Quasi-classical Calculation of Eigenvalues: Examples and Questions

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To the memory of Gérard G. Emch

Abstract. We discuss the Maslov quantization condition, especially a method of quasi-classical calculation of energy levels of Schrödinger operators. The method gives an approximation of eigenvalues of operators in general. We give several concrete examples of Schrödinger operators to which the quasi-classical calculation gives the correct eigenvalues and pose some open problems.

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Introduction

Maslov introduces the so-called Maslov index and the quantization condition for Lagrangian submanifolds and studies the "asymptotic solutions" of the eigenvalue problems in quantum mechanics [7]. The Malsov quantization condition can be regarded as a generalization of the Bohr quantization rule. By means of the quantization condition we can obtain good approximate eigenvalues of Schrödinger operators (see, for example, [4, 8–10]).

On the contrary, there exist several concrete quantum mechanical systems where we obtain exact eigenvalues and multiplicities by means of the Maslov quantization condition (see, for example, [1]). Thus, as far as these systems are concerned, we need not to consider the operator theory to obtain the exact quantum mechanical energy levels and their multiplicities. What we need is only classical mechanics, invariant Lagrangian submanifolds and Maslov's quantization condition.

Our question is:

Why there is such a coincidence?

As far as we know, we have no mathematical proof of the coincidence at present.

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In this note, we explain a concept of quasi-classical calculation of eigenvalues of Schrödinger operators. We also show examples for which the Maslov quantization condition gives exact eigenvalues.

We should also mention the paper of Leray [6], inspired by Malsov's theory, where he constructed a theory of a Lagrangian analysis and treated such a kind of concrete examples.

Maslov quantization condition

Let θ be the canonical 1-form of the cotangent bundle T^*M of a smooth manifold M and $\pi : T^*M \to M$ be the canonical projection. We consider the symplectic manifold $(T^*M, d\theta)$. Consider a Lagrangian submanifold L of $(T^*M, d\theta)$. The Maslov quantization condition is then written as

$$
\frac{1}{2\pi\hbar} \int_c \theta - \frac{1}{4} \langle m_L, [c] \rangle \in \mathbb{Z},
$$

where \hbar (Planck constant) is a positive parameter, $[c] \in H_1(L, \mathbb{Z})$ and m_L is the Maslov class of L.

Example 1: Harmonic oscillator

We explain here how the Maslov quantization condition determines discrete energy levels of a Hamiltonian. We consider the case where $M = \mathbb{R}$ and then the cotangent bundle is $T^*M = T^*\mathbb{R} = \mathbb{R}^2$. We write points as $(x, p) \in \mathbb{R}^2$. Then the cotangent bundle has the canonical symplectic form $d\theta$, where $\theta = pdx$. We consider a Hamiltonian function $H = \frac{1}{2}(p^2 + x^2)$ of the harmonic oscillator.

Now we consider a level set of the function H for every constant $E > 0$, such that

$$
L(E) = \{(x, p) \in \mathbb{R}^2 \mid H(x, p) = E\}.
$$

The level set $L(E)$ is a Lagrangian submanifold of $(\mathbb{R}^2, d\theta)$. We consider the Maslov quantization condition for the Lagrangian submanifold $L(E)$. The equation of motion is

$$
\dot{x} = p, \ \dot{p} = -x
$$

and an orbit in $L(E)$ is

$$
c_E: x(t) = x_0 \cos t + p_0 \sin t, \quad p(t) = p_0 \cos t - x_0 \sin t,
$$

where (x_0, p_0) is a point in $L(E)$ and then $E = H(x_0, p_0) = \frac{1}{2}(p_0^2 + x_0^2)$. Hence the action integral along c_E is

$$
\int_{c_E} \theta = \int_0^{2\pi} p(t)\dot{x}(t)dt = \frac{1}{2}(p_0^2 + x_0^2) 2\pi = 2\pi E.
$$

As to the Maslov index, we prepare the following lemma.

We consider the symplectic manifold $(T^*\mathbb{R}^n, d\theta)$. Let

$$
H_1(x,p), H_2(x,p), \ldots, H_n(x,p)
$$

be smooth functions on a domain D in $T^*\mathbb{R}^n$. Suppose they are in involution, or Poisson commuting each other. We denote their level set by

$$
L(c_1, c_2,..., c_n) = \{(x,p) \in D \mid H_1(x,p) = c_1, H_2(x,p) = c_2,..., H_n(x,p) = c_n\}.
$$

We put $H = (H_1, H_2, \ldots, H_n)$ and define $n \times n$ matrices by

$$
H_x = \left(\frac{\partial H_j}{\partial x_k}\right), \ H_p = \left(\frac{\partial H_j}{\partial p_k}\right), \ j, k = 1, 2, \dots, n.
$$

Then we have (see [11])

Lemma 1. *The Maslov form on* $L(c_1, c_2, \ldots, c_n)$ *is given explicitly as*

$$
m_L = \frac{1}{\pi} d \left(\arg \det(H_p + iH_x) \right).
$$

For the harmonic oscillator $H(x, p) = 1/2$ $(x^2 + p^2)$, we have

$$
\det(H_p + iH_x) = p + ix.
$$

Hence, on the curve

$$
c_E: x(t) = x_0 \cos t + p_0 \sin t, \ p(t) = p_0 \cos t - x_0 \sin t
$$

we see $m_L = (1/\pi) d(\arg \det(H_p + iH_q)) = (1/\pi) dt$, and then the Maslov index for c_E is

$$
\langle m_L, [c_E] \rangle = \int_{c_E} m_L = \frac{1}{\pi} \int_0^{2\pi} dt = 2
$$

Then the Maslov quantization condition for $L(E)$ becomes

$$
\frac{1}{2\pi\hbar}\int_c \theta - \frac{1}{4} \langle m_L, [c] \rangle = \frac{E}{\hbar} - \frac{1}{2} \in \mathbb{Z}
$$

and the level set $L(E)$ satisfies the Malsov quantization condition if and only if the parameter E is given as

$$
E = E_n = \left(n + \frac{1}{2}\right)\hbar, \ n = 0, 1, 2, \dots,
$$

which gives exactly the eigenvalues of the Schrödinger operator of the harmonic oscillator.

Example 2: the hydrogen atom

In this section, we see that the Maslov quantization condition determines the eigenvalues of the Schrödinger operator of the hydrogen atom, the angular momentum operator and the Lenz operator, and also determines multiplicities of the eigenspaces for the hydrogen atom.

The operators of the hydrogen atom, the angular momentum operator and the Lenz operator are respectively given by

$$
\widehat{H}\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) = -\frac{\hbar^2}{2} \triangle - \frac{1}{|x|}, \ |x| = \left(\sum_{k=1}^3 x_k^2\right)^{1/2}
$$
\n
$$
\widehat{l}_1\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) = x_2 \widehat{p}_3 - x_3 \widehat{p}_2,
$$
\n
$$
\widehat{e}_1\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) = x_2 \widehat{p}_1 \widehat{p}_2 + x_3 \widehat{p}_1 \widehat{p}_3 - x_1(\widehat{p}_2^2 + \widehat{p}_3^2) + \widehat{p}_1 + \frac{x_1}{|x|},
$$

where \triangle is the 3-dimensional Laplacian and $\hat{p}_k = \frac{\hbar}{\partial x_k}$, $k = 1, 2, 3$. These opera-
ters are mutually commuting. Denote the corresponding Hamiltonian functions of tors are mutually commuting. Denote the corresponding Hamiltonian functions of \widehat{H} , \widehat{l}_1 and \widehat{e}_1 by

$$
H(x, p) = \frac{1}{2}|p|^2 - \frac{1}{|x|},
$$

\n
$$
l_1(x, p) = x_2p_3 - x_3p_2,
$$

\n
$$
e_1(x, p) = p_1 \langle x, p \rangle - x_1|p|^2 + \frac{x_1}{|x|},
$$

where $(x, p) \in T^*(\mathbb{R}^3 \setminus 0)$ and $\langle x, p \rangle = \sum_{k=1}^3 x_k p_k$. It is easy to see that the functions H, l_1 and e_1 are in involution, or Poisson commuting, with respect to the canonical Poisson bracket. We consider the level set of H, l_1 and e_1 such that

$$
L(\overline{E}, \overline{l}_1, \overline{e}_1) = \left\{ \begin{matrix} (x, p) \in T^*(\mathbb{R}^3 - 0) \mid H(x, p) = -E \ (E > 0) \\ l_1(x, p) = \overline{l}_1, e_1(x, p) = \overline{e}_1 \end{matrix} \right\}.
$$

The functions H, l_1 and e_1 satisfy a priori inequality (see [11, Proposition 1.1])

$$
1/\sqrt{-2H(x,p)} \ge |l_1(x,p)| + |e_1(x,p)|/\sqrt{-2H(x,p)}
$$

for any $(x, p) \in T^*(\mathbb{R}^3 - 0)$. For parameters $(\overline{E}, \overline{l}_1, \overline{e}_1)$ satisfying an inequality such that

 $1/\sqrt{2\overline{E}} > |\overline{l}_1| + \left(|\overline{e}_1|/\sqrt{2\overline{E}}\right)$

it is easy to see that the level sets $L(\overline{E}, \overline{l}_1, \overline{e}_1)$ are compact. Then we have

Proposition 2. The level sets $L(\overline{E}, \overline{l}_1, \overline{e}_1)$ are Lagrangian submanifolds and are *diffeomorphic to* 3 *torus generically.*

Now we calculate action integrals and also the Maslov indices along certain closed curves c_1, c_2, c_3 on $L(\overline{E}, \overline{l}_1, \overline{e}_1)$ which generate $H_1(L(\overline{E}, \overline{l}_1, \overline{e}_1), \mathbb{Z})$ as before, and by a direct calculation we can check the Malsov quantization condition. We see

$$
c_1: \frac{1}{2\pi\hbar}\int_{c_1}\theta-\frac{1}{4}\left\langle m_L,[c_1]\right\rangle=\frac{1}{2\pi\hbar}\left(\frac{1}{\sqrt{2\overline{E}}}+\frac{|\overline{e}_1|}{\sqrt{2\overline{E}}}+\overline{l}_1\right)-\frac{1}{2}\in\mathbb{Z},
$$

$$
c_2: \frac{1}{2\pi\hbar} \int_{c_2} \theta - \frac{1}{4} \langle m_L, [c_2] \rangle = \frac{1}{2\pi\hbar} \left(\frac{1}{\sqrt{2E}} - \frac{|\overline{e}_1|}{\sqrt{2E}} + \overline{l}_1 \right) - \frac{1}{2} \in \mathbb{Z},
$$

$$
c_3: \frac{1}{2\pi\hbar} \int_{c_3} \theta - \frac{1}{4} \langle m_L, [c_3] \rangle = \frac{\overline{l}_1}{\hbar} \in \mathbb{Z}.
$$

Then we have ([11])

Theorem 3. $L(\overline{E}, \overline{l}_1, \overline{e}_1)$ *satisfies the Maslov quantization condition if and only if*

$$
\overline{E} = \overline{E}_n = \frac{1}{2n^2\hbar^2}, \ \overline{l}_1 = \overline{l}_{1,m} = m\hbar, \ \overline{e}_1 = \overline{e}_{1,n_1,n_2} = \frac{n_1 - n_2}{n},
$$

where

 $n = n_1 + n_2 + |m| + 1$, $n, n_1, n_2, m \in \mathbb{Z}, n_1, n_2 \geq 0$.

Theorem 4. *The numbers* E_n , $\bar{l}_{1,m}$ *and* \bar{e}_{1,n_1,n_2} *are just equal to the eigenvalues of the operators* \hat{H} , \hat{l}_1 *and* \hat{e}_1 *, respectively. Moreover, for each* $\overline{E}_n = \frac{1}{2n^2\hbar^2}$ *, the number of level sets* $L(\overline{E}_n, \overline{l}_1, \overline{e}_1)$ *satisfying the Maslov quantization condition* $n =$ $n_1 + n_2 + |m| + 1$, $n_1, n_2 \geq 0$ *is equal to the multiplicity of the eigenspace of* H *belonging to* E_n .

Example 3: MIC-Kepler problem

The MIC-Kepler problem is the Kepler problem under the influence of Dirac's magnetic monopole. The quantized MIC-Kepler problem is formulated and solved by Iwai–Uwano as follows [3]: For every $m \in \mathbb{Z}$, Dirac's monopole field is defined by a closed two-form on $\mathbb{R}^3 \setminus \{0\}$

$$
\widetilde{\Omega}_m = -(m/2)|\widetilde{x}|^{-3}(\widetilde{x}_1 d\widetilde{x}_2 \wedge d\widetilde{x}_3 + \widetilde{x}_3 d\widetilde{x}_1 \wedge d\widetilde{x}_2 + \widetilde{x}_2 d\widetilde{x}_3 \wedge d\widetilde{x}_1),
$$

where $\widetilde{x} = (\widetilde{x}_1, \widetilde{x}_2, \widetilde{x}_3) \in \mathbb{R}^3 \setminus \{0\}$ and $|\widetilde{x}| = (\widetilde{x}_1^2 + \widetilde{x}_2^2 + \widetilde{x}_3^2)^{1/2}$. A simple calculation yields $\int_{S^2} \widetilde{\Omega}_m = 2\pi m$, where S^2 is the unit two-sphere and $\widetilde{\Omega}_m$ is an integral. Then we have a complex line bundle E_m over $\mathbb{R}^3\setminus\{0\}$ with a Hermitian inner product \langle , \rangle_m and a linear connection ∇^m with the curvature form $\tilde{\Omega}_m$. The Hamiltonian of the quantized MC-Kepler problem is given by

$$
\widehat{H}_m = -\frac{\hbar^2}{2} \sum_{j=1}^3 (\nabla_j^m)^2 + \frac{(m/2)^2}{2|\widetilde{x}|^2} - \frac{1}{|\widetilde{x}|},
$$

where ∇_j^m stands for the covariant derivative in the direction of $\partial/\partial \tilde{x}_j$, $j = 1, 2, 3$. The operator \widehat{H}_m has mutually commuting operators

$$
\begin{aligned}\n\widehat{l}_{m,1} &= \frac{\hbar}{i} \left(\widetilde{x}_2 \nabla_3^m - \widetilde{x}_3 \nabla_2^m \right) + \frac{(m/2)}{|\widetilde{x}|} \widetilde{x}_1, \\
\widehat{e}_{m,1} &= \frac{\hbar}{2i} \left(\widehat{l}_{m,2} \nabla_3^m - \widehat{l}_{m,3} \nabla_2^m - \nabla_2^m \widehat{l}_{m,3} + \nabla_3^m \widehat{l}_{m,2} \right) + \frac{\widetilde{x}_1}{|\widetilde{x}|}.\n\end{aligned}
$$

The eigenvalue problem is exactly solved by Iwai–Uwano [3] as follows. Consider a non-negative integer n subject to the condition: $|m| \leq n$ and $n-m$ is even. Then the eigenvalues of \widehat{H}_m and their multiplicities are

$$
E_n^{(m)} = -\frac{2}{(n+2)^2\hbar^2}, \frac{(n-m+2)(n+m+2)}{4},
$$

respectively.

On the other hand, the corresponding classical mechanical system is the following. The symplectic manifold is $(T^*(\mathbb{R}^3 \setminus \{0\}), \sigma_m)$, where

$$
\sigma_m = \sum_{j=1}^3 d\widetilde{p}_j \wedge d\widetilde{x}_j + \pi^* \widetilde{\Omega}_m, \ (\widetilde{x}, \widetilde{p}) \in T^*(\mathbb{R}^3 \setminus \{0\}) = (\mathbb{R}^3 \setminus \{0\}) \times \mathbb{R}^3
$$

and $\pi : T^*(\mathbb{R}^3 \setminus \{0\}) \to \mathbb{R}^3 \setminus \{0\}$ is the canonical projection. The classical Hamiltonian of the operators $\widehat{H}_m, \widehat{l}_{m,1}$ and $\widehat{e}_{m,1}$ are respectively given by

$$
H_m(\tilde{x}, \tilde{p}) = \frac{1}{2} |\tilde{p}|^2 + \frac{(m/2)^2}{2|\tilde{x}|^2} - \frac{1}{|\tilde{x}|},
$$

\n
$$
l_{m,1}(\tilde{x}, \tilde{p}) = \tilde{x}_2 \tilde{p}_3 - \tilde{x}_3 \tilde{p}_2 + \frac{(m/2)}{|\tilde{x}|} \tilde{x}_1,
$$

\n
$$
e_{m,1}(\tilde{x}, \tilde{p}) = -\tilde{x}_1 |\tilde{p}|^2 + \tilde{p}_1 \langle \tilde{x}, \tilde{p} \rangle + \frac{(m/2)(\tilde{x}_2 \tilde{p}_3 - \tilde{x}_3 \tilde{p}_2)}{|\tilde{x}|} + \frac{\tilde{x}_1}{|\tilde{x}|}.
$$

The classical Hamiltonian functions $H_m, l_{m,1}$ and $e_{m,1}$ are in involution, and we consider their level sets

$$
L(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1}) = \left\{ \begin{matrix} (\widetilde{x}, \widetilde{p}) \in T^*(\mathbb{R}^3 - \{0\}) \mid H_m(\widetilde{x}, \widetilde{p}) = -\overline{E}, \ (\overline{E} > 0) \\ l_{m,1}(\widetilde{x}, \widetilde{p}) = \overline{l}_{m,1}, \ e_{m,1}(\widetilde{x}, \widetilde{p}) = \overline{e}_{m,1} \end{matrix} \right\}.
$$

By a similar way as in the Kepler problem, we see that the parameters $(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1})$ satisfy a certain natural inequality, and generically the level set $L(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1})$ is diffeomorphic to 3-torus.

Iwai–Uwano [2] showed that the classical MIC-Kepler problem is obtained by the Marsden–Weinstein reduction by $U(1)$ action on the cotangent bundle $(T^*(\mathbb{R}^4 - \{0\}), d\theta)$. Using this structure Yoshioka–Ii [12] defined a quantization condition on the symplectic manifold $(T^*(\mathbb{R}^3 \setminus \{0\}), \sigma_m)$ which is regarded as a $U(1)$ -reduction of the Maslov quantization condition on the symplectic manifold $(T^*(\mathbb{R}^4 - \{0\}), d\theta).$

Similarly as before, we can check the quantization condition for the level set $L(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1})$ and we obtain ([12])

Theorem 5. *The Lagrangian submanifold* $L(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1})$ *satisfies the quantization condition if and only if the parameters* $(\overline{E}, \overline{l}_{m,1}, \overline{e}_{m,1})$ *coincide with the eigenvalues of the corresponding Hamiltonian operators. For each eigenvalue* $\overline{E} = -E_n^{(m)}$ = $\frac{2}{(n+2)^2\hbar^2}$, the number of the Lagrangian submanifolds $L(E, l_{m,1}, \overline{e}_{m,1})$ satisfying *the quantization condition is equal to the multiplicity of the operator* \widehat{H}_m .

Example 4: The Bochner-Laplacian associated with the harmonic connection on the line bundle over $\mathbb{C}P^n$

In this section, we consider quasi-classical eigenvalues of the Bochner-Laplacian associated with the harmonic connection on the line bundle over $\mathbb{C}P^n$. The harmonic connection is given as follows (see [5]).

We provide $\mathbb{C}^{n+1} = \{z = (z_0, \ldots, z_n)\}\$ with the Hermitian inner product

$$
\langle z,z'\rangle=\sum_{j=0}^nz_j\overline{z}_j
$$

and the real inner product $\langle z, z' \rangle_R = \text{Re}\, \langle z, z' \rangle$. Consider the $2n + 1$ -dimensional sphere with radius 2,

$$
S_{[2]}^{2n+1} = \{ z = (z_0, \dots, z_n) \mid \langle z, z \rangle_R = 4 \},
$$

which is endowed with the canonical Riemannian metric g_s induced from $\langle z, z' \rangle_R$. The action of $U(1) = \{ \lambda \in \mathbb{C} \mid |\lambda| = 1 \}$ on $S^{2n+1}_{[2]}$ denoted by R is given by

$$
R(\lambda)z = \lambda z, \quad \lambda \in U(1), \ z \in S^{2n+1}_{[2]}.
$$

As a quotient space, we get the principal fibre bundle (Hopf fibre bundle) ν_P :
 $S_{[2]}^{2n+1} \to \mathbb{C}P^n$. We fix a Riemannian metric g on $\mathbb{C}P^n$ so that ν_P is a Riemannian submersion. Define a connection on $S_{[2]}^{2n+1}$ by means of the Riemannian metric g_s such that $\beta = g_s(\gamma, *)/|\gamma|$, where γ is the fundamental vector field on $S^{2n+1}_{[2]}$ of the action R. Its curvature form is denoted by Ω . For every $m \in \mathbb{Z}$, we consider a $U(1)$ action ρ on $\mathbb C$ such that

$$
\rho(\lambda)w = \lambda^m w, \quad \lambda \in U(1), w \in \mathbb{C}.
$$

We then have a Hermitian line bundle $(E_m, \langle , \rangle_m)$ associated with $S^{2n+1}_{[2]}$ by ρ_m . The metric connection d_m induced by β is called the *harmonic connection* in $(E_m, \langle , \rangle_m)$. We denote by D_m the Bochner-Laplacian associated with d_m . The eigenvalues and their multiplicities are already known ([5]).

Proposition 6. *The eigenvalues of* D^m *are*

$$
\lambda_m^{(k)} = (k + |m|/2)(k + |m|/2 + n) - m^2/4, \ k = 0, 1, 2, \dots
$$

and the multiplicity of $\lambda_m^{(k)}$ *is*

$$
\binom{k+|m|+n}{k+|m|}\binom{k+n}{k} - \binom{k+|m|+n-1}{k+|m|-1}\binom{k+n-1}{k-1}.
$$

We consider the corresponding quasi-classical calculation. Consider the cotangent bundle $\pi: T^*{\mathbb{C}}P^n \to {\mathbb{C}}P^n$. We denote the energy Hamiltonian of g by H. We consider a symplectic structure on $T^{\ast} \mathbb{C}P^{n}$ such that $\sigma_{m} = d\theta + \pi^{\ast} m\Omega$, where θ is the canonical 1-form of $T^{\ast} \mathbb{C}P^{n}$. The function H is completely integrable and we take certain functions $H_1, \ldots, H_{2n-1}, H_{2n} = H$, which are Poisson commuting. Similarly as before, we consider a level set

$$
L(E_1,\ldots,E_{2n})=\{p\in T^*\mathbb{C}P^n\mid H_j(p)=E_j,\ j=1,2,\ldots,2n\}.
$$

We check the quantization condition directly for the level sets $L(E_1, \dots, E_{2n})$ and we obtain $([13])$

Theorem 7. *The quasi-classical eigenvalues of* H *are*

$$
\begin{aligned} \widetilde{\lambda}_m^{(k)} &= (k+|m|/2)(k+|m|/2+n) - m^2/4 + n^2/4 \\ &= \lambda_m^{(k)} + n^2/4, \ k = 0, 1, 2, \dots \end{aligned}
$$

Remark 8. As to multiplicities, we have that for each k the number of

 $L(E_1,\ldots,E_{2n})$

satisfying the quantization condition is equal to the number of tuples of integers

$$
(\gamma_1,\ldots,\gamma_{n-1},p_0,p_1,\ldots,p_n)
$$

such that

$$
\sum_{l=0}^{n} p_l = m, \quad k \geq \gamma_{n-1} \geq \cdots \geq \gamma_1 \geq \left(\sum_{l=0}^{n} |p_l| - |m|\right)/2.
$$

(For details, see [13].) We can check directly the number of tuples is just equal to the multiplicities of the kth eigenvalue of the Bochner-Laplacian $\lambda_n^{(k)}$ for every k.

Question

Now we would like to ask:

- Can we find other examples which have such coincidence?
- Can we prove mathematically why such coincidence occurs?

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