International Journal of Theoretical Physics, Vol. 46, No. 3, March 2007 (© 2007)
DOI: 10.1007/s10773-005-9006-y

Total Current Operator and its Classical Correspondence for Particles Bounded in Central Force Fields

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Received April 8, 2005; accepted November 24, 2005
Published Online: February 22, 2007

When a particle is bounded in a central force field, the only nonvanishing component of the mean value for current density is along the azimuthal direction; and the total current can therefore be defined. It is found that the total current is in fact a mean value of a newly defined total current operator in the quantum mechanical state. Not only the total current operator itself but also the mean total current has exact classical correspondence.

KEY WORDS: Quantum mechanics.

1. INTRODUCTION

In elementary quantum mechanics, the usual probability density and the usual probability current density come in as two consequences of the fact that the state satisfies Schrödinger equation. As far as we know, it is C. Cohen-Tannoudji, B. Diu, and F. Lalöe who firstly noticed that the probability density and the probability current density are in fact two mean values, in the quantum mechanical state, of the probability density operator $\hat{\rho} = |x\rangle\langle x|$ and probability current density operator $\hat{j} = (|x\rangle\langle x|\hat{\mathbf{P}} + \hat{\mathbf{P}}|x\rangle\langle x|)/(2\mu)$, respectively (Cohen-Tannoudji *et al.*, 1977). In this work, we take a similar study and analyze the total current for particles bounded in central force fields. Results show that a total current operator exists in quantum mechanics for particles bounded in central force fields and its classical correspondence is exact.

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2. THE TOTAL CURRENT IN CENTRAL FORCE PROBLEMS AND ITS CLASSICAL CORRESPONDENCE

In spherical polar coordinates, the (n_r, l, m)th stationary state of a central force problem is usually denoted by $\psi_{n_r lm}(r, \theta, \varphi) = R_{n_r l}(r) Y_{lm}(\theta, \varphi)$ where $R_{n_r l}(r)$ and spherical harmonics $Y_{lm}(\theta, \varphi)$ are the radial and the angular part of the stationary state, respectively. Three components of the mean value for current density in three mutual orthogonal directions $(\vec{e}_r, \vec{e}_\theta, \vec{e}_\varphi)$ are respectively given by (Greiner W, 1994):

$$J_r = 0, \quad J_\theta = 0, \quad J_\varphi = -\frac{em\hbar}{\mu r \sin\theta} |\psi_{n_r lm}(r, \theta, \varphi)|^2. \tag{1}$$

These results reveal that the only nonvanishing component is the azimuthal one. The total current in the stationary state can be carried out by the integration of mean current density J_φ over the half-plane transpierced by the current (e.g., half yz-plane), and the result is

$$\begin{aligned} I_{n_r l} &= -\frac{em\hbar}{\mu} \int_0^\infty \int_0^\pi \frac{1}{r \sin\theta} |\psi_{n_r lm}(r, \theta, \varphi)|^2 r \, dr \, d\theta \\ &= -\frac{em\hbar}{2\pi\mu} \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{r^2 \sin^2\theta} |\psi_{n_r lm}(r, \theta, \varphi)|^2 r^2 \sin\theta \, dr \, d\theta \, d\varphi \qquad (2) \\ &= -\frac{em\hbar}{2\pi\mu} \left\langle n_r l \left| \frac{1}{r^2} \right| n_r l \right\rangle \left\langle lm \left| \frac{1}{\sin^2\theta} \right| lm \right\rangle, \qquad (3) \end{aligned}$$

where

$$\begin{aligned} \left\langle n_r l \left| \frac{1}{r^2} \right| n_r l \right\rangle &= \int_0^\infty \frac{1}{r^2} R^2_{nrl^{r^2}} \, dr, \\ \left\langle lm \left| \frac{1}{\sin^2\theta} \right| lm \right\rangle &= \int_0^\pi \int_0^{2\pi} \frac{|Y_{lm}|^2}{\sin^2\theta} \sin\theta \, d\theta \, d\varphi. \end{aligned} \tag{4}$$

The total current (2) has exact classical correspondence after we can rewrite the Eq. (2) in terms of a mean value for following total current operator in the stationary state $\psi_{n_r lm}(r, \theta, \varphi)$,

$$\hat{I} \equiv \frac{\hat{M}_z}{\hat{A}_z} = \frac{-e}{2\mu} \frac{\hat{L}_z}{\pi (r \sin\theta)^2}, \tag{5}$$

where the factor $-e/(2\mu)$ is the gyromagnetic ratio. This total current operator $\hat{I}$ can be considered as the quantum mechanical quantity obtained by quantization of the classical mechanical relation $I = M_z / A_z$, where $M_z = -e/(2\mu) L_z$ is the circular orbital magnetic moment along the z direction and $A_z = \pi (r \sin\theta)^2$ is the circular orbital area whose radius is $r \sin\theta$. It must be noted that in quantum mechanics, there is no definite orbit, and the particle can appear everywhere in the three-dimensional space with certain probabilities. Therefore the mean value for this total current operator in stationary states should reproduce the classical quantity in classical limit. To see this clearly, we start from the following classical relationship,

$$I = -\frac{e}{T_c}, \tag{6}$$

in which the classical period T_c is (Goldstein, 1980)

$$T_c = 2\pi \left(\frac{\partial H}{\partial J_r}\right)^{-1} = 2\pi \left(\frac{\partial H}{\partial J_\theta}\right)^{-1}, \tag{7}$$

where H is the classical Hamilton function; J_r and J_θ are two classical actions $J_i = \oint p_i\, dq_i$ with i being r and θ, respectively. To compare the total classical current I (6) with quantum mechanical total current $I_{n_r l}$ (2), we rewrite the classical period T_c (7) in terms of quantized actions $J_r = n_r h$ and $J_\theta = lh$ which must hold in either semiclassical quantum mechanics or in classical limit of quantum mechanics, and the results are,

$$T_c \to T_{n_r l} = \left(\frac{\partial E_{n_r l}}{\partial (n_r \hbar)}\right)^{-1} = \left(\frac{\partial E_{nrl}}{\partial (l\hbar)}\right)^{-1}. \tag{8}$$

Combining results (6) and (8), we find that the total classical current becomes,

$$I \to I_{n_r l} = (-e)\frac{\partial E_{n_r l}}{\partial (I\hbar)}. \tag{9}$$

If the exact correspondence works, this current expression (9) is reproducible from the full quantum mechanics. In fact, for the central force field $V(r)$, the radial part of the Hamiltonian operator, or the equivalent Hamiltonian determining the energy eigenvalues $E_{n_r l}$, is given by,

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + l(l+1)\frac{\hbar^2}{2\mu r^2} + V(r). \tag{10}$$

First, Hellmann-Feynman theorem (Cohen-Tannoudji *et al.*, 1977) states that if the Hamiltonian of a bound system H is a function of a particular parameter λ and $\psi_i(\lambda)$ is an eigenfunction corresponding to the eigenvalue $E_i(\lambda)$ that is $H|\psi_i(\lambda)\rangle = E_i(\lambda)|\psi_i(\lambda)\rangle$, then

$$\frac{\partial E_i(\lambda)}{\partial \lambda} = \langle \psi_i(\lambda)|\frac{\partial H(\lambda)}{\partial \lambda}|\psi_i(\lambda)\rangle. \tag{11}$$

Taking angular quantum number l in (10) as the parameter, we have from the above Hellmann-Feynman theorem (Valk, 1986),

$$\frac{\partial E_{n_r l}}{\partial (l\hbar)} = \left\langle n_{rl} \left| \frac{\partial H}{\partial (l\hbar)} \right| n_{rl} \right\rangle = \left(l + \frac{1}{2}\right)\frac{\hbar}{\mu}\left\langle n_{rl} \left| \frac{1}{r^2} \right| n_{rl} \right\rangle. \tag{12}$$

Second, one of the orthogonal relations for spherical harmonics gives (Gradshteyn and Ryzhik, 1994),

$$\left\langle lm \left| \frac{1}{\sin^2\theta} \right| lm \right\rangle = \int_0^{\pi} \int_0^{2\pi} \frac{|Y_{lm}|^2}{\sin^2\theta} \sin\theta \, d\theta \, d\varphi = \frac{2l+1}{2m}, \quad (m \neq 0). \tag{13}$$

Substituting these two relations (12) and (13) into Eq. (3), we obtain exactly $I_{n_r l}$ given by Eq. (9).

Here, two remarks are added to the total current operator (5) and its classical correspondence relation (9). 1, What we prove above is a theorem which holds for the particles bounded in *all* central force fields. 2, It appears unnecessary to define a period operator. If one insists on doing so, the period operator is not so physically reasonable as the total current operator is.

3. TWO EXAMPLES

3.1. Kepler Problem

As well known, the stationary state is for the Kepler problem $\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r)Y_{lm}(\theta, \varphi)$, and the mean value of r^{-2} is,

$$\left\langle nl \left| \frac{1}{r^2} \right| nl \right\rangle = \int_0^{\infty} \frac{1}{r^2} R_{nl}^2 r^2 dr = \frac{1}{n^3\left(l+\frac{1}{2}\right)a_0^2}, \tag{14}$$

where $a_0 = 4\pi\varepsilon_0\hbar^2/(\mu e^2)$ is the Bohr's radius. The mean value for total current is from its definition (3),

$$I_{nl} = -\frac{e}{T_{nl}}, \tag{15}$$

where T_{nl} is,

$$T_{nl} = 2\pi \frac{\mu n^3 a_0^2}{\hbar}. \tag{16}$$

The classical correspondence of the total current (15) is evident from the fact that it reproduces the third law of Kepler's law of planetary motion (Goldstein, 1980),

$$\frac{T_{nl}^2}{T_{msa}^3} = 4\pi^2 \frac{\mu^2 a_0}{\hbar^2} = 4\pi^2 \frac{\mu}{(e^2/4\pi\varepsilon_0)}, \tag{17}$$

where T_{nl} is the classical period and $r_{msa} = n^2 a_0$ is major semi-axis in the elliptical orbit represented by the stationary state $\psi_{nlm}(r, \theta, \varphi)$.

3.2. Isotropic Harmonic Oscillator

The stationary state is $\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r)Y_{lm}(\theta, \varphi)$, $(n = l + 2n_r)$. The mean value of r^{-2} is (Valk, 1986),

$$\langle nl|\frac{1}{r^2}|nl\rangle = \int_0^\infty \frac{1}{r^2} R_{nl}^2 r^2\, dr = \frac{1}{\left(l+\frac{1}{2}\right)} \frac{\mu\omega}{\hbar}. \tag{18}$$

The mean value for total current is from its definition (3),

$$I_{nl} = -\frac{e\omega}{2\pi}.$$

It is exactly what we expect for the classical period T_{nl} which is,

$$T_{nl} = \frac{2\pi}{\omega}. \tag{19}$$

One may argue that our theorem can only apply to these two systems which, according to Bertrand's theorem (Goldstein, 1980), seem to be the only examples that permit closed orbits for all bound particles. It is not the case at all. As pointed out in (Wu and Zeng, 2000) that the usual derivation of Bertrand's theorem assumes that the form of the central potential is to be a power-law function of r as r^n. Furthermore, if the restriction of a power-law form of the central potential is relaxed, Bertrand's theorem may be extended, and there exists an infinite number of closed orbits (rather than elliptic orbits) for a particle in e.g., the screened Coulomb potential and isotropic harmonic oscillator (Wu and Zeng, 2000). However, the results of these examples are essentially the same, but more technical calculations are needed.

4. CONCLUSIONS

When a particle is bounded in a central force field, the total current operator is definable from quantum mechanics. Then a theorem is proved that not only the total current operator itself, but also the mean value for the total current in a stationary state has direct classical correspondence. Two simple examples, Kepler problem and the isotropic harmonic oscillator, are chosen to illustrate the theorem.

ACKNOWLEDGMENTS

This subject is in part supported by Program for New Century Excellent Talents in University, Ministry of Education; and the Key Teaching Reform Program, Hunan Province, China.

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