Semiclassical wave functions and energy levels of Bose-condensed gases in spherically symmetric traps

András Csordás,[1] Robert Graham,[2] and Péter Szépfalusy[3]
[1]*Research Group for Statistical Physics of the Hungarian Academy of Sciences, Múzeum körút 6–8, H-1088 Budapest, Hungary*
[2]*Fachbereich Physik, Universität-Gesamthochschule Essen, 45117 Essen, Germany*
[3]*Institute for Solid State Physics, Eötvös University, Múzeum körút 6–8, H-1088 Budapest, Hungary and Research Institute for Solid State Physics, P.O. Box 49, H–1525 Budapest, Hungary*
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The WKB approximation for the Bogoliubov equations of the quasiparticle excitations in Bose gases with a condensate is worked out in the case of spherically symmetric trap potentials on the basis of the resulting quantization rule. The excitation spectrum is calculated numerically and also analytically in certain limiting cases. [S1050-2947(97)08011-6]

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The experimental realization and study of Bose-Einstein condensates in alkali atom gases confined by magnetic traps [1–5] has induced vivid activity in the theoretical investigation of such systems. From a theoretical point of view, the existence of the external potential requires alternative methods for calculating the physical properties of the quantum gases with Bose condensation. Our aim is to solve the Bogoliubov equations in WKB approximation and to determine the excitation spectrum on the basis of the resulting quantization rule. Our work goes beyond the previous semiclassical calculations, which used the local-density approximation and considered only the classically allowed region [6].

In the Bogoliubov theory the field operator can be expressed as a linear combination of quasiparticle creation and annihilation operators. The corresponding (nonuniform) expansion coefficients $u_j(\boldsymbol{r})$ and $v_j(\boldsymbol{r})$ obey the coupled linear Bogoliubov eigenvalue equations [7]

$$\begin{pmatrix} \hat{H}_{HF} & -K(\boldsymbol{r}) \\ -K^*(\boldsymbol{r}) & \hat{H}_{HF} \end{pmatrix} \begin{pmatrix} u_j(\boldsymbol{r}) \\ v_j(\boldsymbol{r}) \end{pmatrix} = E_j \begin{pmatrix} u_j(\boldsymbol{r}) \\ -v_j(\boldsymbol{r}) \end{pmatrix}, \tag{1}$$

where j denotes one of the quasiparticle states and E_j is the corresponding quasiparticle energy. The Hartree-Fock operator $\hat{H}_{HF}$ takes the form

$$\hat{H}_{HF} = -\frac{\hbar^2}{2m}\Delta + U(\boldsymbol{r}) + 2|K(\boldsymbol{r})| - \mu, \tag{2}$$

where $U(\boldsymbol{r})$ is the trap potential, μ is the chemical potential, and

$$K(\boldsymbol{r}) = \frac{4\pi\hbar^2 a}{m}\psi_0(\boldsymbol{r})^2 \tag{3}$$

denotes the potential-like contribution of the condensate, whose wave function $\psi_0(\boldsymbol{r})$ is normalized as $\int d^3r|\psi_0(\boldsymbol{r})|^2 = N_0$. N_0 is the number of particles in the condensate and a is the s-wave scattering length. In the following we shall assume that $a>0$. The quasiparticle amplitudes $u_j(\boldsymbol{r})$ and $v_j(\boldsymbol{r})$ are normalized according to [7]

$$\int d^3r[u_j^*(\boldsymbol{r})u_k(\boldsymbol{r}) - v_j^*(\boldsymbol{r})v_k(\boldsymbol{r})] = \delta_{jk}. \tag{4}$$

For the sake of simplicity, we choose the external potential as spherically symmetric. Moreover, we shall take $\psi_0(\boldsymbol{r})$ and hence also $K(\boldsymbol{r})$ as real and shall also make frequent use of the Thomas-Fermi approximation [8], which leads to

$$|\psi_0(\boldsymbol{r})|^2 = \begin{cases} \dfrac{m}{4\pi\hbar^2 a}[\mu_{TF} - U(r)] & \text{if } r < r_{TF} \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Here $U(r_{TF}) = \mu_{TF}$ and μ_{TF} is fixed by normalization. One can introduce spherical coordinates r, θ, ϕ, and separate variables in the usual way:

$$\begin{pmatrix} u_j(\boldsymbol{r}) \\ v_j(\boldsymbol{r}) \end{pmatrix} = \frac{1}{r}\begin{pmatrix} u_{nl}(r) \\ v_{nl}(r) \end{pmatrix} Y_{lm}(\theta,\phi), \tag{6}$$

where j denotes the usual quantum numbers (n,l,m) for isotropic problems and the Y_{lm} are the spherical harmonics.

To solve the coupled, radial equations obtained from Eq. (1) it is advantageous to use the linear combinations [9]

$$G_{nl}^{\pm}(r) = u_{nl}(r) \pm v_{nl}(r), \tag{7}$$

which satisfy the uncoupled equations

$$\{\hat{H}_{HF}^2 - K(r)^2 - E^2 \mp [\hat{H}_{HF}, K(r)]\}G^{\pm}(r) = 0. \tag{8}$$

Here $[,]$ denotes the commutator. (For brevity we have omitted the indices n and l.) Furthermore, it follows from the original equations that

$$G^{\pm} = \frac{1}{E}[\hat{H}_{HF} \pm K(r)]G^{\mp}, \tag{9}$$

which is compatible with Eq. (8).

Now the operator $\hat{H}_{HF}$ has the form

$$\hat{H}_{HF} = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + U_{eff}(r), \tag{10}$$

where

$$U_{eff}(r)=\frac{\hbar^2 l(l+1)}{2mr^2}+U(r)+2K(r)-\mu. \tag{11}$$

In our WKB treatment we use Langer's rule by replacing $l(l+1)$ by $(l+1/2)^2$. In the following $U_{eff}(r)$ is considered as a classical potential.

We shall consider two types of solutions

$$G^+(r)=\exp\left[\frac{i}{\hbar}\left(S_0+\frac{\hbar}{i}S_1+\cdots\right)\right], \tag{12}$$

$$G^+(r)=\exp\left[-\frac{1}{\hbar}(\widetilde{S}_0+\hbar\widetilde{S}_1+\cdots)\right], \tag{13}$$

with real functions $S_0(r), S_1(r), \ldots$ and $\widetilde{S}_0(r), \widetilde{S}_1(r), \ldots$, respectively. Gathering terms having different powers of $\hbar$, one gets first-order ordinary differental eqations for the unknown quantities occurring in Eqs. (12) and (13).

First we consider solutions of the form (12). The $O(\hbar^0)$ equation is the classical Hamilton-Jacobi equation for the radial action $S_0(r)$, from which one can express the classical radial momenta as

$$|p_r|\equiv\left|\frac{dS_0}{dr}\right|=\sqrt{2m(\pm\sqrt{E^2+K^2}-U_{eff})}. \tag{14}$$

We shall assume that $U_{eff}>0$, in which case only the plus sign is allowed to have p_r real. This is the case, for instance, in the Thomas-Fermi approximation (5). We introduce the radial velocity in the usual way $v_r=\partial H/\partial p_r$ by regarding E in (14) as the classical Hamiltonian $H(p_r,r)$. The obtained expression [10]

$$v_r=\sqrt{\frac{E^2+K^2(r)}{E}}\frac{p_r}{m} \tag{15}$$

reflects the peculiarity of the classical quasiparticle dynamics in traps. The effective quasiparticle mass, which can be read off from Eq. (14), is energy and space dependent. It approaches the particle mass at the boundary of the condensate, but can become much smaller yet remains nonzero even in the center of very large condensates in traps. This is a fundamental difference to the untrapped case, where the limit $E\to 0$ can be taken, in which the quasiparticle mass vanishes.

By solving Eq. (8) with the ansatz (12) up to S_1, then using Eq. (9) for $G^-(r)$, and finally transforming back from $G^{\pm}(r)$ to $u_{nl}(r)$ and $v_{nl}(r)$, particular solutions of the radial Bogoliubov equations are obtained in the form

$$\begin{pmatrix}u_{nl}(r)\\ v_{nl}(r)\end{pmatrix}\simeq\text{const}\times\begin{pmatrix}u_B(r)\\ v_B(r)\end{pmatrix}\frac{1}{\sqrt{|v_r|}}\exp\left(\pm\frac{i}{\hbar}\int^r p_r(r)dr\right), \tag{16}$$

where $u_B^2=\{\sqrt{1+[K(r)/E]^2}+1\}/2$ and $u_B^2-v_B^2=1$ are the generalizations of the usual Bogoliubov coefficients for the case without trapping potential. Note that the classical probability distribution is inversely proportional to $|v_r|$, as expected physically.

Solutions (16) are valid in the classically allowed region, i.e., between the classical turning points r_{t1} and $r_{t2}>r_{t1}$ defined by the condition $p_r(r_{ti})=0$, $i=1,2$. We shall assume that there are two turning points only. There may be three cases: case A, if $r_{t1}<r_{TF}<r_{t2}$, in other words, the classical particle enters the condensate, then leaves it, and returns again, etc.; case B, if $r_{TF}<r_{t1}<r_{t2}$, i.e., we have only a simple classical motion in the trapping potential; case C, if $r_{t1}<r_{t2}<r_{TF}$, in which case the classical motion is confined to the condensate.

Next we construct solutions of the form (13) proceeding similarly to before. Using the ansatz (13) in Eq. (8), there can exist two different solutions for $\widetilde{S}_0$,

$$|q_r^{(i)}|\equiv\left|\frac{d\widetilde{S}_0^{(i)}}{dr}\right|=\sqrt{2m[U_{eff}+(-1)^i\sqrt{E^2+K^2}]},$$

$$i=1,2. \tag{17}$$

Both signs are allowed, for example, in the Thomas-Fermi approximation (5). The solution for $i=1$ is defined only outside the classically accessible region, while the other one ($i=2$) is permissible for all r values, if $U_{eff}>0$ (as we suppose), and represents a solution that can only occur in the present two-component quasiparticle dynamics. Let us define furthermore quantities $w_r^{(i)}$ similar to those in Eq. (15) by the relation

$$w_r^{(i)}=\sqrt{\frac{E^2+K^2(r)}{E}}\frac{q_r^{(i)}}{m}. \tag{18}$$

Let us now consider the allowed solutions in case A. Requiring normalizibily and performing turning point matching at r_{tj}, one obtains

$$\begin{pmatrix}u_{nl}\\ v_{nl}\end{pmatrix}\simeq\frac{C_{1j}}{\sqrt{|w_r^{(2)}|}}\begin{pmatrix}v_B\\ -u_B\end{pmatrix}\exp\left[\frac{(-1)^j}{\hbar}\int_r^{r_{TF}}q_r^{(2)}(r)dr\right]+\frac{C_{2j}}{\sqrt{|Z_r|}}\begin{pmatrix}u_B\\ v_B\end{pmatrix}F(r), \tag{19}$$

where $j=1$ and $j=2$ correspond to $r<r_{TF}$ and $r>r_{TF}$, respectively. C_{1j} and C_{2j} are arbitrary constants and

$$F(r)=\exp\left[\frac{(-1)^j}{\hbar}\int_r^{r_{tj}}q_r^{(1)}(r)dr\right],$$

$$Z_r=w_r^{(1)}\quad\text{for}\begin{cases}0<r<r_{t1} & (j=1)\\ r_{t2}<r & (j=2),\end{cases} \tag{20}$$

and

$$F(r)=2\sin\left[\frac{(-1)^j}{\hbar}\int_r^{r_{tj}} p_r(r)dr+\frac{\pi}{4}\right],$$

$$Z_r=v_r \quad \text{for} \quad \begin{cases} r_{t1}<r<r_{TF} & (j=1) \\ r_{TF}<r<r_{t2} & (j=2). \end{cases} \tag{21}$$

Requiring that $u(r)$, $v(r)$ and their first derivatives are continuous at r_{TF}, one gets four homogeneous linear equations for the four unknown constants. In order to get nontrival solutions the determinant of the coefficient matrix should vanish. This leads to the semiclassical quantization rule

$$0=-\frac{p_A}{\hbar}\cos\left(\frac{I_A+I_B}{\hbar}\right)+\sin\left(\frac{I_A}{\hbar}+\frac{\pi}{4}\right) \times\sin\left(\frac{I_B}{\hbar}+\frac{\pi}{4}\right)\left[\frac{mL}{p_A^2}-\left(\frac{L}{2E}\right)^2\frac{\hbar p_B^2}{2p_B^3+\hbar mL}\right], \tag{22}$$

where we have introduced the notations $p_A\equiv p_r(r_{TF})$, $p_B\equiv q_r^{(2)}(r_{TF})$, $L=(\partial K/\partial r)_{r_{TF}+0}-(\partial K/\partial r)_{r_{TF}-0}$, $I_A=\int_{r_{t1}}^{r_{TF}}p_r dr$, and $I_B=\int_{r_{TF}}^{r_{t2}}p_r dr$.

Keeping only the first term on the right-hand side of Eq. (22) leads to the usual Bohr-Sommerfeld quantization rule

$$\left(n+\frac{1}{2}\right)=\frac{1}{\pi\hbar}\int_{r_{t1}}^{r_{t2}}dr\,\sqrt{2m[\sqrt{E^2+K^2(r)}-U_{eff}(r)]}, \tag{23}$$

with the integer radial quantum number $n\geqslant 0$ and including the Maslov indices due to the two turning points in the radial motion. Case B can be treated in an analogous way, leading to the quantization rule (23) with $K(r)=0$ within the range of integration.

We discuss first the energy levels on the basis of Eq. (23) and will return to the consequences of the general expression (22) afterward. To evaluate Eq. (23) we choose a harmonic potential $U(r)=m\omega_0^2 r^2/2$ often used in theoretical consideration [8,9,11]. To distinguish between cases A and B let us use the dimensionless variables $\tilde{J}=\hbar\omega_0(l+1/2)/2\mu$, $\tilde{E}=E/\mu$. For energies and angular momenta in the region $1<2\tilde{J}-1<\tilde{E}<\tilde{J}^2$ case B occurs and the energy spectrum is simply that of a harmonic oscillator shifted by μ

$$E_{n,l}^{(osc)}=\hbar\omega_0\left(2n+l+\frac{3}{2}\right)-\mu. \tag{24}$$

The self-consistency condition for case B is then $l+1/2>2\mu/\hbar\omega_0+\sqrt{4\mu(2n+1)/\hbar\omega_0}$. One can check that case C, i.e., the classical motion is entirely inside the condensate, is not possible.

Considering the nontrivial case A in region $0<\tilde{J}^2<\tilde{E}$, the action integral in Eq. (23) can still be performed analytically, but the result is rather cumbersome and the energies E_{nl} cannot be expressed explicitly. However, due to Eq. (23) the semiclassical energies fulfill the scaling relation $E_{n,l}=\hbar\omega_0 G_{n,l}(\mu/\hbar\omega_0)$. We discuss here some limiting cases. One interesting limit is when one considers the high-lying levels, i.e., when $E_{n,l}\gg\mu$ is fulfilled. Then the main contribution to the action integral in Eq. (23) comes from the region outside of the condensate, leading to a spectrum that is almost that of a harmonic oscillator. Expanding the action integral to the next to leading correction in $\mu/E_{n,l}$ one gets

$$E_{n,l}=E_{n,l}^{(osc)}+\hbar\omega_0\delta_{n,l}$$

$$\delta_{n,l}\simeq\frac{1}{3\pi}\frac{\left[\frac{4\mu}{\hbar\omega_0}\left(2n+l+\frac{3}{2}-\frac{\mu}{\hbar\omega_0}\right)-\left(l+\frac{1}{2}\right)^2\right]^{3/2}}{\left[2n+l+\frac{3}{2}-\frac{\mu}{\hbar\omega_0}\right]^2}. \tag{25}$$

This result and that of the perturbation theoretical calculation [12] agree for large $(2n+l)$ values.

The other interesting limit is the region of excitation energies small compared to the chemical potential. To reach it formally, the angular momentum and the radial quantum numbers l and n are kept fixed, but $\mu/\hbar\omega_0$ tends to infinity. The main contribution to the radial action integral (23) comes from those r values that are within the condensate. To leading order

$$E_{n,l}\simeq\hbar\omega_0[2n^2+2nl+3n+l+1]^{1/2}. \tag{26}$$

Our result (26) almost coincides with that of Stringari's hydrodynamic calculation [11], except for the last constant 1 within $[\,]^{1/2}$ in Eq. (26), which has an appreciable effect only on the lowest levels. It is, of course, not unexpected that a WKB approach may fail there. For somewhat higher energies at fixed but large chemical potential there is a considerable region where the two spectra calculated in WKB and in hydrodynamical approximations, respectively, overlap. For even higher energies the applicability of the hydrodynamical approach loses its validity. The task of solving Eq. (23) for E can be carried out numerically in a straightforward manner for given scattering length a, trapping potential (i.e., ω_0), and number N_0 of atoms in the condensate, fixing the single parameter $2\mu/\hbar\omega_0=(15N_0a/\sqrt{\hbar/m\omega_0})^{2/5}$ on which the spectrum depends. An example of the results obtained is depicted in Fig. 1.

Let us turn now to the discussion of Eq. (22). By solving Eq. (22) numerically for the energies we have found that the corrections $\Delta E_{n,l}$ to the levels defined by Eq. (23) are small, except when the classical inner turning point r_{t1} gets close to the surface of the condensate [the border between regions A and B in the (n,l) plane], in which case the radial wave number p_A goes to zero. $\Delta E_{n,l}$ then becomes large, but decreases rapidly when going away from this situation. Note that in this case the classical orbits are just glancing at the surface of the condensate. The solution of the Bogoliubov equations then contains an anomalous contribution, namely, the first term on the right-hand side of Eq. (19), which is exponentially localized at the surface. The effect remains even for high energies when v_B becomes negligible. At such energies it is generally assumed that the Bogoliubov equations go over to the Hartree-Fock equations. Our results suggest that there might be exceptional states at the border of regions A and B. Physically, the effect is caused by the narrow boundary layer of the condensate, which looks effectively sharp for orbits glancing on the surface. Its qualitative

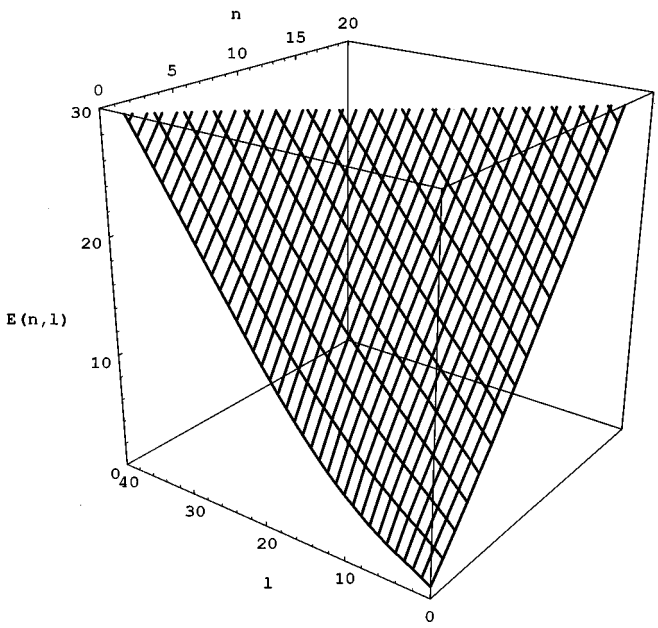

FIG. 1. Energy levels $E(n,l)=E_{nl}/\hbar\omega_0$ obtained numerically from Eq. (23) for an isotropic harmonic-oscillator trap potential $U(r)=m\omega_0^2 r^2/2$ as a function of the radial quantum number n and of the angular-momentum quantum number l. The chemical potential was chosen to be $8\hbar\omega_0$.

aspects can therefore be expected to be independent from the WKB and Thomas-Fermi approximations in a preasymptotic region in energy, when the WKB solution is valid only outside the boundary layer. If in this energy region one uses a condensate potential (3), which is smooth (i.e., exceeds the Thomas-Fermi approximation), one has to solve the Bogoliubov equations within the boundary layer appropriately and matching the result with the WKB solutions outside. Such a procedure goes beyond the scope of the present paper and is left as a future work. Finally, we note that experimentally such anomalous states could be observed by their excitation via modulations of the trapping potentials as in [4,5] or by light scattering.

In this paper we have restricted ourselves, for the sake of simplicity, to the case of the spherically symmetric trap potential. Calculations along these lines for anisotropic harmonic-oscillator trap potentials as they are used in the experiments [4,5] will be discussed elsewhere. Here we only mention that the corresponding classical Hamiltonian shows chaotic behavior [13], especially for energies comparable to the chemical potential.

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[10] It is worth noting that the classical current related to the velocity field has a quantum-mechanical counterpart also in this quasiparticle dynamics. To obtain it one has to subtitute for the energy eigenvalue the time derivative operator $i\hbar\partial/\partial t$ in Eq. (1) in order to consider the time-dependent solutions $u(\boldsymbol{r},t)$ and $v(\boldsymbol{r},t)$. Through the usual steps one arrives at the continuity equation $(\partial\rho/\partial t)+\mathrm{div}\boldsymbol{j}=0$, with $\rho=|u|^2-|v|^2$ and $\boldsymbol{j}=(\hbar/m)\mathrm{Im}(u^*\nabla u+v^*\nabla v)$. The appearance of different signs for the contributions of v in the expressions for ρ and $\boldsymbol{j}$ leads to the unusual relation (15) between velocity and momentum in the classical limit.

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