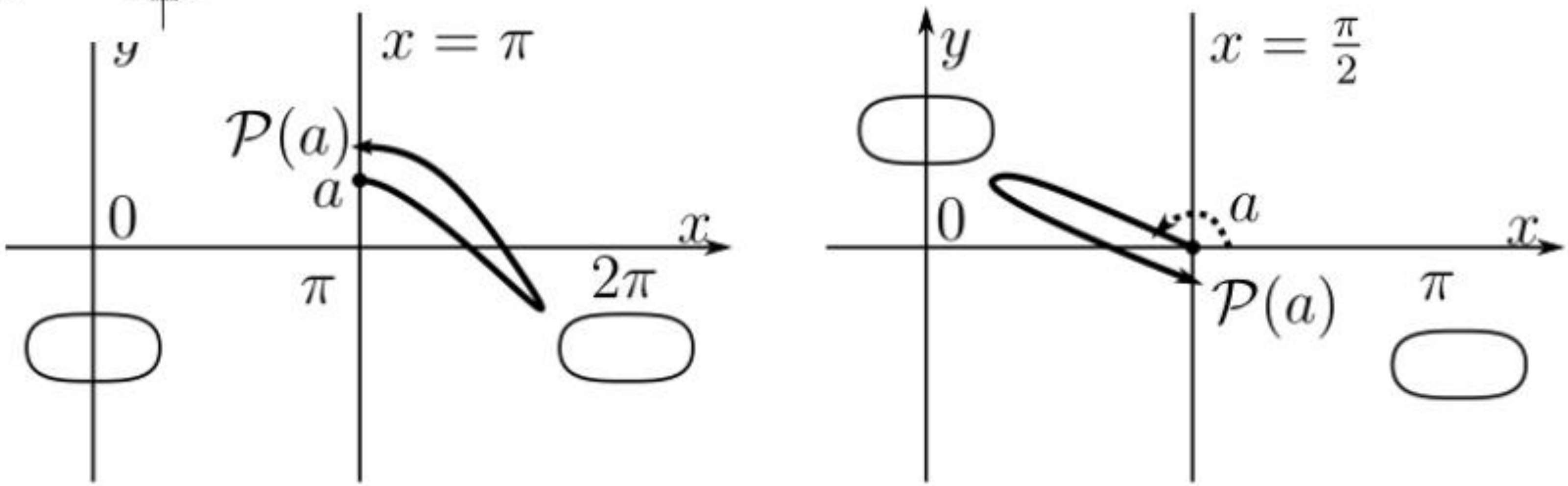


Figure 7: Seeking a libration numerically. In Case 1 (on the left) we shoot from the line $x = \pi$ with the initial velocity parallel to the x-axis. The magnitude of the velocity is determined by energy E. The varying parameter a is the initial y-coordinate. In Case 2 for a 'vertical' libration (on the right) we shoot from the point $x = \pi/2$, $y = 0$ with the velocity magnitude determined by energy E. The varying parameter a is the shooting angle.

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THANK YOU FOR YOUR ATTENTION !

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