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The Classical Limit of some Stationary State wave Functions

Guo Shiqi
(Computer Institute, Beijing Polytechnic University, 100044)
Qian Shangwu
(Department of Physics, Beijing University, 100871)

Abstract The classical limits of the one dimensional harmonic oscillator wave function and the hydrogen wave function are studied in this paper. It is proved that these classical limits, described classically, are for a single particle ensemble, not a single particle.

Keywords classical limits, stationary state wave function, ensemble

1 Introduction

There are two kinds of view on the meaning of the classical limit of a quantum mechanical state, one is that it describes classically a single particle, the another is that it describes classically a single particle ensemble, we shall call such ensemble "homogeneous ensemble", which is introduced and defined in this article in section 2. In section 3 we derive the classical limit of one dimensional harmonic oscillator wave function. In section 4 we derive the classical limit of the hydrogen atom wave function.

2 Homogeneous ensemble

We consider an ensemble of single particle, for which the physical quantities G_1, G_2, G_3 are kept constant. Let h_1, h_2, h_3 be the corresponding conjugate coordinates of G_1, G_2, G_3, then the distribution function(DF) in the $\vec{h}$, $\vec{G}$ phase space can be written as

$$P(\vec{h}, \vec{G})=P(\vec{h})\delta(\vec{G}-\vec{G}') \quad (1)$$

(1) can also be used to describe a single particle with constant value of $\vec{G}$ ($\vec{G}:=G_1$, G_2, G_3), in this case

$$P(\vec{h})=\delta(\vec{h}-\vec{h}') \quad (2)$$

where $\vec{h}'(\vec{h}':=h_1', h_2', h_3')$ are functions of time t, which are determined by equations

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of motion and initial conditions. We introduce such a single particle ensemble, that its DF in $\vec{h}$ space is a costant, i.e.

$$P(\vec{h})=A=\text{const} \tag{3}$$

we call it a "homogeneous ensemble" (HMES).

Now, let us turn to find HMES of a classical harmonic oscillator, the conserved quantity is energy E, its canonical conjugate coordinate is time t, the DF in t, E space is

$$P(t,\ E)=P(t)\delta(E-E') \tag{4}$$

Let $P(x)$ be DF in configuration space, then we have

$$P(x)\,\mathrm{d}x=2P(t)\,\mathrm{d}t \tag{5}$$

The factor 2 comes from the fact that in one period of time the particle pass twice the same position. From the classical equation of motion we obtain

$$x=\frac{1}{\omega}\sqrt{\frac{2E'}{m}}\sin(\omega t+\Phi) \tag{6}$$

from the normalization condition

$$\int_0^T P(t)\,\mathrm{d}t=1 \tag{7}$$

we get $A=1/T$, hence DF of HMES for classical harmonic oscillator in x space is

$$P(x)=\frac{1}{\pi\sqrt{\frac{2E'}{m\omega^2}-x^2}} \tag{8}$$

Next, we turn to find HMES of the classical electron in the hydrogen atom. The motion of election in time is given by the following equations[1]:

$$r=a(1-\varepsilon\cos\psi) \tag{9}$$

$$\tan\frac{\chi}{2}=\sqrt{\frac{1+\varepsilon}{1-\varepsilon}}\tan\frac{\psi}{2} \tag{10}$$

$$\omega t=\psi-\varepsilon\sin\psi \qquad \left(\omega=\frac{2\pi}{T}=\frac{e}{\sqrt{ma^3}}\right) \tag{11}$$

where χ is the polar angle in the orbit plane, ψ is eccentric anomaly, ε is eccentricity,

$$\varepsilon=\sqrt{1+\frac{2EL^2}{me^4}} \tag{12}$$

where e, m, E are the charge, mass, energy of electron respectively. In this case there are three conserved quantities, which are E, angular momentum L, z component of L, denoted by L_z. The corresponding conjugate coordinates are t, χ, Φ. By the definition of HMES, the DF in t, χ, Φ space is

$$P(t,\ \chi,\ \Phi)=A \tag{13}$$

DF in the spherical polar coordinates r, θ, Φ space $P(r, \theta, \Phi)$ is given by

$$A\,\mathrm{d}t\,\mathrm{d}\chi\,\mathrm{d}\Phi = P(r, \theta, \Phi)\, r^2 \sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\Phi \tag{14}$$

since

$$\mathrm{d}r\,\mathrm{d}\theta = \frac{\partial(r, \theta)}{\partial(\chi, t)}\,\mathrm{d}\chi\,\mathrm{d}t \tag{15}$$

hence

$$P(r, \theta, \Phi) = \frac{A}{\dfrac{\partial(r, \theta)}{\partial(\chi, t)}\, r^2 \sin\theta} \tag{16}$$

from (9) and (11) we obtain

$$\frac{\partial r}{\partial t} = \frac{\varepsilon a \omega \sin\psi}{1-\varepsilon\cos\psi} \qquad \frac{\partial r}{\partial \chi} = 0 \tag{17}$$

let θ_N be the polar angle of the normal of the orbit plane, then

$$\cos\theta_N = L_z / L \tag{18}$$

$$\sin\theta_N \sin\chi = \cos\theta \tag{19}$$

from (19),

$$\frac{\partial\theta}{\partial\chi} = -\frac{\cos\chi\sin\theta_N}{\sin\theta} \tag{20}$$

using (9), (17) ~ (20), we obtain

$$\frac{\partial(r, \theta)}{\partial(\chi, t)} = \frac{\varepsilon a \omega \sin\psi \cos\chi \sin\theta_N}{(1-\varepsilon\cos\psi)\sin\theta}$$

$$= \frac{\omega a^2 \sqrt{\varepsilon^2 - (1-\dfrac{r}{a})^2}\,\sqrt{\sin^2\theta - L_z^2/L^2}}{r\sin\theta} \tag{21}$$

from the normalization condition

$$\int_0^T\int_0^\pi\int_0^\pi A\,\mathrm{d}t\,\mathrm{d}\chi\,\mathrm{d}\Phi = 1 \tag{22}$$

we get $A = \omega / 2\pi^3$, finally we obtain

$$P(r, \theta, \Phi) = \frac{1}{\pi a^2 r\sqrt{\varepsilon^2 - (1-\dfrac{r}{a})^2}} \cdot \frac{1}{2\pi^2\sqrt{\sin^2\theta - L_z^2/L^2}} \tag{23}$$

3 Classical limit of the harmonic oscillator wave function

The quantum mechanical stationary state wave function of harmonic oscillator is[2]

$$\psi_n(x) = \frac{1}{\sqrt{x_0}}\, e^{-\xi^2/2} H_n(\xi)$$

$$= \frac{1}{\sqrt{x_0}} \frac{(-1)^n}{\sqrt{n!\sqrt{\pi}}} 2^{(\frac{n}{2}+\frac{1}{4})}(\sqrt{2}\xi)^{-\frac{1}{2}} W_{\frac{n}{2}+\frac{1}{4}, -\frac{1}{4}}(\xi^2) \tag{24}$$

where $W_{\frac{n}{2}+\frac{1}{4}, -\frac{1}{4}}(\xi^2)$ is whittaker function[3], and

$$\xi^2 = \frac{x^2}{x_0^2} = \frac{m\omega x^2}{h} = 4\frac{(n+\frac{1}{2})}{2}\frac{\frac{1}{2}m\omega^2 x^2}{E_n} = 4k\cos^2\tau \tag{25}$$

where $k = \frac{1}{2}(n+\frac{1}{2})$, $\cos^2\tau = \frac{1}{2}m\omega^2 x^2/E_n$, $E_n = (n+\frac{1}{2})\hbar\omega$.

Using the asympototic formula of whittaker function:

$$\lim_{k\to\infty} W_{k,m}^2(4k\cos^2\tau) = 2k^{2k}e^{-2k}(\tan\tau)^{-1} \tag{26}$$

and

$$\lim_{n\to\infty}(1+\frac{1}{2n})^n = e^{\frac{1}{2}} \qquad \lim_{n\to\infty} n! = n^n e^{-n}\sqrt{2\pi n} \tag{27}$$

we can easily obtain the classical limit of $\psi_n^2(x)$. The totality of the two limits, the large quantum number limit and the $h\to 0$ limit, is called the classical limit. The result obtained under the conditions

$$n\to\infty,\ \hbar\to 0,\ E_n = (n+\frac{1}{2})\hbar\omega = E' = \text{const} \tag{28}$$

is

$$P(x) = \psi_n^2(x) \to \lim_{n\to\infty} \frac{2n^n\sqrt{n}\,(1+\frac{1}{2n})^n}{n!\sqrt{2\pi}\,e^{n+\frac{1}{2}}\sqrt{\frac{2E'}{m\omega^2}-x^2}}$$

$$= \frac{1}{\pi\sqrt{\frac{2E'}{m\omega^2}-x^2}} \tag{29}$$

hence we prove the conclusion that the oscillator wave function in the classical limit describes HMES for classical harmonic oscillators.

4 Classical limit of the hydrogen wave function

In hydrogen atom electron position probability in the volume element $r^2\sin\theta\,dr\,d\theta\,d\Phi$ situated at the point (r, θ, Φ) is

$$|\psi_{nlm}(r, \theta, \Phi)|^2 r^2\sin\theta\,dr\,d\theta\,d\Phi \tag{30}$$

hence

$$P(r, \theta, \Phi) = |\psi_{nlm}(r, \theta, \Phi)|^2 = |R_{nl}(r)|^2\,|Y_{lm}(\theta, \Phi)|^2 \tag{31}$$

the classical limit of the radial wave function is given by WKB method, which is[4]

$$\left|R_{nl}(r)\right|^2 \to \frac{C_1}{r^2 p(r)} \tag{32}$$

where

$$p^2(r)=2m[E_n+\frac{e^2}{r}-\frac{l(l+\frac{1}{2})\hbar^2}{2mr^2}]=$$

$$=\frac{2m|E_n|a^2}{r^2}[\varepsilon^2-(1-\frac{r}{a})^2]\quad(\varepsilon=\sqrt{1-\frac{l(l+\frac{1}{2})}{n^2}})\tag{33}$$

the constant C_1 can be obtained by

$$\int_0^\infty R_{nl}^2(r)\,\mathrm{d}r=1\tag{34}$$

hence in the classical limit

$$|R_{nl}(r)|^2\rightarrow\frac{1}{\pi a^2 r\sqrt{\varepsilon^2-(1-\frac{r}{a})^2}}\tag{35}$$

we turn to find the classical limit of $|Y_{lm}(\theta,\Phi)|^2$

$$|Y_{lm}(\theta,\Phi)|^2=\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}|P_l^{|m|}(\cos\theta)|^2\tag{36}$$

the associated Legendre polynomial $y=P_l^{|m|}(x)$ satisfy the following differential equation:

$$y''-\frac{2x}{1-x^2}y'+k^2(x)y=0\tag{37}$$

where

$$k^2(x)=\frac{[1-x^2-m^2/l(l+1)]}{(1-x^2)/l(l+1)}\tag{38}$$

the classical limit of y obtained by WKB method is[5]

$$y=\frac{C_2}{[1-x^2-m^2/l(l+1)]^{1/4}}\mathrm{Re}\exp(\pm i\int k(x)\,\mathrm{d}x)\tag{39}$$

C_2 can be determined by the normalization condition of spherical harmonics. Finally we obtain the classical limit:

$$|Y_{lm}(\theta,\Phi)|^2\rightarrow\frac{1}{2\pi\sqrt{\sin^2\theta-L_z^2/L^2}}\tag{40}$$

Substitute (35) and (40) in (31) we obtain (23), hence the hydrogen wave function in the classical limit describes HMES for classical electrons[6].

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一些定态波函数的经典极限

郭世琪 钱尚武

（北京工业大学计算学院，100044） （北京大学物理系，100871）

摘 要 研究了一维谐振子的波函数和氢原子波函数的经典极限．首先定义了一种特殊的单粒子系综，即均匀系综．其次明确了经典极限是一种综合极限，即量子数 $n\to\infty$，普朗克常数 $h\to 0$ 但保持能量 $E(n, h)$ 为某一固定值的极限，这种极限实质是大量子数极限但可使能量变化取无限小量．引入均匀系综定义并用综合极限方法，严格证明了一维谐振子的定态波函数和氢原子的定态波函数的精典极限都是某种均匀系综．

关键词 经典极限，定态波函数，系综

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