

Asymptotic Evaluation of an Integral Arising in Quantum Harmonic Oscillator Tunnelling Probabilities

R. B. Paris

Division of Computing and Mathematics
University of Abertay Dundee, Dundee DD1 1HG, UK

Copyright © 2015 R. B. Paris. This article is distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Abstract

We obtain an asymptotic evaluation of the integral

$$\int_{\sqrt{2n+1}}^{\infty} e^{-x^2} H_n^2(x) dx$$

for $n \rightarrow \infty$, where $H_n(x)$ is the Hermite polynomial. This integral is used to determine the probability for the quantum harmonic oscillator in the n th energy eigenstate to tunnel into the classically forbidden region. Numerical results are given to illustrate the accuracy of the expansion.

Mathematics Subject Classification: 33C45, 34B05, 41A30, 41A60

Keywords: Quantum oscillator, tunnelling, asymptotic expansion

1. Introduction

The quantum harmonic oscillator in dimensionless variables has the Hamiltonian given by $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2)$, where \hat{x}, \hat{p} are the position and momentum operators satisfying $[\hat{x}, \hat{p}] = i$. The normalised eigenstates are

$$\psi_n(x) = \pi^{-1/4} (2^n n!)^{-1/2} e^{-x^2/2} H_n(x),$$

where $H_n(x)$ is the n th Hermite polynomial. The corresponding probability densities $P_n(x)$ are then given by $|\psi_n(x)|^2$, that is

$$P_n(x) = a_n e^{-x^2} H_n^2(x), \quad a_n = \frac{1}{\sqrt{\pi 2^n n!}}. \quad (1.1)$$

The classical turning points are situated at $x = \pm\sqrt{2n+1}$, so that the probability of tunnelling into the classically forbidden region is expressed as

$$P_{n,tun} = 2a_n Q_n, \quad Q_n = \int_{\sqrt{2n+1}}^{\infty} e^{-x^2} H_n^2(x) dx. \quad (1.2)$$

It has been pointed out recently by Jadczyk [1] that the tunnelling probabilities $P_{n,tun}$ are rarely discussed in the literature on quantum mechanics. In [1], he has shown that $P_{n,tun}$ has the approximate representation for large values of n given by

$$P_{n,tun} = \frac{1}{n^{1/3}} \left\{ 0.133975 - \frac{0.0122518}{n^{2/3}} + O(n^{-1}) \right\} \quad (n \rightarrow \infty). \quad (1.3)$$

Our aim in this note is to obtain more precise information on the large- n behaviour of $P_{n,tun}$. We carry this out by exploiting the uniform asymptotic expansion of the parabolic cylinder function $U(-n - \frac{1}{2}, 2^{\frac{1}{2}}x)$ given in [4], valid for $n \rightarrow \infty$ and $x \geq \sqrt{2n+1}$.

2. A representation of Q_n

We set $\nu := \sqrt{2n+1}$ and rescale the variable x to write the integral Q_n in (1.2) as

$$Q_n = \nu \int_1^{\infty} e^{-(\nu x)^2} H_n^2(\nu x) dx.$$

The integrand can be expressed in terms of the parabolic cylinder function $U(a, z)$ by [3, Eq. (18.15.28)]

$$e^{-(\nu x)^2/2} H_n(\nu x) = 2^{\frac{1}{4}\nu^2 - \frac{1}{4}} U(-\frac{1}{2}\nu^2, 2^{\frac{1}{2}}\nu x).$$

The asymptotic expansion of this last function in terms of the Airy function $\text{Ai}(z)$ and its derivative is given by [4, Eq. (3.23)]

$$U(-\frac{1}{2}\nu^2, 2^{\frac{1}{2}}\nu x) = \frac{2^{\frac{1}{4}\nu^2 + \frac{1}{4}} e^{\nu^2/4} \Gamma(\frac{1}{2} + \frac{1}{2}\nu^2)}{\nu^{\frac{1}{2}\nu^2 + \frac{1}{6}}} \left(\frac{\zeta}{x^2 - 1} \right)^{1/4} \Upsilon_{\nu}(\zeta), \quad (2.1)$$

$$\Upsilon_{\nu}(\zeta) = \text{Ai}(\nu^{4/3}\zeta) F_{\nu}(\zeta) + \nu^{-8/3} \text{Ai}'(\nu^{4/3}\zeta) G_{\nu}(\zeta) \quad (2.2)$$

as $\nu \rightarrow +\infty$ uniformly valid for $x \geq 1$, where

$$\zeta^{3/2} = \frac{3}{4}x\sqrt{x^2 - 1} - \frac{3}{4} \text{arccosh}x \quad (x \geq 1). \quad (2.3)$$

The functions $F_{\nu}(\zeta)$ and $G_{\nu}(\zeta)$ have the asymptotic expansions

$$F_{\nu}(\zeta) \sim \sum_{k=0}^{\infty} f_k(\zeta) \nu^{-2k}, \quad G_{\nu}(\zeta) \sim \sum_{k=0}^{\infty} g_k(\zeta) \nu^{-2k},$$

where, from [4, §3.2], we have

$$f_0(\zeta) = 1, \quad f_1(\zeta) = \frac{1}{24}, \quad f_2(\zeta) = a_1(\zeta) + \frac{1}{576},$$

$$g_0(\zeta) = b_0(\zeta), \quad g_1(\zeta) = \frac{b_0(\zeta)}{24},$$

with

$$a_1(\zeta) = \frac{1}{1152} \left\{ \frac{145 + 249x^2 - 9x^4}{(x^2 - 1)^3} - \frac{7x(x^2 - 6)}{(x^2 - 1)^{3/2}\zeta^{3/2}} - \frac{455}{4\zeta^3} \right\}, \tag{2.4}$$

$$b_0(\zeta) = -\frac{1}{2\zeta^{\frac{1}{2}}} \left\{ \frac{x(x^2 - 6)}{12(x^2 - 1)^{3/2}} + \frac{5}{24\zeta^{3/2}} \right\}. \tag{2.5}$$

Then, from (2.1) and (2.2) it follows that

$$Q_n = \frac{2^{2n+1}(n!)^2 e^{n+\frac{1}{2}}}{\nu^{2n+\frac{1}{3}}} \int_1^\infty \left(\frac{\zeta}{x^2 - 1} \right)^{1/2} \Upsilon_\nu^2(\zeta) dx.$$

The quantity ζ is a monotonically increasing function for $x \geq 1$ and $\zeta = 0$ when $x = 1$. Furthermore

$$\frac{d\zeta}{dx} = \left(\frac{\zeta}{x^2 - 1} \right)^{-1/2},$$

so that we can introduce the new integration variable ζ to find [1]

$$Q_n = \frac{2^{2n+1}(n!)^2 e^{n+\frac{1}{2}}}{\nu^{2n+\frac{1}{3}}} \int_0^\infty \phi(\zeta) \Upsilon_\nu^2(\zeta) d\zeta, \quad \phi(\zeta) := \frac{\zeta}{x^2 - 1}. \tag{2.6}$$

From (2.2), we have

$$\begin{aligned} \Upsilon_\nu^2(\zeta) &= \text{Ai}^2(\nu^{4/3}\zeta) F_\nu^2(\zeta) + 2\nu^{-8/3} \text{Ai}(\nu^{4/3}\zeta) \text{Ai}'(\nu^{4/3}\zeta) F_\nu(\zeta) G_\nu(\zeta) \\ &\quad + \nu^{-16/3} \text{Ai}'^2(\nu^{4/3}\zeta) G_\nu^2(\zeta) \\ &= \text{Ai}^2(\nu^{4/3}\zeta) \left(1 + \frac{1}{12\nu^2} + \frac{1+1152f_2(\zeta)}{576\nu^4} + O(\nu^{-6}) \right) \\ &+ \nu^{-8/3} b_0(\zeta) [\text{Ai}^2(\nu^{4/3}\zeta)]' \left(1 + \frac{1}{12\nu^2} + O(\nu^{-4}) \right) + \nu^{-16/3} b_0^2(\zeta) \text{Ai}'^2(\nu^{4/3}\zeta) (1 + O(\nu^{-2})). \end{aligned}$$

Retaining terms up to and including $\nu^{-14/3}$, we therefore find

$$\begin{aligned} \int_0^\infty \phi(\zeta) \Upsilon_\nu^2(\zeta) d\zeta &= \int_0^\infty \phi(\zeta) \left\{ \text{Ai}^2(\nu^{4/3}\zeta) \left(1 + \frac{1}{12\nu^2} + \frac{1+1152f_2(\zeta)}{576\nu^4} \right) \right. \\ &\quad \left. + \nu^{-8/3} b_0(\zeta) [\text{Ai}^2(\nu^{4/3}\zeta)]' + O(\nu^{-16/3}) \right\} d\zeta \tag{2.7} \end{aligned}$$

as $\nu \rightarrow \infty$.

3. The asymptotic expansion of two integrals

To evaluate the integrals appearing in (2.7) we employ the modification of Watson's lemma given in Olver's book [2, p. 337]. This is possible since $\text{Ai}(x)$ possesses the asymptotic behaviour

$$\text{Ai}(x) \sim \frac{1}{2}\pi^{-1/2}x^{-1/4}\exp[-\frac{2}{3}x^{3/2}] \quad (x \rightarrow +\infty).$$

Inversion of (2.3) with the help of *Mathematica* yields¹

$$x = 1 + 2^{-1/3}\zeta - \frac{2^{-2/3}\zeta^2}{10} + \frac{11\zeta^3}{700} - \frac{823 \cdot 2^{-1/3}\zeta^4}{12600} + \dots \quad (|\zeta| < \zeta_0),$$

where $\zeta_0 = (\frac{3}{4}\pi)^{2/3}$; see [3, Eq. (12.10.41)]. Then we have

$$\phi(\zeta) = \sum_{m=0}^{\infty} \alpha_m \zeta^m \quad (|\zeta| < \zeta_0), \quad (3.1)$$

where

$$\alpha_0 = 2^{-2/3}, \quad \alpha_1 = -\frac{1}{5}, \quad \alpha_2 = \frac{2^{5/3}}{35}, \quad \alpha_3 = -\frac{2^{10/3}}{225}, \quad \alpha_4 = \frac{1548}{67375}, \dots$$

Now for a fixed positive integer M , and with $t = \nu^{4/3}\zeta$,

$$\int_0^{\infty} \phi(\zeta) \text{Ai}^2(\nu^{4/3}\zeta) d\zeta = \sum_{m=0}^{M-1} \frac{\alpha_m}{\nu^{\frac{4}{3}m + \frac{4}{3}}} \int_0^{\infty} t^m \text{Ai}^2(t) dt + R_M,$$

where

$$R_M = \int_0^{\infty} \phi_M(\zeta) \text{Ai}^2(\nu^{4/3}\zeta) d\zeta, \quad \phi_M(\zeta) := \phi(\zeta) - \sum_{m=0}^{M-1} \alpha_m \zeta^m.$$

It follows that $\phi_M(\zeta) = O(\zeta^M)$ as $\zeta \rightarrow 0+$ and it is known [1] that $\phi(\zeta) \leq 2^{-2/3}$ for $\zeta \geq 0$. Hence we can find a constant C such that the inequality $|\phi_M(\zeta)| < C\zeta^M$ holds when $\zeta \geq 0$. Then

$$|R_M| \leq C \int_0^{\infty} \zeta^M \text{Ai}^2(\nu^{4/3}\zeta) d\zeta = O(\nu^{-\frac{4}{3}M - \frac{4}{3}})$$

as $\nu \rightarrow \infty$, upon use of the evaluation [3, Eq. (12.11.15)]

$$\int_0^{\infty} t^m \text{Ai}^2(t) dt = \frac{2m! 12^{-\frac{1}{3}m - \frac{7}{6}}}{\sqrt{\pi}\Gamma(\frac{1}{3}m + \frac{7}{6})} \quad (m = 0, 1, 2, \dots). \quad (3.2)$$

¹The function $\zeta(x)$ is real for $x > -1$, being given by $(-\zeta)^{3/2} = \frac{3}{4}(\arccos x - x\sqrt{1-x^2})$ in the interval $-1 < x \leq 1$. The finite radius of convergence results from the singularity in the inversion at $x = -1$, where $\zeta = -(\frac{3}{4}\pi)^{2/3}$.

Thus we obtain the asymptotic expansion

$$\int_0^\infty \phi(\zeta) \text{Ai}^2(\nu^{4/3}\zeta) d\zeta \sim \frac{2}{\sqrt{\pi}} \sum_{m=0}^\infty \frac{\alpha_m m! \nu^{-4m/3-4/3}}{12^{\frac{1}{3}m+\frac{7}{6}} \Gamma(\frac{1}{3}m + \frac{7}{6})} \quad (\nu \rightarrow \infty). \quad (3.3)$$

A similar reasoning can be applied to the second integral on the right-hand side in (2.7), when we observe that the function $-b_0(\zeta)$ in (2.5) decreases monotonically from the value $9 \cdot 2^{-2/3}/140$ to zero for $\zeta \geq 0$ (we omit these details). With the help of *Mathematica*, the product $\phi(\zeta)b_0(\zeta)$ has the series expansion

$$\phi(\zeta)b_0(\zeta) = - \sum_{m=0}^\infty \beta_m \zeta^m \quad (|\zeta| < \zeta_0),$$

where the first few coefficients are

$$\beta_0 = \frac{9}{280} 2^{-1/3}, \quad \beta_1 = -\frac{179}{6300} 2^{-2/3}, \quad \beta_2 = \frac{28687}{2425500}, \quad \beta_3 = -\frac{750979}{78828750} 2^{-1/3}.$$

Then we find upon using an integration by parts, combined with (3.2) and the result $\text{Ai}(0) = 3^{-2/3}/\Gamma(\frac{2}{3})$, that

$$\int_0^\infty \phi(\zeta) b_0(\zeta) [\text{Ai}^2(\nu^{4/3}\zeta)]' d\zeta \sim \frac{\beta_0 (3\nu)^{-4/3}}{\Gamma^2(\frac{2}{3})} + \frac{2}{\sqrt{\pi}} \sum_{m=1}^\infty \frac{\beta_m m! \nu^{-4m/3-4/3}}{12^{\frac{1}{3}m+\frac{5}{6}} \Gamma(\frac{1}{3}m + \frac{5}{6})} \quad (3.4)$$

as $\nu \rightarrow \infty$.

4. The asymptotic calculation of $P_{n,tun}$ for $n \rightarrow \infty$

The function $-a_1(\zeta)$ appearing in (2.4) is found to be monotonically decreasing for $\zeta \geq 0$ with the series expansion

$$-a_1(\zeta) = \frac{249}{28800} - \frac{6849}{616000} 2^{-1/3}\zeta + \frac{737}{65000} 2^{-2/3}\zeta^2 - \dots \quad (|\zeta| < \zeta_0).$$

Then the $O(\nu^{-4})$ term multiplying $\text{Ai}^2(\nu^{4/3}\zeta)$ in (2.7) has the expansion

$$-\frac{1}{576} \phi(\zeta) (1 + 1152 f_2(\zeta)) = \frac{29}{2400} 2^{-2/3} - \frac{25013}{1848000} \zeta + \dots \quad (|\zeta| < \zeta_0).$$

From (2.7), (3.3) and (3.4) we therefore find

$$\begin{aligned} & \nu^{4/3} \int_0^\infty \phi(\zeta) \Upsilon_\nu^2(\zeta) d\zeta \\ &= \frac{2}{\sqrt{\pi}} \left(1 + \frac{1}{12\nu^2} - \frac{29}{2400\nu^4} \right) \left(\frac{1}{12^{7/6}\Gamma(\frac{7}{6})} + \frac{2\alpha_1\nu^{-4/3}}{12^{3/2}\sqrt{\pi}} + \frac{2\alpha_2\nu^{-8/3}}{12^{11/6}\Gamma(\frac{11}{6})} + \frac{6\alpha_3\nu^{-4}}{12^{13/6}\Gamma(\frac{13}{6})} \right) \end{aligned}$$

$$+\nu^{-8/3}\left(1 + \frac{1}{12\nu^2}\right)\left(\frac{3^{-4/3}\beta_0}{\Gamma^2(\frac{2}{3})} + \frac{2\beta_1\nu^{-4/3}}{\sqrt{\pi} 12^{7/6}\Gamma(\frac{7}{6})}\right) + O(\nu^{-16/3}).$$

Hence, from (1.2) and (2.6), we obtain

$$P_{n,tun} = \frac{2^{n+2}(n!)e^{n+\frac{1}{2}}}{\sqrt{\pi} \nu^{2n+5/3}} \times \left\{ \left(1 + \frac{1}{12\nu^2} - \frac{29}{2400\nu^4}\right) \left\{ \frac{6^{-2/3}}{\Gamma^2(\frac{1}{3})} - \frac{\nu^{-4/3}}{30\pi\sqrt{3}} + \frac{4}{525} \frac{6^{-1/3}\nu^{-8/3}}{\Gamma^2(\frac{2}{3})} - \frac{16}{525} \frac{6^{-2/3}\nu^{-4}}{\Gamma^2(\frac{1}{3})} \right\} + \nu^{-8/3} \left(1 + \frac{1}{12\nu^2}\right) \left\{ \frac{3}{280} \frac{6^{-1/3}}{\Gamma^2(\frac{2}{3})} - \frac{179}{6300} \frac{6^{-2/3}\nu^{-4/3}}{\Gamma^2(\frac{1}{3})} \right\} + O(\nu^{-16/3}) \right\} \quad (4.1)$$

upon use of the properties of the gamma function to simplify the coefficients.

On noting that

$$\frac{2^{n+2}n!e^{n+\frac{1}{2}}}{\sqrt{\pi} \nu^{2n+5/3}} = \frac{2^{5/3}}{n^{1/3}} \left(1 - \frac{5}{12\nu^2} - \frac{23}{288\nu^4} + O(\nu^{-6})\right) \quad (n \rightarrow \infty),$$

we then finally obtain from (4.1) that

$$P_{n,tun} = \frac{2^{5/3}}{n^{1/3}} \left\{ \left(1 - \frac{1}{3\nu^2}\right) \left(\frac{6^{-2/3}}{\Gamma^2(\frac{1}{3})} - \frac{\nu^{-4/3}}{30\pi\sqrt{3}} + \frac{11}{600} \frac{6^{-1/3}\nu^{-8/3}}{\Gamma^2(\frac{2}{3})}\right) - \frac{167}{900} \frac{6^{-2/3}\nu^{-4}}{\Gamma^2(\frac{1}{3})} + O(\nu^{-16/3}) \right\} \quad (4.2)$$

as $n \rightarrow \infty$. Insertion of numerical values for the coefficients yields the alternative form

$$P_{n,tun} = \frac{1}{n^{1/3}} \left\{ \left(1 - \frac{1}{3\nu^2}\right) \left(0.1339750 - \frac{0.0194484}{\nu^{4/3}} - \frac{0.0174687}{\nu^{8/3}}\right) - \frac{0.0248598}{\nu^4} + O(\nu^{-16/3}) \right\}, \quad \nu = \sqrt{2n+1}.$$

The first two leading terms in this expansion can be seen to agree with the approximation stated in (1.3).

We conclude by presenting the results of numerical calculations to illustrate the accuracy of the asymptotic expression in (4.2). In Table 1 we show the values of the absolute relative error in the computation of $P_{n,tun}$ using (4.2) for different n .

Table 1: Values of the absolute relative error in the computation of $P_{n,tun}$ from (4.2).

n	$P_{n,tun}$	Error	n	$P_{n,tun}$	Error
10	0.0601438	1.323×10^{-5}	200	0.0228302	6.975×10^{-9}
20	0.0483977	2.528×10^{-6}	400	0.0181454	1.130×10^{-9}
50	0.0360132	2.534×10^{-7}	500	0.0168499	6.276×10^{-10}
100	0.0286973	4.250×10^{-8}	800	0.0144138	1.815×10^{-10}

References

- [1] A. Jadczyk, Asymptotic formula for quantum harmonic oscillator tunneling probabilities. arXiv: 1501.07483. Reports on Math. Phys. (2015) [to appear].
- [2] F. W. J. Olver, Asymptotics and Special Functions, Academic Press, New York 1974. Reprinted in A. K. Peters, Massachusetts, 1997.
- [3] F. W. J. Olver, D. W. Lozier, R. F. Boisvert and C. W. Clark (eds.), NIST Handbook of Mathematical Functions, Cambridge University Press, Cambridge, 2010.
- [4] N. M. Temme, Numerical and asymptotic aspects of parabolic cylinder functions, J. Comput. Appl. Math. **121** (2000) 221–246. [http://dx.doi.org/10.1016/s0377-0427\(00\)00347-2](http://dx.doi.org/10.1016/s0377-0427(00)00347-2)

Received: March 20, 2015; Published: April 27, 2015