Asymptotic formula for the condensate wave function of a trapped Bose gas

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An analytical property is pointed out for the universal differential equation first derived by Dalfovo, Pitaevskii, and Stringari for the condensate wave function at the boundary of a trapped Bose gas. Specifically, the constant multiplying the Airy function of the solution asymptotically outside the trap is $\sqrt{2}$. Accordingly, the Wentzel-Kramers-Brillouin approximation is determined in the case of a spherically symmetric harmonic potential. This calculation is related to Josephson-type currents flowing between well-separated traps.

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In an insightful paper [1], Dalfovo, Pitaevskii, and Stringari give the condensate wave function at the boundary of a boson gas with repulsive interactions at $T=0$ in terms of an ordinary differential equation of universal form; the focus is on spherically symmetric traps. They proceed to compute the leading term of the kinetic energy per atom of the condensate. This differential equation connects the so-called Thomas-Fermi approximation, by neglect of the ∇^2 operator inside the trap, to the Wentzel-Kramers-Brillouin (WKB) formula, by neglect of the nonlinear term outside the trap. In the notation of Ref. [1], the equation is

$$\phi''(\xi)-\phi(\xi)^3-\xi\phi(\xi)=0, \tag{1}$$

with the boundary conditions

$$\lim_{\xi\to+\infty}\phi(\xi)=0, \qquad \lim_{\xi\to-\infty}(-\xi)^{-1/2}\phi(\xi)=1. \tag{2}$$

Because of the first of these conditions, the nonlinear term in Eq. (1) can be neglected for $\xi\to+\infty$, yielding Airy's equation. The solution to Eq. (1) becomes

$$\phi(\xi)\sim C\,\mathrm{Ai}(\xi) \quad \text{as} \quad \xi\to+\infty, \tag{3}$$

where Ai is the usual Airy function [2]. It is the purpose of this report to point out the beautiful formula

$$C=\sqrt{2}, \tag{4}$$

which has been known in relation to a boundary-value problem in plasma physics [3,4], and to outline its possible implication for the physics of Bose-Einstein condensation. The value for C signifies the effect of a boundary layer [5]; its importance lies in the fact that Eq. (1) can be extended to a class of sufficiently smooth and slowly varying external potentials, where ξ expresses the local normal to the boundary [6,7]. In Ref. [6], Wu recognizes the solution $\phi(\xi)$ to be a special case of the second Painlevé transcendent [8–10].

In an attempt to verify Eq. (4) numerically, one may treat $\phi''(-\xi)$ as small for $\xi\to+\infty$ according to the scheme [11]

$$\phi_{n+1}(-\xi)=\sqrt{\xi}\sqrt{1+\frac{\phi_n''(-\xi)}{\xi\phi_n(-\xi)}},$$

$$\phi_0(-\xi)=\sqrt{\xi}\sim\phi(-\xi), \tag{5}$$

$$|\phi_n''(-\xi)/[\xi\phi_n(-\xi)]|\ll 1,$$

where $n=0,1,2,\ldots$, and the subscript denotes the order of iteration. Hence,

$$\phi(-\xi)=\sqrt{\xi}-\xi^{-5/2}w(\xi), \qquad \xi>0, \tag{6}$$

$$w(\xi)\sim d_0+d_1\xi^{-3}+d_2\xi^{-6}+d_3\xi^{-9}+d_4\xi^{-12}+d_5\xi^{-15} \quad \text{as} \quad \xi\to+\infty. \tag{7}$$

After some straightforward algebra,

$$d_0=\frac{1}{8}, \quad d_1=\frac{73}{128}, \quad d_2=\frac{10\,657}{1024},$$
$$d_3=\frac{13\,912\,277}{32\,768}, \quad d_4=\frac{8\,045\,883\,943}{262\,144},$$
$$d_5=\frac{14\,518\,450\,612\,315}{4\,194\,304}. \tag{8}$$

The ensuing expansions for $\phi(-\xi)$ and its derivative for $\xi\to+\infty$ are

$$\phi(-\xi)\sim\sqrt{\xi}-\frac{1}{8}\xi^{-5/2}-\frac{73}{128}\xi^{-11/2}-\frac{10\,657}{1024}\xi^{-17/2}-\frac{13\,912\,277}{32\,768}\xi^{-23/2}-\frac{8\,045\,883\,943}{262\,144}\xi^{-29/2}-\frac{14\,518\,450\,612\,315}{4\,194\,304}\xi^{-35/2}, \tag{9}$$

$$\phi'(-\xi)\sim-\frac{1}{2}\xi^{-1/2}-\frac{5}{16}\xi^{-7/2}-\frac{803}{256}\xi^{-13/2}-\frac{181\,169}{2048}\xi^{-19/2}-\frac{319\,982\,371}{65\,536}\xi^{-25/2}-\frac{233\,330\,634\,347}{524\,288}\xi^{-31/2}-\frac{508\,145\,771\,431\,025}{8\,388\,608}\xi^{-37/2}. \tag{10}$$

The prime here denotes differentiation with respect to the argument. A suitable number of terms of these expansions can be employed for the numerical calculation of the constant C introduced in formula (3). This program is carried out by use of the routine DIVPRK of the FORTRAN IMSL mathematical library. C is found to be

$$C=1.414\,213\,649\,795. \tag{11}$$

It is remarkable that Eq. (4) is then implied with an accuracy of seven decimal places.

In the following, the WKB solution is discussed briefly for the spherically symmetric potential $V_{\rm ext}=\frac{1}{2}m\omega_0^2 r^2$, by taking Eq. (4) seriously. With

$$\Lambda=(4a^2N^2m\omega_0/\hbar)^{1/4}, \quad \lambda=\sqrt{2\mu/\hbar\omega_0}, \tag{12}$$

$$r\psi(\mathbf{r})=\left(\frac{N^2m\omega_0}{16\pi^2\hbar}\right)^{1/4}q(\overline{r}), \quad \overline{r}=\sqrt{m\omega_0/\hbar}\,r, \tag{13}$$

the Gross-Pitaevskii equation employed in Ref. [1] reduces to

$$-q''(\overline{r})+\overline{r}^2q(\overline{r})+\Lambda^2\frac{q(\overline{r})^3}{\overline{r}^2}=\lambda^2q(\overline{r}). \tag{14}$$

μ is the relevant chemical potential and $\psi(\mathbf{r})$ is the normalized condensate wave function $[N^{-1}\int d\mathbf{r}|\psi(\mathbf{r})|^2=1]$. For comparison with Ref. [6], note that

$$\mu=E+\frac{\hbar\omega_0\Lambda^2}{4}\int_0^\infty\frac{d\overline{r}}{\overline{r}^2}q(\overline{r})^4, \tag{15}$$

E being the energy per particle of the condensate.

When $\Lambda\gg1$, $\lambda\sim(\frac{15}{2}\Lambda^2)^{1/5}$ [12]. For $\overline{r}-\lambda\gg\lambda^{-1/3}$, the WKB method yields

$$q(\overline{r})\sim\mathcal{C}(\overline{r}^2-\lambda^2)^{-1/4}\lambda^{-1}\exp\{-(\lambda^2/2)[(\overline{r}/\lambda)\sqrt{(\overline{r}/\lambda)^2-1}-\cosh^{-1}(\overline{r}/\lambda)]\}. \tag{16}$$

For fixed Λ, $\overline{r}$ has to be large. This new constant $\mathcal{C}$ is independent of $\overline{r}$. On the other hand, the neglect of the second derivative in Eq. (14) furnishes

$$q(\overline{r})\sim(\overline{r}/\Lambda)\sqrt{\lambda^2-\overline{r}^2}, \quad 0\leqslant\overline{r}<\lambda, \quad \lambda-\overline{r}\gg\lambda^{-1/3}, \tag{17}$$

which is in accord with the approximation in Ref. [1] and connects smoothly to the leading term of expansion (9). For $\lambda^{-1/3}\ll\overline{r}-\lambda\ll\lambda^{1/5}$, expression (16) reduces to

$$q(\overline{r})\sim2^{-1/4}\mathcal{C}\lambda^{-3/2}(\overline{r}/\lambda-1)^{-1/4}\times\exp[-2\sqrt{2}\lambda^2(\overline{r}/\lambda-1)^{3/2}/3]. \tag{18}$$

This formula connects to expression (3) via the replacements

$$\xi=(2\lambda^4)^{1/3}(\overline{r}/\lambda-1), \quad q(\overline{r})=\frac{(2\lambda^4)^{1/3}}{\Lambda}\phi(\xi) \tag{19}$$

in Eq. (14) where $\overline{r}^2\sim\lambda^2+2\lambda(\overline{r}-\lambda)$. By virtue of the known large-argument approximation for the Airy function and Eq. (4) for C,

$$\mathcal{C}=\sqrt{\frac{15}{2\pi}}. \tag{20}$$

This equation enables an explicit analytical description for the Josephson-type current flowing between two sufficiently separated, spherically symmetric traps, in the spirit of Ref. [1].

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