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On the validity of the WKB approximation

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Abstract. We consider the WKB approximation to the non-relativistic Schrödinger equation for an N-particle system with a possibly time-dependent potential. A recent rigorous and explicit error estimate given by Molzahn is investigated by means of examples. To this end we extend the class of potentials considered by Molzahn and find that his estimates are almost optimal. However, these examples also reveal an inherent drawback of the WKB method.

1. Introduction

According to the approximation scheme known among physicists as the Wentzel–Kramers–Brillouin (WKB) approximation, the exact solution ψ of some wave equation is approximated by ψ_{WKB} which can be obtained by solving the corresponding classical problem.

A heuristical derivation of the WKB scheme can be obtained by a formal series expansion of the exact solution in terms of the 'parameter' $\hbar$, cf [5]. In contrast to the vast amount of literature on the WKB method, very little is known about the error of approximation, say, $\|\psi(\cdot,t)-\psi_{\mathrm{WKB}}(\cdot,t)\|$, where $\|\cdot\|$ denotes the $L^2(\mathbb{R}^d, dx)$-norm, and, for example, $d = 3N$. But, of course, exact results on the error estimate would be very useful for assessing the applicability of the method to concrete problems. Maslov and Fedoriuk [5] obtained exact estimates for a large class of problems which for the lowest-order approximation is

$$\sup_{|t|<T} \|\psi(\cdot,t) - \psi_{\mathrm{WKB}}(\cdot,t)\| < C\hbar \tag{1}$$

for some $C > 0$ and $\hbar$, T sufficiently small. Because the constants involved are not specified this result represents some kind of justification of the WKB approximation but is of little use for concrete applications. The first rigorous and explicit estimate has, to our knowledge, been given by Molzahn [6]. He considers the non-relativistic Schrödinger equation for N particles with mass m and potential $V(x,t)$, $x \in \mathbb{R}^{3N}$, and an initial wavefunction of the form

$$\psi(x,0) = \phi(x)\exp\left[\frac{\mathrm{i}}{\hbar}(p_0\cdot x)\right]. \tag{2}$$

His result is, essentially,

$$\|\psi(\cdot,t) - \psi_{\mathrm{WKB}}(\cdot,t)\| < C(t)\frac{\hbar t}{m} \qquad \text{for } t \in \Omega \tag{3}$$

where Ω and $C(t)$ are given explicitly in terms of ϕ and V, see below.

In this paper we want to apply and scrutinize Molzahn's result for concrete examples. The purpose is to improve the physical interpretation of the estimate (3) and to better understand the nature of the error in the WKB approximation. A related question is whether the RHS term in (3) really represents the main part of the error, i.e. whether Molzahn's estimate is optimal or 'almost' optimal for numerical purposes. Hence we should consider examples where ψ and ψ_{WKB} and thus the exact L^2-norm difference could be explicitly calculated. Here we are confronted with the difficulty that Molzahn, in order to apply his technique of a constructive series representation of the classical action, developed in [7], has to impose strong restrictions to the potential $V(x,t)$. They are stronger than boundedness and real analyticity and essentially require that the Fourier transform of V decreases 'very' rapidly. Examples of potentials falling into the Molzahn class are Bessel functions of integer order, $\sin^n(ax)/x^n$, and $\sin(\lambda x)$, but no non-trivial polynomial will be in this class. From the examples only $\sin(\lambda x)$ is 'in principle' solvable but the calculations would become very complicated. We do not know, for example, how to compose a wavepacket out of Mathieu functions, etc.

However, there is another way to get solvable examples, namely to extend the Molzahn class in such a way that (3) remains valid. We may consider sequences of Molzahn potentials $V^{(\lambda)}$ converging (in some appropriate sense) towards V, which is not in the Molzahn class, such that $\psi^{(\lambda)}$, $\psi^{(\lambda)}_{\mathrm{WKB}}$, $\Omega^{(\lambda)}$ and $C^{(\lambda)}$ converge and their limits satisfy (3). This appears as a natural way to extend the Molzahn class. We will indicate the technical details of the procedure below.

It turns out that at least linear and quadratic potentials can be obtained by extending the Molzahn class. These are, of course, exactly solvable and we can compute $\Omega, C(t)$ for these cases and compare the exact norm difference of ψ and ψ_{WKB} for, say, Gaussian wavepackets, especially coherent states.

We will see that Molzahn's estimate is almost optimal for both examples. The reason is probably that his estimate correctly accounts for the first two terms in the expansion of $\|\psi - \psi_{\mathrm{WKB}}\|$ according to powers of t, where the t^2-term is vanishing.

Hence, for numerical purposes, the first term already gives the correct order of magnitude of the approximation error. This will be illustrated by a further example ($V(x) = \mathrm{sech}^2(x)$) which is not covered by Molzahn's theorem.

Finally, we will give a physical explanation of the t-linear part of the error. It is of purely kinematical nature and due to the fact that the WKB approximation corresponds to an ensemble of particles flying in formation for a moment, whereas the exact solution diffuses according to the spread of momentum. At least, this interpretation is possible for the case of a linear potential.

Some remarks on notation are in order. n denotes a multi-index $(n_1, n_2, \ldots, n_d)$ and $|n| = \sum_{i=1}^{d} n_i$. Let $A \in \mathbb{C}^{d\times d}$ be a $d \times d$ complex-valued matrix then the Hilbert–Schmidt norm reads $\|A\|_2 = (\sum_{i,j=1}^{d} |A_{i,j}|^2)^{1/2}$. $\nabla\nabla\phi$ denotes the matrix of spatial second derivations ('Hessian').

2. WKB approximation and Molzahn's result

We consider the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi \tag{4}$$

where $\psi(\cdot, t) \in \mathrm{L}^2(\mathbb{R}^d, dx)$ and

$$\psi(x, 0) = \phi(x) \exp\left(\frac{\mathrm{i}}{\hbar} S_0(x)\right). \tag{5}$$

Let $S(x, t)$ be a solution of the corresponding Hamilton–Jacobi equation

$$\partial_t S(x, t) + \frac{1}{2m}(\nabla_x S)^2 + V(x) = 0 \tag{6}$$

with initial values $S(x, 0) = S_0(x)$. Further, define

$$p_0(x) = \nabla_x S_0(x) \tag{7}$$

and let $x(x_0, t)$ be the solution of the corresponding classical equation of motion

$$\frac{\partial^2}{\partial t^2} x(x_0, t) = -\frac{1}{m}\nabla_x V(x(x_0, t)) \tag{8}$$

with initial values

$$x(x_0, 0) = x_0 \tag{9}$$

$$\frac{\partial}{\partial t} x(x_0, 0) = \frac{1}{m} p_0(x_0). \tag{10}$$

Let $x_0(x, t)$ be the inverse function of $x(x_0, t)$ and denote its Jacobian by

$$D(x, t) = \det \frac{\partial x_0(x, t)}{\partial x}. \tag{11}$$

Then the WKB approximation to the solution of (4), (5) has the form

$$\psi_{\mathrm{WKB}}(x, t) = \sqrt{D(x, t)}\, \phi(x_0(x, t)) \exp\left[\frac{\mathrm{i}}{\hbar} S(x, t)\right]. \tag{12}$$

Molzahn [6] is slightly more general in considering a time-dependance of the potential $V(x, t)$, and slightly more special in assuming

$$S_0(x) = p_0 \cdot x \qquad p_0 \in \mathbb{R}^d. \tag{13}$$

One may indicate the dependence on the 'parameter' p_0 in the functions $S(x, t; p_0)$, $D(x, t; p_0)$, and $x_0(x, t; p_0)$. The latter may be obtained by

$$x_0(x, t; p_0) = \nabla_{p_0} S(x, t; p_0). \tag{14}$$

Hence ψ_{WKB} can be completely specified if only $S(x, t; p_0)$ is known. It can be shown [6] that ψ_{WKB} satifies an 'approximate Schrödinger equation'. With the Hamiltonian operator

$$H = -\frac{\hbar^2}{2m}\Delta + V(x) \tag{15}$$

it reads

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\mathrm{WKB}}(x,t) = H\psi_{\mathrm{WKB}}(x,t) + \frac{\hbar^2}{2m}g_t \tag{16}$$

where

$$g_t(x) = D(x,t;p_0)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}S(x,t;p_0)\right)\left[\left(\frac{\Delta_x D}{2D} - \left(\frac{\nabla_x D}{2D}\right)^2\right)\phi(x_0(x,t)) \right.$$
$$\left. + \frac{1}{D}\nabla_x D\cdot\nabla(\phi\circ x_0)(x,t) + \Delta(\phi\circ x_0)(x,t)\right]. \tag{17}$$

From (16) one easily derives the estimate

$$\|\psi(\cdot,t) - \psi_{\mathrm{WKB}}(\cdot,t)\| \leqslant \frac{\hbar}{2m}t\sup_{\tau\in[0,t]}\|g_\tau\|. \tag{18}$$

It is worthwhile noting that according to (18) and (17), an error estimate of the WKB-approximation can, in principle, be determined if only the classical problem is solved. But even then the task to calculate the RHS of (18) may become very complicated and a simpler estimate is desirable.

Molzahn derived such a simpler estimate but he had to impose severe restrictions on the class of potentials. We will formulate his restrictions only for the special case $d = 1$ and time-independent potentials that will be used in later examples.

Definition. $V \in \mathcal{U}$ iff

(1) V is bounded and $V \in C^\infty(\mathbb{R})$, and
(2) there exist $U, K \in (0,\infty)$ such that for all $n \in \mathbb{N}$ $\|V^{(n)}(\cdot)\|_\infty \leqslant UK^n$.

It follows that $V \in \mathcal{U}$ is real analytic and that $\mathcal{U}$ contains all functions V, the Fourier transform of which has a compact support. $\mathcal{U}$ is an $\mathbb{R}$-algebra with the usual addition and multiplication of functions. It separates points, and hence approximates continuous functions on compact subsets (Stone–Weierstrass theorem). With the following definitions

$$T_H = \frac{1}{K}\sqrt{\frac{m}{eU}} \tag{19}$$

$$\lambda_\sigma = \frac{1}{1 + 1/\sigma\sqrt{2\pi}} \tag{20}$$

$$t(\sigma) = T_H\sqrt{\lambda_\sigma} \tag{21}$$

$$\sigma(t) = \frac{1}{\sqrt{2\pi}}\frac{t^2}{T_H^2 - t^2} \tag{22}$$

$$\Omega = \left(-\sqrt{\lambda_1}T_H, \sqrt{\lambda_1}T_H\right) \tag{23}$$

$$\gamma(\lambda_\sigma, l) = \sum_{n=1}^{\infty}\lambda_\sigma^n n^l \tag{24}$$

$$C_0(\sigma) = (1-\sigma)^{-2}\left[(K/\sqrt{2\pi})\gamma(\lambda_\sigma,1)\right]^2\tfrac{5}{4} + \tfrac{1}{2}(1-\sigma)^{-1}\left(K^2/\sqrt{2\pi}\right)\gamma(\lambda_\sigma,2) \tag{25}$$

$$C_1(\sigma) = \left(K/\sqrt{2\pi}\right)\gamma(\lambda_\sigma,1)\left[\frac{1+\sigma}{1-\sigma} + 1\right] \tag{26}$$

$$C_2(\sigma) = (1+\sigma)^2 \tag{27}$$

$$C_\phi(\sigma) = \tfrac{1}{2}\|C_0(\sigma)|\phi| + C_1(\sigma)|\nabla\phi| + C_2(\sigma)\|\nabla\nabla\phi\|_2\|. \tag{28}$$

Molzahn obtains the result that, if $V \in \mathcal{U}$,

$$\|\psi(\cdot,t) - \psi_{\mathrm{WKB}}(\cdot,t)\| \leqslant C_\phi(t)\frac{t\hbar}{m} \qquad \text{for } t \in \Omega\,. \tag{29}$$

The RHS of (29) can be calculated by means of integrals involving only the initial wavefunction ϕ. The potential V only has an influence on the estimate by means of the constants U and K.

3. Extension of the class $\mathcal{U}$ of admissible potentials

Before testing the estimate (29) in concrete examples, we have to extend the class $\mathcal{U}$ in such a way that (29) will remain true. To this end we consider a sequence $V_n \in \mathcal{U}$ and set

$$H_n = -\frac{\hbar^2}{2m}\Delta + V_n\,. \tag{30}$$

The dependence on H_n of the various wavefunctions will be indicated by a superscript. H_n shall converge towards an operator $H = -(\hbar^2/2m)\Delta + V$ in a sense to be explained below, and the extended class $\tilde{\mathcal{U}}$ will consist of all such limits V.

By triangle inequality

$$\begin{aligned}\|\psi^H(\cdot,t) - \psi^H_{\mathrm{WKB}}(\cdot,t)\| \leqslant{}& \underbrace{\|\psi^H(\cdot,t) - \psi^{H_n}(\cdot,t)\|}_{(1)} + \underbrace{\|\psi^{H_n}(\cdot,t) - \psi^{H_n}_{\mathrm{WKB}}(\cdot,t)\|}_{(2)}\\ &+ \underbrace{\|\psi^{H_n}_{\mathrm{WKB}}(\cdot,t) - \psi^H_{\mathrm{WKB}}(\cdot,t)\|}_{(3)}\,.\end{aligned} \tag{31}$$

In order to retain the result (29) the terms (1) and (3) should converge to 0 as $n \to \infty$, and (2) should approach a stable Molzahn estimate. We will consider the three terms separately.

(1) Sufficient for the norm convergence $\psi^{H_n} \to \psi^H$ is the strong resolvent convergence $H_n \to H$, cf [11] theorem 9.18.

(2) The obvious conditions for obtaining a stable Molzahn estimate for $n \to \infty$ are

$$\overline{\lim_{n\to\infty}} K_n = K \in [0,\infty) \tag{32}$$

$$\overline{\lim_{n\to\infty}} K_n\sqrt{U_n} \in [0,\infty)\,. \tag{33}$$

The first condition guarantees that the RHS of (29) can be chosen independently of n. The second condition implies that T_H does not vanish in the limit $n \to \infty$.

(3) One has to invoke the theorem that the solution of an ordinary differential equation depends smoothly on its parameters. A closer inspection shows that sufficient condition will be

(*a*) $V \in C^4(\mathbb{R})$
(*b*) V_n, ∇V_n and $\nabla\nabla V_n$ converge pointwise towards V, ∇V and $\nabla\nabla V$.

The condition $V_n(x) \to V(x)$ is also sufficient for strong resolvent convergence, $H_n \to H$, if these operators have a common core.

We leave it to the reader to formulate a theorem which extends Molzahn's result to the larger class $\tilde{\mathcal{U}}$. It is difficult to say whether $\tilde{\mathcal{U}}$ is really an improvement of $\mathcal{U}$. We only know two potentials which are in $\tilde{\mathcal{U}}$ but not in $\mathcal{U}$; the linear and the quadratic one. These will be investigated in the next section.

An alternative to extending the potential class is simply to include the quadratic parts of the potential into the unperturbed Hamiltonian. Recently Molzahn and Osborn [8] Corns [9] have obtained propagator cluster expansions for pertubations of $(\hat{q}, \hat{p})$-quadratic operators, and conjectured tree-graph series for the action S have been extracted. However, an analogous error estimation seems not to be known.

4. Examples

4.1. The linear potential

We consider the one-dimensional linear potential

$$V(x) = -mgx \tag{34}$$

and an initial wavefunction

$$\psi(x, 0) = C \exp\left(- \frac{(x - \xi_0)^2}{4\Delta^2} \right) \mathrm{e}^{\mathrm{i}p_0 x} \tag{35}$$

with normalization $C = (2\pi)^{-1/4}\Delta^{-1/2}$. Then $\psi(x, t)$ and $\psi_{\mathrm{WKB}}(x, t)$ can be explicitly calculated (see [2]):

$$\begin{aligned}
\psi(x, t) = {} & C\Delta \frac{1}{\sqrt{\Delta^2 + \mathrm{i}\hbar t/2m}} \exp\left[- \Delta^2 \left(\frac{mgt}{\hbar} + p_0 \right)^2 \right] \\
& \times \exp\left\{ \left[16\Delta^6 \left(\frac{mgt}{\hbar} + p_0 \right)^2 - 4\Delta^2 \left(\xi_0 - x - \frac{gt^2}{2} \right)^2 \right.\right. \\
& \left.\left. - 8\Delta^2 \frac{\hbar t}{m} \left(\frac{mgt}{\hbar} + p_0 \right) \left(\xi_0 - x - \frac{gt^2}{2} \right) \right] \Big/ \left(16\Delta^4 + \frac{4\hbar^2 t^2}{m^2} \right) \right\} \\
& \times \exp\left[\left[\frac{\mathrm{i}}{\hbar} \left\{ \left[- 16\Delta^4 \left(mgt + p_0\hbar \right) \left(\xi_0 - x - \frac{gt^2}{2} \right) - 8\Delta^4 \frac{\hbar^2 t}{m} \left(\frac{mgt}{\hbar} + p_0 \right)^2 \right.\right.\right.\right. \\
& \left.\left.\left.\left. + \frac{2\hbar^2 t}{m} \left(\xi_0 - x - \frac{gt^2}{2} \right)^2 \right] \Big/ \left(16\Delta^4 + \frac{4\hbar^2 t^2}{m^2} \right) \right\} \right]\right] \\
& \times \exp\left[\frac{\mathrm{i}}{\hbar} \left(\xi_0 mgt + \xi_0 p_0 \hbar - \frac{1}{6} mg^2 t^3 \right) \right]
\end{aligned} \tag{36}$$

$$\begin{aligned}
\psi_{\mathrm{WKB}}(x, t) = {} & C \exp\left(- \frac{(x - (p_0/m)t - gt^2/2 - \xi_0)^2}{4\Delta^2} \right) \\
& \times \exp\left(\frac{\mathrm{i}}{\hbar} \left(p_0 x + \left(mgx - \frac{p_0^2}{2m} \right) t - \frac{1}{2} g p_0 t^2 - \frac{1}{6} mg^2 t^3 \right) \right).
\end{aligned} \tag{37}$$

After some lengthy calculation we obtain

$$\|\psi - \psi_{\mathrm{WKB}}\| = \sqrt{2 - 2\mathrm{Re}\left(\frac{1}{\sqrt{1 + \mathrm{i}\hbar t/4\Delta^2 m}}\right)}. \tag{38}$$

Expanding (38) with respect to t yields

$$\|\psi(\cdot, t) - \psi_{\mathrm{WKB}}(\cdot, t)\| = \frac{\sqrt{3}}{8}\frac{\hbar t}{\Delta^2 m} - \frac{35\sqrt{3}}{12\,288}\left(\frac{\hbar t}{\Delta^2 m}\right)^3 + \mathrm{O}(t^5). \tag{39}$$

Next we approximate the linear potential by a family of potentials $V_\lambda \in \mathcal{U}, \lambda \to 0$,

$$V_\lambda(x) = -mg\frac{\sin(\lambda x)}{\lambda}. \tag{40}$$

Obviously

$$|V_\lambda^{(n)}(x)| \leqslant \frac{m|g|}{\lambda}\lambda^n \tag{41}$$

hence

$$U_\lambda = \frac{m|g|}{\lambda} \qquad K_\lambda = \lambda. \tag{42}$$

It follows that $K = \lim K_\lambda = 0$ and $T_H = (1/\lambda)\sqrt{\lambda/e|g|} \to \infty,\ \lambda \to 0$. We conclude

$$C_\phi(\sigma) = \frac{1}{2}\|\phi''\| = \frac{\sqrt{3}}{8\Delta^2} \tag{43}$$

and the Molzahn estimate reads

$$\|\psi(\cdot, t) - \psi_{\mathrm{WKB}}(\cdot, t)\| \leqslant \frac{\sqrt{3}}{8}\frac{\hbar t}{\Delta^2 m} \tag{44}$$

which is exactly the linear term of (39), see figure 1.

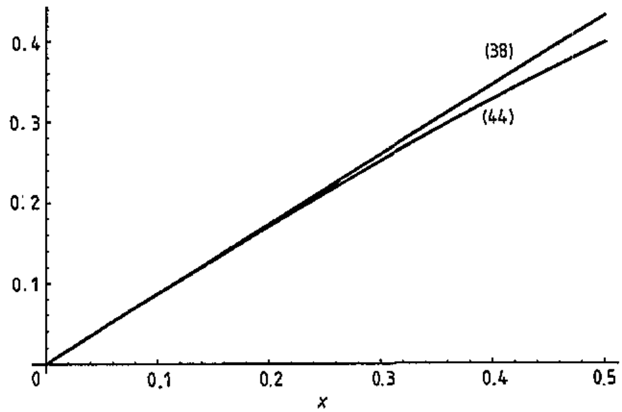

Figure 1. The norm difference (38) and the Molzahn estimation (44) are plotted as a function of the dimensionless quantity $x = (\hbar t/4\Delta^2 m)$.

4.2. *The harmonic oscillator*

We consider the potential

$$V(x) = \frac{m}{2}\omega^2 x^2 \tag{45}$$

and the time evolution of a coherent state (see [4])

$$\psi(x,t) = C\exp\bigg(-\frac{\alpha^2}{2}[x - Q\cos(\omega t+\delta)]^2 - \mathrm{i}xQ\alpha^2\sin(\omega t+\delta) - \frac{\mathrm{i}\omega t}{2} + \frac{\alpha^2 Q^2}{4}\,\mathrm{i}[\sin(2(\omega t+\delta)) - \sin(2\delta)]\bigg) \tag{46}$$

with

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} \tag{47}$$

and

$$\xi_0 + \frac{\mathrm{i}p_0}{m\omega} = Q\,\mathrm{e}^{-\mathrm{i}\delta}. \tag{48}$$

The WKB approximation is

$$\psi_{\mathrm{WKB}}(x,t) = \frac{1}{\sqrt{\cos(\omega t)}} C\exp\bigg(-\frac{\alpha^2}{2}\bigg[\frac{x}{\cos(\omega t)} - \frac{p_0}{m\omega}\tan(\omega t) - \xi_0\bigg]^2\bigg) \times\exp\bigg(\frac{\mathrm{i}}{\hbar}\bigg(-\frac{1}{2}\bigg[m\omega x^2 + \frac{p_0^2}{m\omega}\bigg]\tan(\omega t) + \frac{p_0 x}{\cos(\omega t)}\bigg)\bigg). \tag{49}$$

We may calculate three different estimates. The exact norm difference is

$$\|\psi - \psi_{\mathrm{WKB}}\| = \bigg[2 - 2\mathrm{Re}\bigg(\frac{\sqrt{2}\exp(-\frac{1}{2}\mathrm{i}\omega t)}{\sqrt{\cos(\omega t) + 1/\cos(\omega t) - \mathrm{i}\sin(\omega t)}}\bigg)\bigg]^{1/2} \tag{50}$$

$$= \frac{\sqrt{3}}{4}\omega t + \frac{31\sqrt{3}}{512}(\omega t)^3 + \mathrm{O}(t^5). \tag{51}$$

The estimate (18) according to the 'approximate Schrödinger equation' reads

$$\|\psi - \psi_{\mathrm{WKB}}\| \leqslant \frac{1}{\cos(\omega t)}\frac{\sqrt{3}}{4}\omega t \tag{52}$$

$$= \frac{\sqrt{3}}{4}\omega t + \frac{\sqrt{3}}{8}(\omega t)^3 + \mathrm{O}(t^5). \tag{53}$$

Molzahn's estimate is in this case

$$\|\psi - \psi_{\mathrm{WKB}}\| \leqslant (1+\sigma(t))^2\frac{\sqrt{3}}{4}\omega t \tag{54}$$

$$= \frac{\sqrt{3}}{4}\omega t + \frac{\sqrt{6}\mathrm{e}}{4\sqrt{\pi}}(\omega t)^3 + \mathrm{O}(t^5). \tag{55}$$

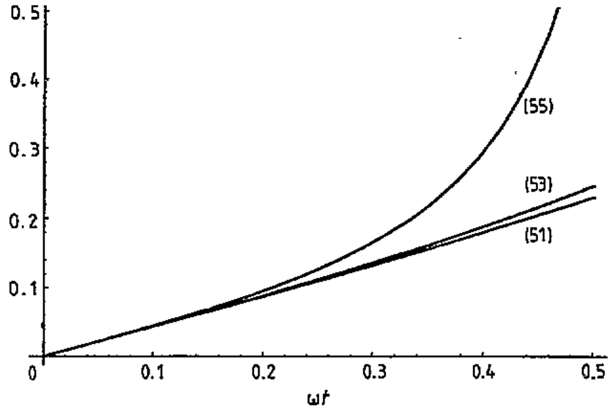

Figure 2. The three estimates plotted as functions of ωt. (55) is the Molzahn estimation, (53) represents the approximate Schrödinger equation and (51) is the exact result.

For obtaining the latter we approximated $V(x) = \frac{1}{2}m\omega^2x^2$ by $V_\lambda(x) = \frac{1}{2}m\omega^2(\sin(\lambda x)/\lambda)^2$ for $\lambda \to 0$. It follows that

$$U_\lambda = \frac{m\omega^2}{4\lambda^2} \qquad K_\lambda = 2\lambda \to 0 \tag{56}$$

and

$$T_H = \frac{1}{\sqrt{e}\omega} \tag{57}$$

independent from λ. The other conditions for extending the result of Molzahn to the class $\tilde{\mathcal{U}}$ are also satisfied. The result is graphically represented in figure 2.

4.3. Discussion

The above figures show that, for both examples, Molzahn's estimate is 'almost' optimal, at least for small t/T_H. The reason for this is twofold. First, Molzahn's estimate is exact with respect to the linear term in the t-expansion of $\|\psi - \psi_{\mathrm{WKB}}\|$. Second, this linear term is the dominating contribution for small t/T_H, since the quadratic term vanishes in the examples.

The question arises whether this result is only valid for the particular examples or generally true. We will now show the latter.

First, we expand ψ and ψ_{WKB} up to $\mathrm{O}(t^3)$-terms (writing $\psi_0 = \psi(0)$, etc)

$$\psi(t) = \psi_0 - \frac{\mathrm{i}t}{\hbar}H\psi_0 - \frac{t^2}{2\hbar^2}H^2\psi_0 + \mathrm{O}(t^3) \tag{58}$$

$$\psi_{\mathrm{WKB}}(t) = \psi_0 - \frac{\mathrm{i}t}{\hbar}H\psi_0 - \frac{\mathrm{i}\hbar t}{2m}g_0 - \frac{t^2}{2}\left(\frac{1}{\hbar^2}H^2\psi_0 + \frac{1}{2m}Hg_0 + \frac{\mathrm{i}\hbar}{2m}\dot{g}_0\right) + \mathrm{O}(t^3) \tag{59}$$

where, according to the definition (17) of g_t

$$g_0 = \exp\left(\frac{\mathrm{i}}{\hbar}S_0\right)\phi''. \tag{60}$$

Expanding the square root

$$\|\psi - \psi_{\mathrm{WKB}}\| = \sqrt{\langle\psi - \psi_{\mathrm{WKB}}|\psi - \psi_{\mathrm{WKB}}\rangle} \tag{61}$$

we obtain

$$\|\psi - \psi_{\mathrm{WKB}}\| = \frac{\hbar t}{2m}\|g_0\| + \frac{2mt^2}{\hbar\|g_0\|}\mathrm{Re}\left[\frac{-\mathrm{i}\hbar}{4m}\left(\frac{1}{2m}\langle g_0|Hg_0\rangle + \frac{\mathrm{i}\hbar}{2m}\langle g_0|\dot{g}_0\rangle\right)\right] + \mathrm{O}(t^3)\,. \tag{62}$$

The quadratic term vanishes, because $\langle g_0|Hg_0\rangle$ is real and

$$\dot{g}_0 = -\frac{\mathrm{i}}{\hbar}\left(\frac{p_0^2}{2m} + V\right)g_0 - \frac{p_0}{m}\,\mathrm{e}^{\mathrm{i}S_0/\hbar}\phi''' \tag{63}$$

hence

$$\langle g_0|\dot{g}_0\rangle = -\frac{\mathrm{i}}{\hbar}\left(\frac{p_0^2}{2m}\|g_0\|^2 + \langle g_0|Vg_0\rangle\right) - \frac{p_0}{m}\langle\phi''|\phi'''\rangle \tag{64}$$

is purely imaginary. The linear term can be shown to be identical with the linear term of Molzahn's estimate, using

$$C_\phi(\sigma) = \tfrac{1}{2}\|\phi''\| + \mathrm{O}(t)\,. \tag{65}$$

The foregoing considerations suggest the following 'rule of thumb', which is not an exact error bound, but very simple and not confined to the restricted class of potentials $\mathcal{U}$:

$$\|\psi - \psi_{\mathrm{WKB}}\| \approx \frac{\hbar t}{2m}\|\phi''\| \tag{66}$$

if

$$\psi(x,0) = \phi(x)\exp\left(\frac{\mathrm{i}}{\hbar}p_0 x\right). \tag{67}$$

The usefulness of this rule of thumb will be illustrated by a further example.

4.4. The sech^2-potential

We consider the potential

$$V(x) = -V_0\mathrm{sech}^2\left(\frac{x}{2a}\right) \qquad V_0 > 0 \tag{68}$$

representing an attractive potential well of depth V_0 and width $a > 0$. V is not contained in the Molzahn class $\mathcal{U}$. Using the Taylor series of $\tanh x$ we obtain

$$\left|\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{2n-2}\mathrm{sech}^2(0)\right| = \frac{16^n - 4^n}{(2\pi)^n}\frac{\zeta(n)}{n}(2n)!\,. \tag{69}$$

Hence $V^{(m)}(0)$ grows faster than UK^m (recall that Riemann's zeta function satisfies *$\zeta(n) \to 1$ for $n \to \infty$). It is well known [3] that V admits a finite number of bound* states which can be expressed in terms of the hypergeometric function. If we choose

$$V_0 = \frac{15}{32}\frac{\hbar^2}{ma^2} \tag{70}$$

there are exactly two eigenvalues of H and the corresponding eigensolutions of the Schrödinger equation assume the simple form

$$\psi_1(x,t) = \frac{1}{\sqrt{\pi a}} \cosh^{-3/2}(x/2a)\, \mathrm{e}^{-\mathrm{i}\omega_1 t} \qquad \text{with} \qquad \omega_1 = -\frac{9}{32}\frac{\hbar}{ma^2} \tag{71}$$

$$\psi_2(x,t) = \frac{1}{\sqrt{\pi a}} \cosh^{-3/2}(x/2a) \sinh(x/2a)\, \mathrm{e}^{-\mathrm{i}\omega_2 t} \qquad \text{with} \qquad \omega_2 = -\frac{1}{32}\frac{\hbar}{ma^2}. \tag{72}$$

Choosing $p_0 = 0$ in (2), we take the superposition

$$\psi(x,t) = \frac{1}{\sqrt{2}}(\psi_1(x,t) + \psi_2(x,t)) \tag{73}$$

as the exact solution to be approximated by ψ_{WKB}. To obtain the latter we consider the solution of the classical equation of motion

$$x(x_0,t) = 2a \sinh^{-1}\left[\sinh(x_0/2a)\cos\left(\frac{Bt}{2a}\right)\right] \qquad \text{with} \qquad B = \sqrt{\frac{2V_0}{m\cosh^2(x_0/2a)}} \tag{74}$$

and the classical action

$$\tilde{S}(x_0,t) = -\frac{V_0 t}{\cosh^2(x_0/2a)} + 4a\sqrt{\frac{mV_0}{2}} \arctan\left[\frac{\tan(Bt/2a)}{\cosh(x_0/2a)}\right] \tag{75}$$

where the tilde ($\sim$) denotes the choice of x_0 as the argument of a function (as opposed to x). From (74) we obtain

$$\begin{aligned} J(x_0,t) &\stackrel{\text{def}}{=} \frac{1}{\tilde{D}(x_0,t)} = \frac{\partial x(x_0,t)}{\partial x_0} \\ &= \frac{\cosh(x_0/2a)\cos(Bt/2a) + \sin(Bt/2a)\tanh^2(x_0/2a)\sqrt{2V_0/m(t/2a)}}{\sqrt{\sinh^2(x_0/2a)\cos^2(Bt/2a)+1}} \end{aligned} \tag{76}$$

and, finally,

$$\tilde{\psi}_{\mathrm{WKB}}(x_0,t) = \frac{1}{\sqrt{J(x_0,t)}}\psi(x_0,0)\exp\left(\frac{\mathrm{i}}{\hbar}\tilde{S}(x_0,t)\right). \tag{77}$$

In order to calculate $\langle\psi|\psi_{\mathrm{WKB}}\rangle$ we choose x_0 as the integration variable and obtain

$$\begin{aligned} \langle\psi(\cdot,t)|\psi_{\mathrm{WKB}}(\cdot,t)\rangle &= \frac{1}{2\pi a}\int_{-\infty}^{\infty} \mathrm{d}x_0 \left[\sinh^2(x_0/2a)\cos^2\left(\frac{Bt}{2a}\right)+1\right]^{-3/4} \\ &\quad \times \left(\mathrm{e}^{\mathrm{i}\omega_1 t} + \sinh(x_0/2a)\cos\left(\frac{Bt}{2a}\right)\mathrm{e}^{\mathrm{i}\omega_2 t}\right) \\ &\quad \times \sqrt{J(x_0,t)}\cosh^{-3/2}(x_0/2a)(1+\sinh(x_0/2a))\exp\left(\frac{\mathrm{i}}{\hbar}\tilde{S}(x_0,t)\right). \end{aligned} \tag{78}$$

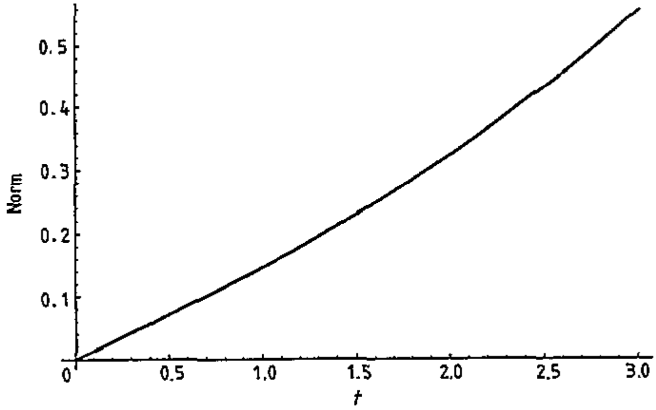

Figure 3. The norm difference for the hyperbolic potential as a function of $\hbar t/ma^2$.

It turns out that the integral and hence $\|\psi - \psi_{\rm WKB}\|$ only depends on the dimensionless variable

$$\tau = \frac{t}{T_{\rm K}} \tag{79}$$

where

$$T_{\rm K} = \frac{4\pi m a^2}{\hbar\sqrt{15}} \tag{80}$$

is the classical caustic time. The integral (78) can only be numerically determined, see figure 3. For the t-linear term we obtain an anlaytical result

$$\|\psi(\cdot, t) - \psi_{\rm WKB}(\cdot, t)\| = \frac{\sqrt{326}}{128}\frac{\hbar t}{ma^2} + \mathrm{O}(t^2) \tag{81}$$

which is numerically in accordance with (66).

5. Explanation of the error of the WKB approximation

The result of Molzahn is confined to the time interval $|t| < \sqrt{\lambda_1}\, T_H \approx 0.8\, T_H$. It is well known [1] that $\psi_{\rm WKB}$ has to be modified for times greater than $T_{\rm C}$, the time where the classical motion exhibits caustics. This is plausible if one construes $\psi_{\rm WKB}$ as the stationary phase approximation of the Feynman path integral representation of ψ. For $t > T_{\rm C}$ there are more than one paths joining $(x_0, 0)$ and (x, t) which make the classical action stationary. It remains to show that

$$T_H = \frac{1}{K}\sqrt{\frac{m}{eU}} \approx T_{\rm C}\,. \tag{82}$$

We will provide a heuristic argument. If V has a minimum at $x = 0$, $V(x) \approx m/2\omega^2 x^2$, where $m\omega^2 = V''(0)$. For the quadratic potential it is known that $T_{\rm C} = \pi/2\omega$. Hence

$$T_{\rm C} \approx \frac{\pi}{2}\left(\frac{V''(0)}{m}\right)^{-1/2} \geqslant \frac{\pi}{2}\left(\frac{UK^2}{m}\right)^{-1/2} = \frac{\pi}{2}\frac{1}{K}\sqrt{\frac{m}{U}} \approx T_H\,. \tag{83}$$

Generally, it is clear that $T_C \notin \Omega$ since $x \to x_0(x,t)$ is a diffeomorphism [6].

We have seen that, for small t/T_H, the main part of the error of WKB approximation is $\|\psi - \psi_{\mathrm{WKB}}\| \approx (\hbar t/2m)\|\Delta\phi\|$. This term can be heuristically explained. The WKB approximation can be associated with a classical ensemble of particles, all having momentum p_0 at $t = 0$. These particles obey (8), (9) for x_0 in supp ϕ. But the quantum initial data (5) has a momentum dispersion δp obeying the uncertainty relation

$$\delta q\,\delta p \geqslant \hbar/2\,. \tag{84}$$

If we consider a second classical ensemble satisfying (84), then these two ensembles will become significantly different after a typical time

$$T \cong \frac{\delta q}{\delta v} = \frac{m\delta q}{\delta p}\,. \tag{85}$$

Now δp can be bounded above by

$$(\delta p)^2 = \langle P^2\rangle - \langle P\rangle^2 \leqslant \langle P^2\rangle \leqslant \langle P^4\rangle^{1/2} = \|P^2\phi\| = \hbar^2\,\|\Delta\phi\|\,. \tag{86}$$

From these two relations we obtain an estimate for T,

$$T \geqslant \frac{m\hbar}{2(\delta p)^2} \geqslant \frac{m}{2\hbar}\|\phi''\|^{-1} \tag{87}$$

which is in agreement with the time region where (66) indicates a poor approximation.

These heuristic considerations can be confirmed by comparing the Wigner transforms of ψ and ψ_{WKB}. Recall its definition ($\hbar = 1$)

$$F(x,p) = \frac{1}{\pi}\int \mathrm{d}y\, \mathrm{e}^{-2\mathrm{i}py}\,\psi^*(x-y)\,\psi(x+y) \tag{88}$$

and that the Wigner transform maps Gaussians onto Gaussians and the quantum time evolution onto the classical one if the Hamiltonian is at most quadratic in P and Q; see, for example, [10].

For the linear potential and ψ, ψ_{WKB} according to (36), (37) we obtain the Wigner transforms

$$F(x,p,t) = \frac{1}{\pi}\exp\left[-\frac{\left(x-(p/m)t+\frac{1}{2}gt^2-\xi_0\right)^2}{2\Delta^2} - 2\Delta^2(p+mgt-p_0)^2\right] \tag{89}$$

and

$$F_{\mathrm{WKB}}(x,p,t) = \frac{1}{\pi}\exp\left[-\frac{\left(x-(p_0/m)t+\frac{1}{2}gt^2-\xi_0\right)^2}{2\Delta^2} - 2\Delta^2(p+mgt-p_0)^2\right]. \tag{90}$$

We see that F 'swims' with the classical flow in phase space, whereas F_{WKB} represents a rigid motion of a Gaussian through phase space such that only its peak follows a classical path.

For the quadratic potential and coherent states the situation is a bit different because here F follows a rigid rotation in phase space whereas F_{WKB} is (periodically) distorted:

$$F(x,p,t) = \frac{1}{\pi}\exp\left[-\alpha^2\left(x\cos(\omega t) - \frac{p}{m\omega}\sin(\omega t) - \xi_0\right)^2 - \frac{1}{\alpha^2}(p\cos(\omega t) + m\omega x\sin(\omega t) - p_0)^2\right] \tag{91}$$

$$F_{\mathrm{WKB}}(x,p,t) = \frac{1}{\pi}\exp\left[-\alpha^2\left(\frac{x}{\cos(\omega t)} - \frac{p_0}{m\omega}\tan(\omega t) - \xi_0\right)^2 - \frac{1}{\alpha^2}(p\cos(\omega t) + m\omega x\sin(\omega t) - p_0)^2\right]. \tag{92}$$

In any case, it becomes obvious that the main t-linear part of $\|\psi - \psi_{\mathrm{WKB}}\|$ is of purely kinematical nature and due to the unability of the WKB approximation of first order to correctly account for the diffusion of the wavepacket. It is completely independent of the potential, contrary to the folklore which says that the WKB approximation is good if the potential is sufficiently smooth.

Of course the applicability of the WKB approximation requires $t < T_C$ which according to (83) means that the potential must be slowly varying.

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