Maslov index and other potential parameters away from the semiclassical limit

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Reflection phase and Maslov index, modified quantization rule

Examples: sharp step, inverse-square potential

Applications: circle billard, homogeneous potentials \( V(r) = \pm \frac{C}{r^\alpha} \)

Quantization in molecular potentials

Near-threshold quantization

Near-threshold scattering and quantum reflection

Real experiments on the quantum reflection of cold atoms

(former) students
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Michael J. Moritz
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Reflexion phase and Maslov index

On classically allowed side of a classical turning point \( r_t \):
\[
(p(r) = \sqrt{2M[E - V(r)]})
\]

\[
\psi_{\text{WKB}}(r) \propto \frac{1}{\sqrt{p(r)}} \left[ e^{-\frac{i}{\hbar} \int_{r_t}^{r} p(r')dr'} + Re^{\frac{i}{\hbar} \int_{r_t}^{r} p(r')dr'} \right]
\]
\[
\propto \frac{1}{\sqrt{p(r)}} \cos \left[ \frac{1}{\hbar} \int_{r_t}^{r} p(r')dr' - \frac{\phi}{2} \right]. \quad R = e^{-i\phi}
\]

\( \phi \) is the phase loss due to reflection, the reflection phase

Quantization in potential well \( r_1 < r < r_r \):
\[
\cos \left[ \frac{1}{\hbar} \int_{r_1}^{r} p(r')dr' - \frac{\phi_1}{2} \right] =
\]
\[
\pm \cos \left[ \frac{1}{\hbar} \int_{r}^{r_r} p(r')dr' - \frac{\phi_r}{2} \right]
\]
\[
\frac{1}{\hbar} \int_{r_1}^{r_r} p(r)dr = n\pi + \frac{\phi_1 + \phi_r}{2} = \left( n + \frac{\mu_M}{4} \right) \pi, \quad \mu_M = \frac{\phi_1 + \phi_r}{\pi/2}
\]

Potential linear around \( r_t \) \( \Rightarrow \phi = \frac{\pi}{2} \) \( \Rightarrow \mu_M \) counts number of reflections. This assumption of conventional WKB quantization is far too restrictive.
Example: Sharp step

\[ V(r) = \begin{cases} 
  V_0 = \frac{\hbar^2 (K_0)^2}{2M}, & r < L \\
  0, & r > L 
\end{cases} \]

WKB approximation is exact everywhere, except at \( r = L \).

\[ 0 < E = \frac{\hbar^2 k^2}{2M} < V_0 : \quad \phi = 2 \arctan \frac{\kappa}{k}, \quad \kappa = \sqrt{(K_0)^2 - k^2} \]

With this choice of \( \phi \), \( \psi_{\text{WKB}} \) is exact in class. allowed region.

Example: inverse-square potential, \( V(r) = \frac{\hbar^2}{2M} \frac{\gamma}{r^2} \)

At energy \( E = \frac{\hbar^2 k^2}{2M} \), CTP is: \( kr_t = \sqrt{\gamma} \)

\[ \psi_{\text{WKB}} \xrightarrow{kr \to \infty} \left( \frac{1 - \gamma(\gamma - 2)}{8(kr)^2} \right) \cos \left[ kr - \sqrt{\gamma} \frac{\pi}{2} - \frac{\phi}{2} \right] - \frac{\gamma}{2kr} \sin \left[ kr - \sqrt{\gamma} \frac{\pi}{2} - \frac{\phi}{2} \right] \]

Exact wave function: \( \psi_{\text{exact}} \propto \sqrt{kr} J_\mu(kr), \quad \mu = \sqrt{\gamma + 1/4} \)

\[ \psi_{\text{exact}} \xrightarrow{kr \to \infty} \left( \frac{1 - \gamma(\gamma - 2)}{8(kr)^2} \right) \cos \left[ kr - \mu \frac{\pi}{2} - \frac{\pi}{4} \right] - \frac{\gamma}{2kr} \sin \left[ kr - \mu \frac{\pi}{2} - \frac{\pi}{4} \right] \]

\( \phi = \frac{\pi}{2}, \quad \gamma \to \gamma + \frac{1}{4} \) (Lang.mod.) \( \Rightarrow \psi_{\text{WKB}} \xrightarrow{kr \to \infty} \psi_{\text{exact}} + O \left( \frac{1}{kr} \right) \)

\( \phi = \frac{\pi}{2} + \pi \left( \sqrt{\gamma + \frac{1}{4}} - \sqrt{\gamma} \right) \) \( \Rightarrow \psi_{\text{WKB}} \xrightarrow{kr \to \infty} \psi_{\text{exact}} + O \left( \frac{1}{(kr)^3} \right) \)
\[ V(r) = \frac{\hbar^2}{2Mr^2} \Rightarrow \text{refl. phase} [1]: \quad \phi = \frac{\pi}{2} + \pi \left( \sqrt{\gamma + \frac{1}{4}} - \sqrt{\gamma} \right) \]

centrifugal potentials: \( \gamma = l_3(l_3+1), \ l_3 = 0, 1, 2, 3, \ldots \) (3D)
\[ \gamma = (l_2)^2 - \frac{1}{4}, \ l_2 = 0, \pm 1, \pm 2, \ldots \] (2D)

Circle billard, free particle inside circle of radius \( R \)
\[ \psi(r, \varphi) = \frac{\psi_{l_2}(r)}{\sqrt{r}} e^{il_2\varphi}, \quad l_2 = 0, \pm 1, \pm 2, \ldots \]

radial wave function \( \psi_{l_2}(r) \) obeys 1D Schrödinger equation with inverse-square potential, \( \gamma = (l_2)^2 - \frac{1}{4} \).

Exact wave functions:
\( \psi_{\text{exact}} \propto \sqrt{kr} J_{l_2}(kr) \), boundary condition: \( \psi_{\text{exact}}(R) = 0 \)

Energy eigenvalues:
\( E_{n,l_2} = \hbar^2 (k_{n,l_2})^2 / (2M) \)

exact: \( k_{n,l_2} = x_{n,l_2} / R \), \( x_{n,l_2} = n\)-th zero of \( J_{l_2}(x) \)

conv. WKB quantiz.: \( \gamma = (l_2)^2 \), \( \phi_1 = \frac{\pi}{2}, \ \phi_r = \pi \), \( \mu_M = 3 \)

mod. WKB: \( \gamma = (l_2)^2 - \frac{1}{4} \), \( \phi_1 = \frac{\pi}{2} + \pi(\lvert l_2 \rvert - \sqrt{\gamma}) \), \( \phi_r = \pi \)
(special treatment for \( l_2 = 0 \) [2])

Conventional WKB quantization yields essentially the same eigenvalues as EBK quantization (torus quantization)

Application of higher-order periodic orbit theory by Main [3]
Energy eigenvalues $E_{n,l_2}$ [in units of $\hbar^2/(2MR^2)$] for angular momentum quantum numbers $l_2 = 0$ and $|l_2| = 1$ in the circle billiard. The superscript “WKB” refers to conventional WKB quantization of the radial degree of freedom, “mqr” refers to the modified quantization rule (82), “exact” labels the exact results and “(1)” the results obtained by Main [22] in higher-order semiclassical periodic orbit theory.

<table>
<thead>
<tr>
<th>n</th>
<th>$E_{n,0}^{WKB}$</th>
<th>$E_{n,0}^{mqr}$</th>
<th>$E_{n,0}^{exact}$</th>
<th>$E_{n,0}^{(1)}$</th>
<th>$E_{n,1}^{WKB}$</th>
<th>$E_{n,1}^{mqr}$</th>
<th>$E_{n,1}^{exact}$</th>
<th>$E_{n,1}^{(1)}$</th>
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</thead>
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<td>843.7182</td>
<td>843.7182</td>
</tr>
</tbody>
</table>

- $l_2 = 0$
- $|l_2| = 1$

$\log_{10}(\text{error})$ vs. $n$ for different quantum numbers $l_2$.
Reflection phase for inverse-square potential:

\[ \phi = \frac{\pi}{2} + \pi \left( \sqrt{a^2 + \frac{1}{4}} - a \right), \quad a = \sqrt{\gamma} = kr_t \]

Repulsive homogeneous potential,

\[ V^{\text{rep}}_\alpha(r) = \frac{C_\alpha}{r^{\alpha}} = \frac{\hbar^2}{2M} \frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha}; \quad \alpha > 0, \ C_\alpha > 0 \]

reflection phase as function of "reduced CTP"

\[ a = kr_t = \frac{\text{classical turning point}}{\text{asymptotic wave length} / 2\pi} = (k/\beta_\alpha)^{1-2/\alpha} = \frac{p_{\text{as}}r_t}{\hbar} \]

\begin{figure}
\centering
\includegraphics[width=\textwidth]{graph.png}
\end{figure}

semiclassical limit \( a \to \infty \): \( E \to 0 \) if \( 0 < \alpha < 2 \)

\[ |E| \to \infty \] if \( \alpha > 2 \)

anticlassical limit \( a \to 0 \): \( |E| \to \infty \) if \( 0 < \alpha < 2 \)

\[ E \to 0 \] if \( \alpha > 2 \)
semiclassical expansion [4] for reflection phase for \( V_{\alpha}^{\text{rep}} \),

\[
\phi \underset{a \to \infty}{\sim} \frac{\pi}{2} + \frac{\sqrt{\pi}}{a} \frac{(\alpha + 1) \Gamma \left( \frac{1}{\alpha} \right)}{12 \alpha \Gamma \left( \frac{1}{2} + \frac{1}{\alpha} \right)} + O \left( \frac{1}{a^3} \right)
\]

ansatz:

\[
\phi = \frac{\pi}{2} + \pi \left( \sqrt{\left( a_S \right)^2 + \frac{1}{4}} - a_S \right)
\]

with

\[
a_S = \frac{a}{S(\alpha)} \quad , \quad S(\alpha) = \frac{2(\alpha + 1) \Gamma \left( \frac{1}{\alpha} \right)}{3 \alpha \sqrt{\pi} \Gamma \left( \frac{1}{2} + \frac{1}{\alpha} \right)}
\]

---

Scattering phase shift:

\[
\psi \underset{r \to \infty}{\propto} \sin(kr + \delta)
\]

\[
\psi \underset{r \to \infty}{\propto} \cos \left( \Phi_{\text{WKB}} - \frac{\phi}{2} \right)
\]

\[
\Phi_{\text{WKB}} = \frac{1}{\hbar} \int_{r_t}^{r} p(r') \, dr'
\]

\[
\delta = \frac{\pi}{2} - a \frac{\sqrt{\pi}}{2} \frac{\Gamma \left( \frac{1}{\alpha} \right)}{\Gamma \left( \frac{3}{2} - \frac{1}{\alpha} \right)} - \left[ \frac{\pi}{4} + \frac{\pi}{2} \left( \sqrt{\left( a_S \right)^2 + \frac{1}{4}} - a_S \right) \right]
\]
Attractive homogeneous potential,

\[ V_{\alpha}^{\text{att}}(r) = \frac{C_{\alpha}}{r^{\alpha}} = -\frac{\hbar^2}{2M} \frac{(\beta_{\alpha})^{\alpha-2}}{r^\alpha}; \quad \alpha > 2, \quad C_{\alpha} > 0 \]

\[ E = -\frac{\hbar^2}{2M} \kappa^2 < 0; \quad \text{CTP: } r_t = \frac{\beta_{\alpha}}{(k\beta_{\alpha})^{2/\alpha}}; \quad \text{reduced CTP: } a = \kappa r_t = \frac{\text{classical turning point}}{\text{asymptotic penetration depth}} \]

\[ = \left( \kappa \beta_{\alpha} \right)^{1-2/\alpha} = \frac{|p_{\text{as}}| r_t}{\hbar} \]

anticlásica límite \[ [5]: \quad \phi \xrightarrow{a \to 0} \frac{\pi}{2} + \frac{\pi}{\alpha - 2} \]

semiclásica límite: \[ \phi \xrightarrow{a \to \infty} \frac{\pi}{2} + \frac{\sqrt{\pi}}{a} \frac{(\alpha + 1) \Gamma \left( \frac{1}{\alpha} \right)}{12 \alpha \Gamma \left( \frac{1}{2} + \frac{1}{\alpha} \right)} \tan \left( \frac{\pi}{\alpha} \right) \]

ansatz:

\[ \phi = \frac{\pi}{2} + \frac{2\pi}{\alpha - 2} \left( \sqrt{(a_R)^2 + \frac{1}{4}} - a_R \right) \]

\[ a_R = \frac{a}{R(\alpha)}, \quad R(\alpha) = \frac{(\alpha + 1)(\alpha - 2) \Gamma \left( \frac{1}{\alpha} \right)}{3\alpha \sqrt{\pi} \Gamma \left( \frac{1}{2} + \frac{1}{\alpha} \right)} \tan \left( \frac{\pi}{\alpha} \right) \]
Quantization in molecular potentials

Lennard-Jones: \[ V(r) = \varepsilon \left[ \left( \frac{r_{\text{min}}}{r} \right)^{12} - 2 \left( \frac{r_{\text{min}}}{r} \right)^6 \right] \]

attractive tail: \[ \alpha = 6, \quad R(6) = 2.083 \]

For \( B_{\text{LJ}} := \varepsilon / \left( \frac{\hbar^2}{2M(r_{\text{min}})^2} \right) = 10^4 \): 24 bound states

![Graph showing the energy levels for different n values](image)
Performance of quantization rules for Lennard-Jones potential

\[ \frac{1}{\hbar} \int_{r_{in}}^{r_{out}} p(r) dr = \left( n + \frac{\mu_M}{4} \right) \pi , \quad \mu_M = \frac{\phi_{in} + \phi_{out}}{\pi/2} \]

conventional WKB: \( \phi_{in} = \phi_{out} = \frac{\pi}{2} \)

modified quantization rule: \( \phi_{in} = \frac{\pi}{2} \),

\[ \phi_{out} = \frac{\pi}{2} + \frac{\pi}{2} \left( \sqrt{\left( a_R \right)^2 + \frac{1}{4} - a_R} \right) , \quad a_R = \frac{(k \beta_6)^{2/3}}{2.083} \]

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_n )</th>
<th>( 10^3 \times \Delta E_n^{\text{conv}} )</th>
<th>( 10^3 \times \Delta E_n^{R} )</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>-0.941046032</td>
<td>-85841</td>
<td>-17508</td>
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<td>23</td>
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<td>-1021</td>
<td>+42</td>
</tr>
</tbody>
</table>

relative error:
\[ |\Delta E_n|/(E_n - E_{n-1}) \]

\( \Delta \): conventional WKB

■: modified quant. rule

\( \Delta \): WKB in higher \((2N + 1)\) order [6]
Near-threshold quantization

Zero-energy solutions of the Schrödinger equation:

\[ \psi_0(r) \sim 1, \quad \psi_1(r) \sim r. \]

In WKB region:

\[ \psi_0(r) = \frac{D_0}{\sqrt{p_0(r)}} \cos \left( \frac{1}{\hbar} \int_r^\infty p_0(r')dr' - \frac{\phi_0}{2} \right) \]

\[ p_0(r) = \sqrt{-2MV(r)} \]

\( \phi_0 \) is the zero-energy reflection phase, i.e. the reflection phase at the outer turning point, \( r_{\text{out}} = \infty \) for \( E = 0 \).

In WKB region:

\[ \psi_1(r) = \frac{D_1}{\sqrt{p_0(r)}} \cos \left( \frac{1}{\hbar} \int_r^\infty p_0(r')dr' - \frac{\phi_1}{2} \right) \]

Just below threshold: Asymptotic penetration depth \( \kappa \) enters in Schrödinger equation via \( E = -\hbar^2 \kappa^2 / (2M) \), zero-energy solutions are still correct to order less than \( O(E) = O(\kappa^2) \)

example: \( \psi_\kappa(r) = \psi_0 - \kappa \psi_1 \sim 1 - \kappa r = e^{-\kappa r} + O(\kappa^2) \)

matching \( \psi_\kappa = \psi_0 - \kappa \psi_1 \) in WKB region to

\[ \psi_{\text{WKB}}(r) \propto \frac{1}{\sqrt{p_0(r)}} \cos \left( \frac{1}{\hbar} \int_{r_{\text{in}}(0)}^r p_0(r')dr' - \frac{\phi_{\text{in}}(0)}{2} \right) + O(E) \]

gives

\[ n\pi = n_{\text{th}}\pi - b\kappa + O(\kappa^2), \quad b = \frac{D_1}{D_0} \sin \left( \frac{\phi_0 - \phi_1}{2} \right) \]

\[ n_{\text{th}}\pi = \frac{1}{\hbar} \int_{r_{\text{in}}(0)}^\infty p_0(r)dr - \frac{\phi_{\text{in}}(E=0) + \phi_0}{2} \]
Universal near-threshold quantization rule: \[ n = n_{\text{th}} - \frac{b}{\pi} \]
(for all potentials falling off faster than \(1/r^2\))

Homogeneous pot.: \( \frac{\phi_0}{\pi} = \frac{1}{2} + \nu \), \( \frac{b}{\beta_\alpha} = \frac{\pi \nu^{1+2\nu}}{\Gamma(1+\nu)^2} \), \( \nu = \frac{1}{\alpha - 2} \)

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>( \infty )</th>
</tr>
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<tbody>
<tr>
<td>( b/\beta_\alpha )</td>
<td>( \pi )</td>
<td>1</td>
<td>0.6313</td>
<td>0.4780</td>
<td>0.3915</td>
<td>( \pi/\alpha )</td>
</tr>
</tbody>
</table>

Classical scaling would suggest \( n = n_{\text{th}} - \text{const.} \kappa^{1-2/\alpha} \),
BUT: leading energy dependence of \( \phi_{\text{out}} \) exactly cancels corresponding term in classical action integral.

Demonstration of performance for Lennard-Jones potential:
\( B_{\text{LJ}} = 10^4 \Rightarrow E_{23} = -0.000002697 \epsilon \), reduced CTP: \( a = 1.562 \).
Gradually reducing \( B_{\text{LJ}} \) pushes \( E_{23} \) closer to threshold;
\( E_{23} \) reaches threshold for \( B_{\text{LJ}} = 9800, [a = 0] \)

near-thr. qu. rule:
\( \phi_{\text{in}}(0) = \frac{\pi}{2} \)
\( \alpha = 6 \Rightarrow \phi_0 = \frac{3}{4} \pi, \)
\( b = 0.4780 \beta_\alpha \)
Generalization to longer ranged potential tails

$E = -\frac{\hbar^2 \kappa^2}{2M} \to 0$

Summary of near-threshold quantization rules for attractive and repulsive potential tails. The second column gives the leading term(s) to the quantization rule in the limit of vanishing energy, $E = -\hbar^2 \kappa^2/(2M) \to 0$. The third column lists equations where explicit expressions for the constants appearing in the second column can be found; these can apply quite generally, as in the first row, or to special models of potential tails with the asymptotic behaviour given in the first column.

<table>
<thead>
<tr>
<th>$V(r)$ for $r \to \infty$</th>
<th>quantization rule for $E \to 0$</th>
<th>refs. for constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-\frac{\hbar^2}{2M}(\beta\alpha)^{\alpha-2}/r^{\alpha}$, $0 &lt; \alpha &lt; 2$</td>
<td>$n \sim \frac{1}{\pi} F(\alpha)/(\kappa\beta\alpha)^{(2/\alpha)-1}$</td>
<td>$F(\alpha)$: Eq. (163)</td>
</tr>
<tr>
<td>$\frac{\hbar^2}{2M} \gamma/r^2$, $\gamma &lt; -\frac{1}{4}$</td>
<td>$n \sim -\frac{1}{2\pi} \ln\left(-E/E_0\right)/\sqrt{</td>
<td>\gamma</td>
</tr>
<tr>
<td>$\gamma = -\frac{1}{4}$</td>
<td>$n \sim n_{th} + A/\ln(-E/B)$</td>
<td>$n_{th}$: (205)</td>
</tr>
<tr>
<td>$-\frac{1}{4} &lt; \gamma &lt; \frac{3}{4}$</td>
<td>$n \sim n_{th} - B(-E)^{\gamma+1/4}$</td>
<td>$B$: (207)</td>
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<td>$\gamma \geq \frac{3}{4}$</td>
<td>$n \sim n_{th} - O(E)$</td>
<td>$n_{th}$: (205)</td>
</tr>
<tr>
<td>$\alpha + 1/r^\alpha$, $0 &lt; \alpha &lt; 2$</td>
<td>$n \sim n_{th} - O(E)$</td>
<td>$n_{th}$: (148)</td>
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<tr>
<td>$\alpha \pm 1/r^\alpha$, $\alpha &gt; 2$</td>
<td>$n \sim n_{th} - \frac{1}{\alpha} b\kappa$</td>
<td>$b$: (154), (159), (187)</td>
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<td>(188), (189), Tab. 3,</td>
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<tr>
<td></td>
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<td>Eq. (60) in Ref. [97]</td>
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</table>

From [7]
Just above threshold: \( E = \frac{\hbar^2 k^2}{2M} > 0 \)

Below order \( O(E) \) can be deduced from the zero-energy solutions of the Schrödinger equation, \( \psi_0 \sim \infty 1 \), \( \psi_1 \sim \infty r \)

**Example: near-threshold s-wave scattering**

\[
\psi_{\text{reg}}(r) \propto \sin(kr + \delta), \quad \delta \to 0 \quad k = n\pi - ka_0, \quad a_0 = \text{scattering length}
\]

\[
\psi_{\text{reg}}(r) \propto k(r - a_0) \propto k(\psi_1 - a_0\psi_0)
\]

Matching to

\[
\frac{1}{\sqrt{p_0(r)}} \cos \left( \frac{1}{\hbar} \int_{r_{\text{in}}(0)}^r p_0(r')dr' - \frac{\phi_{\text{in}}(0)}{2} \right)
\]

in the WKB region gives:

\[
a_0 = \frac{b}{\tan \left[ \frac{\phi_0 - \phi_1}{2} \right]} + \frac{b}{\tan(n_{\text{th}}\pi)}, \quad b = \frac{D_1}{D_0} \sin \left( \frac{\phi_0 - \phi_1}{2} \right)
\]

\[
n_{\text{th}}\pi = \frac{1}{\hbar} \int_{r_{\text{in}}(0)}^\infty p_0(r)dr - \frac{\phi_{\text{in}}(0) + \phi_0}{2}, \quad \frac{b}{\tan \left[ \frac{\phi_0 - \phi_1}{2} \right]} \equiv \bar{a}_0
\]

\( \bar{a}_0 = \text{mean scattering length. Hom. pot.,} \quad V = -\frac{\hbar^2}{2M} \frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha} \),

\[
b = \beta_\alpha \frac{\pi \nu^{1+2\nu}}{\Gamma(1+\nu)^2} \quad [8] \quad \text{and} \quad \bar{a}_0 = \frac{b}{\tan(\pi\nu)} \quad [9], \quad \nu = \frac{1}{\alpha - 2}
\]

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>( \infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b/\beta_\alpha )</td>
<td>\pi</td>
<td>1</td>
<td>0.6313</td>
<td>0.4780</td>
<td>0.3915</td>
<td>( \pi/\alpha )</td>
</tr>
<tr>
<td>( \bar{a}<em>0/\beta</em>\alpha )</td>
<td>-</td>
<td>0</td>
<td>0.3645</td>
<td>0.4780</td>
<td>0.5389</td>
<td>1</td>
</tr>
</tbody>
</table>
Example: near threshold quantum reflection

\[ \psi(r) \to r^{-\infty} e^{-ikr} + Re^{+ikr} \]

\[ k \to 0 \quad 1 + R - ikr(1 - R) \]

\[ = (1 + R) \psi_0 - ik(1 - R) \psi_1 \]

matching to \( \frac{T}{\sqrt{p_0(r)}} \exp \left( \frac{i}{\hbar} \int_{r_{\text{ref}}}^{r} p_0(r') dr' \right) \) in WKB region:

\[ R \underset{k \to 0}{\sim} \frac{1 - ik \frac{D_1}{D_0} e^{-i(\phi_0 - \phi_1)/2}}{1 + ik \frac{D_1}{D_0} e^{-i(\phi_0 - \phi_1)/2}} = |R| e^{i\theta} \]

\[ |R| \underset{k \to 0}{\sim} 1 - 2kb = e^{-2kb} + O(k^2), \quad \theta = \arg R \underset{k \to 0}{\sim} \pi - 2k\bar{a}_0 \]

where \( b \) and \( \bar{a}_0 \) are the previously introduced tail parameters

Quantum reflection probability: \( P_R = |R|^2 \underset{k \to 0}{\sim} e^{-4kb} + O(k^2) \)

When a wave packet with momentum sharply peaked around \( \hbar k_0 = M v_0 \) undergoes quantum reflection, it experiences a time gain (relative to a free particle reflected at \( r = 0 \)),

\[ \Delta t = -\hbar \frac{d\theta}{dE} \bigg|_{E=\hbar^2 k_0^2/(2M)} \underset{E \to 0}{\sim} \frac{2M}{\hbar k_0} \bar{a}_0 \]

This corresponds to the time evolution of a free particle reflected not at \( r = 0 \) but at \( r = \Delta r \), where \( \Delta t = 2v_0 \Delta r \):

\[ \Delta r = \frac{-1}{2d\bar{a}} \bigg|_{k_0} \underset{E \to 0}{\sim} \bar{a}_0. \]
Summary of near-threshold properties

Consider a potential \( V(r) \) that falls off asymptotically \( (r \to \infty) \) faster than \( 1/r^2 \), which has a WKB-region of moderate \( r \) values, where WKB wave functions are accurate approximations to exact solutions of the Schrödinger equation.

Near-threshold properties of bound states (near-threshold quantization rule \( n = n_{\text{th}} - (b/\pi)\kappa \), near-threshold level density \( dn/dE \)), and of continuum states (scattering length, modulus and phase of quantum reflection amplitude) are determined by three "tail parameters" which depend only on the behaviour of the potential beyond the WKB region. They are derived from zero-energy solutions \( \psi_0 \overset{r \to \infty}{\sim} 1, \psi_1 \overset{r \to \infty}{\sim} r \) of the Schrödinger equation via their phases \( (\phi_0, \phi_1) \) and amplitudes \( (D_0, D_1) \) as WKB wave functions in the WKB region,

\[
\begin{align*}
\text{zero-energy reflection phase:} & \quad \phi_0, \\
\text{characteristic length:} & \quad b = \frac{D_1}{D_0} \sin \left( \frac{\phi_0 - \phi_1}{2} \right), \\
\text{mean scattering length:} & \quad \bar{a}_0 = \frac{b}{\tan \left( \frac{\phi_0 - \phi_1}{2} \right)}.
\end{align*}
\]

The tail parameters depend not only on leading asymptotic behaviour of the potential, but on its behaviour in the whole quantal region beyond the WKB region. They can be derived numerically for any potential tail, and analytically, if the zero energy solutions \( \psi_0 \) and \( \psi_1 \) are known for the potential tail.
Characteristic length \( b \), mean scattering length \( \bar{a}_0 \) and zero-energy reflection phase \( \phi_0 \) for several attractive potential tails, \( V(r) = -v(r) \times h^2/(2M) \).

<table>
<thead>
<tr>
<th>( v(r) )</th>
<th>( b )</th>
<th>( \bar{a}_0 )</th>
<th>( \phi_0 )</th>
<th>comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>((K_0)^2 \Theta(L-r))</td>
<td>(1/K_0)</td>
<td>(L)</td>
<td>(0)</td>
<td>(\nu = \frac{1}{\alpha-2} &lt; 1)</td>
</tr>
<tr>
<td>(\frac{(\beta_\alpha)^{\alpha-2}}{r^\alpha})</td>
<td>(\frac{\pi \beta_\alpha \nu^{1+2\nu}}{\Gamma(1+\nu)^2})</td>
<td>(\beta_\alpha \nu^{2\nu} \frac{\Gamma(1-\nu)}{\Gamma(1+\nu)} \cos(\pi \nu))</td>
<td>(\pi \left(\nu + \frac{1}{2}\right))</td>
<td>(\nu = \frac{1}{\alpha-2} &lt; 1)</td>
</tr>
<tr>
<td>(\frac{\beta_3}{r^3})</td>
<td>(\pi \beta_3)</td>
<td>(-)</td>
<td>(\frac{3}{2} \pi)</td>
<td>(\rho = \left(\frac{\beta_\alpha}{\beta_\alpha_1}\right)^{1/\nu})</td>
</tr>
<tr>
<td>(\frac{(\beta_\alpha)^{\alpha-2}}{r^{\alpha-1}} + \frac{(\beta_\alpha_1)^{\alpha-2}}{r^{\alpha-1}})</td>
<td>(\frac{\beta_\alpha \nu^{2\nu} \Gamma(1-\nu)}{\Gamma(1+\nu)} \left</td>
<td>\frac{\Gamma(z_+)}{\Gamma(z_-)}\right</td>
<td>\times\frac{\beta_\alpha_1 \nu^{2\nu} \Gamma(1-\nu)}{\Gamma(1+\nu)} \left</td>
<td>\frac{\Gamma(z_+)}{\Gamma(z_-)}\right</td>
</tr>
<tr>
<td>(\frac{\beta_3}{r^3} + \frac{(\beta_4)^2}{r^4})</td>
<td>(\frac{\pi \beta_3}{2} \left[1 + \coth\left(\frac{\pi \rho}{2}\right)\right])</td>
<td>(-)</td>
<td>(\pi + \rho \left(1 - \ln\left(\frac{\rho}{\nu}\right)\right))</td>
<td>(\rho = \frac{\beta_3}{\beta_4})</td>
</tr>
<tr>
<td>(\frac{(\beta_4)^2}{r^4} + \frac{(\beta_5)^3}{r^5})</td>
<td>(\frac{3(\beta_5)^3}{\pi (\beta_4)^2} F(z)^{-1})</td>
<td>(-\frac{(\beta_5)^3}{2(\beta_4)^2} \left(1 + \rho \frac{F'(z)}{F(z)}\right))</td>
<td>(\frac{5}{6} \pi - \frac{4}{3} \rho - 2 \arctan\left[\frac{J_{\frac{1}{3}}(z)}{Y_{\frac{1}{3}}(z)}\right])</td>
<td>(\rho = \left(\frac{\beta_4}{\beta_5}\right)^3)</td>
</tr>
<tr>
<td>(\left[\frac{r^3}{\beta_3} + \frac{r^4}{(\beta_4)^2}\right]^{-1})</td>
<td>(\frac{(\beta_4)^2}{\pi \beta_3} F(z)^{-1})</td>
<td>(-\frac{(\beta_4)^2}{2 \beta_3} \left(1 + \rho \frac{F'(z)}{F(z)}\right))</td>
<td>(\frac{3}{2} \pi - 4 \rho - 2 \arctan\left[\frac{J_{\frac{1}{3}}(z)}{Y_{\frac{1}{3}}(z)}\right])</td>
<td>(\rho = \frac{\beta_3}{\beta_4})</td>
</tr>
<tr>
<td>(\frac{(K_0)^2}{1 + \exp[(r-L)/\beta]})</td>
<td>(\pi \beta \coth(\pi K_0 \beta))</td>
<td>(L - 2 \beta (\gamma_E + \Re(z)))</td>
<td>(\pi + 4K_0 \beta \ln 2)</td>
<td>(z = \psi_1(i K_0 \beta))</td>
</tr>
<tr>
<td>((K_0)^2 \exp\left(-\frac{r}{\beta}\right))</td>
<td>(\pi \beta)</td>
<td>(2 \beta \ln(K_0 \beta))</td>
<td>(\frac{1}{2} \pi)</td>
<td>†</td>
</tr>
</tbody>
</table>

† Here the semiclassical region of "small" \( r \) is \( r \to -\infty \). \( \gamma_E \) is Euler's constant and \( \psi_1 \) the digamma function.
Quantum reflection of cold atoms by surfaces

retarded van der Waals potential \cite{10}

\[-\frac{\hbar^2 \beta_3}{2M r^3} = -\frac{C_3}{r^3} \quad \text{for } r \to \infty \quad -\frac{C_4}{r^4} = -\frac{\hbar^2}{2M} \frac{(\beta_4)^2}{r^4}\]

conducting surface:

\[C_3^\infty = \frac{1}{4\pi} \int_0^\infty \alpha_d(i\omega) d\omega; \quad C_4^\infty = \frac{3}{8\pi} \frac{\alpha_d(0)}{\alpha_{fs}}\]

Length scales involved are very large [atomic units]:

<table>
<thead>
<tr>
<th></th>
<th>H</th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C_3)</td>
<td>0.25</td>
<td>1.447</td>
<td>1.576</td>
<td>2.153</td>
<td>2.291</td>
<td>2.589</td>
</tr>
<tr>
<td>(C_4)</td>
<td>73.6</td>
<td>2683</td>
<td>2662</td>
<td>4789</td>
<td>5221</td>
<td>6579</td>
</tr>
<tr>
<td>(\beta_3)</td>
<td>919</td>
<td>36610</td>
<td>132100</td>
<td>306900</td>
<td>713900</td>
<td>1255000</td>
</tr>
<tr>
<td>(\beta_4)</td>
<td>520</td>
<td>8239</td>
<td>14940</td>
<td>26130</td>
<td>40330</td>
<td>56460</td>
</tr>
<tr>
<td>(C_4/C_3)</td>
<td>294</td>
<td>1854</td>
<td>1690</td>
<td>2225</td>
<td>2278</td>
<td>2540</td>
</tr>
</tbody>
</table>

Dependence of quantum reflection amplitude on power \(\alpha\)

near threshold: \(\log |R|, \arg (-R) \propto k, \text{ const.} = F(\alpha)\beta_\alpha\)

beyond threshold \cite{11}:

\[|R| \sim e^{-B_\alpha k r_E}, \quad |V(r_E)| = E\]

\[k r_E = (k/\beta_\alpha)^{1-2/\alpha} = \frac{p_{as} r_E}{\hbar}\]

<table>
<thead>
<tr>
<th>(\alpha)</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>(\infty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(B_\alpha)</td>
<td>2.2405</td>
<td>1.6944</td>
<td>1.3515</td>
<td>1.1202</td>
<td>0.9545</td>
<td>2\pi/\alpha</td>
</tr>
</tbody>
</table>

conjecture \cite{12}:

\[\theta = \arg R \sim \infty c_0 - c_1 k r_E\]
\[ \theta = \lim_{k \to \infty} c_0 - c_1 k r_E \implies \Delta r \sim r_E \]

Classical time gains and space shifts:

\[
(\Delta t)_{\text{cl}} = 2 \lim_{r \to \infty} \int_0^r \left( \frac{1}{v_0} - \frac{1}{|v(r')|} \right) dr' \\
= 2M \int_0^\infty \left( \frac{1}{\hbar k_0} - \frac{1}{p(r)} \right) dr > 0
\]

For homogeneous potentials:

\[
(\Delta t)_{\text{cl}} = \frac{2M}{\hbar k_0} r_E \tau(\alpha) , \quad (\Delta r)_{\text{cl}} = r_E \tau(\alpha)
\]

\[
\tau(\alpha) = \frac{1}{\sqrt{\pi}} \Gamma \left( \frac{1}{2} + \frac{1}{\alpha} \right) \Gamma \left( 1 - \frac{1}{\alpha} \right)
\]

<table>
<thead>
<tr>
<th>(\alpha)</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>(\infty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\tau(\alpha))</td>
<td>0.8624</td>
<td>0.8472</td>
<td>0.8526</td>
<td>0.8624</td>
<td>0.8725</td>
<td>1</td>
</tr>
</tbody>
</table>

Quantum reflected wave packet experiences a time gain relative to the free particle (as long as \(\Delta r > 0\)), but the time gain of the classical particle accelerated in the attractive potential is larger, the associated space shift diverges as \(r_E\) towards threshold whereas the space shift of the quantum particle is bounded by a distance of the order of \(\beta \alpha\).

The quantum particle is always delayed relative to the classical (accelerated) particle.
Specular Reflection of Very Slow Metastable Neon Atoms from a Solid Surface

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Institute for Laser Science and CREST, University of Electro-Communications, Chofu-shi, Tokyo 182-8585, Japan
(Received 7 July 2000)

FIG. 1. The cross-sectional view of the experimental setup. The $1s_3$ metastable neon atoms were generated by focusing an optical pumping laser at 598 nm into the trap of the $1s_5$ atoms. The mask, the top of the reflecting plate and the MCP were placed 37, 39, and 112 cm below the trap, respectively.

FIG. 3. The reflectivity vs the normal incident velocity on the Si(1,0,0) surface. The solid curve is the reflectivity calculated by using the potential Eq. (1) with $\lambda = 0.4 \, \mu m$ and $C_4 = 6.8 \times 10^{-36} \, J \, m^4$, which corresponds to $\alpha = 2.0 \times 10^{-39} \, F \, m^2$ of Casimir's theory.

FIG. 4. The reflectivity vs the normal incident velocity on the BK7 glass surface. The solid curve is the reflectivity calculated by using the potential Eq. (1) with $C_4 = 7.3 \times 10^{-36} \, J \, m^4$ and $\lambda = 5.0 \, \mu m$. 
low energy [1]: \( |R| \stackrel{k \to 0}{\sim} 1 - 2b_\alpha k \approx \exp(-2b_\alpha k) \)

high energy [2]: \( |R| \stackrel{k \to \infty}{\sim} \exp[-B_\alpha (k/\beta_\alpha)^{(1-2/\alpha)}] \)

\[
|R| = \exp[-B(k/\beta)^\mu] \Rightarrow \\
\log(-\log |R|) = \log B + \mu \log (k/\beta)
\]
Experimental Observation of Quantum Reflection far from Threshold

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(Received 7 November 2002; published 6 November 2003)

FIG. 1. Schematic representation of the experimental setup.

FIG. 2. Reflection coefficient as a function of the dimensionless incident wave number \( k/a \) \((\approx \cos \theta_i) \). Open circles: experimental data from the stepped surface. Full circles: corrected data, representing QR from the smooth surface. Solid line: computer simulation using the potential (2) parametrized with \( C_4 = 23.6 \) eV Å\(^4\) and \( l = 10 \) Å. Inset: replot of the same data. The straight of slope \( = 1/3 \) shows the asymptote (4) with \( \beta_3 = 347 \) Å; the straight at small \( \ln(k_a) \), with slope \( = 1 \) and ordinate axis intercept: \( \ln(2.4\beta_3/a) \) for \( \rho \approx 1.9 \) [12], is the near-threshold asymptote.
SUMMARY

- Accuracy of WKB wave functions is a local property of the Schrödinger eq.
- Assumption $\phi_{\text{refl}} = \frac{\pi}{2}$ far too restrictive.
- Allowing more general $\phi_{\text{refl}}$ (nonintegral Maslov index) enhances applicability of WKB.
- Matching exact wave functions from quantal regions to WKB wave functions where accurate $\rightarrow$ highly accurate, often asymptotically exact results all the way to the anti-classical limit.
- Three tail parameters $b$, $\bar{a}_0$, $\phi_0$ determine: near-thr. qu. rule, level density, quantum reflection amplitude for $r^2 V(r) \to 0$.

- Direct applications to experiments with cold atoms — e.g. quantum reflection
References


