Finding way to bridge the gap between quantum and classical mechanics

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Abstract

We have calculated the momentum distributions of nanoparticles in diffraction and interference dependent on the effective screening mass parameter or size parameter and presented the calculations for a nanoparticle inside an infinite square potential well and for a tunnelling nanoparticle through a square potential barrier. These results display the transition from quantum to classical mechanics and the simultaneous wave-particle duality of nanoparticles. The concept that the effective screening effect increases with increasing size of an object paves way for development of nanomechanics and nanotechnology.

1 Introduction

It is well known that there is a gap between quantum and classical mechanics. Nanomechanics is required for the development of nanotechnology that was proposed first in 1959 by Richard Feynman [1]. Now it becomes possible to find way to bridge the gap due to the understanding of quantum reality and interference phenomena as presented in Ref.[2]. In the article a particle is described as a non-spreading wave packet satisfying a linear equation within the framework of special relativity and quantum interference experiments are explained with a hypothesis that there is a coupling interaction between the peaked and non-peaked pieces of the wave packet. It has also been mentioned that concerning a macroscopic object, for example, a tiny grain of sand, roughly speaking, because the outer matter in it,
like a barrier, screens nearly completely the off-peak part of the inner matter, the
diffraction and interference of the grains fundamentally do not take place when
they pass through slits. The concept that the effective screening effect increases
with increasing size of an object gives a logical description of transition from
quantum to classical mechanics and paves way for development of nanomechan-
ics and nanotechnology. This article will present some typical consequences of
the concept to display the transition and the simultaneous wave-particle duality of
nanoparticles. The explanation of the transition in terms of environment-induced
decoherence proposed by such as Zurek [3] seems to be untenable.

2 Diffraction and interference of nanoparticles

A grain of matter in size larger than 100 nm is generally considered as a macro-
scopic object and a particle up to 1 nm as a perfect quantum particle such as
fullerene C_{60} [4]. In order to illustrate the behavior of nanoparticles we con-
sider a spherical nanoparticle as a model as shown in Fig.1(a). Let $m$ denote

\begin{align*}
\text{Figure 1: (a) Sketch of the effective screening layer in a spherical nanoparticle.} \\
\text{(b) Illustration of momentum components of the diffracted nanoparticle.}
\end{align*}

the mass of the effective screening layer, $M$ the total mass and $\alpha = m/M$ the
effective screening mass parameter (ESMP). Furthermore, let $\rho$ denote the aver-
age mass density of the spherical nanoparticle, $r_M$ the radius of the nanoparticle
and $r_m$ the thickness of the effective screening layer, so $M = 4\pi r_M^3 \rho / 3$ and
\[ M - m = 4\pi r_{M-m}^3/3. \] Therefore the ratio \( \sigma = r_m/r_M \) as an effective screening size parameter (ESSP) is

\[
\sigma = \frac{r_m}{r_M} = \frac{r_M - r_{M-m}}{r_M} = \frac{M^{1/3} - (M - m)^{1/3}}{M^{1/3}} = 1 - (1 - \alpha)^{1/3} \tag{1}
\]

\[
\alpha = 1 - (1 - \sigma)^3 \tag{2}
\]

Since the thickness of the screening layer having quantum behavior can be assumed to have a value around a certain value, say 5 nm, the larger the size of the nanoparticle is, the more it is like a classical particle. Now we can investigate diffraction of nanoparticles from a single slit and interference from a double slit in terms of the screening effect.

### 2.1 Diffraction of nanoparticles from a single slit

Assuming that \( x \) axis is perpendicular to a slit in the slit plane and \( z \) axis perpendicular to the slit plane, according to quantum mechanics, if the wave function at the slit is \( \psi(x) \), the diffraction of a particle can be calculated by using the Fourier transformation [5]

\[
\phi(p_x) = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left(-\frac{ip_x x}{\hbar}\right)\psi(x)dx \tag{3}
\]

The momentum of the diffracted particle is

\[
p = \sqrt{m^2v_z^2 + p_x^2} \tag{4}
\]

where \( v_z \) is the velocity component of the particle along \( z \) axis. For a nanoparticle with the ESMP \( \alpha \), its momentum is

\[
p^{(\alpha)} = \sqrt{M^2v_z^2 + p_x^{(\alpha)}^2}, \quad p_x^{(\alpha)} = \alpha p_x \tag{5}
\]

where \( p_x^{(\alpha)} \) is the diffraction contribution of the effective screening layer and is equal to \( \alpha p_x \) as illustrated in Fig.1(b).

The normalized function of the single slit of width, say, 50 nm, as shown in Fig.2(a) is

\[
\Psi(x) = \frac{1}{\sqrt{50}}, \quad |x| < 25 \tag{6}
\]
Figure 2: Slit functions: (a) at the single slit, (b) at the double slit.

\[ \Psi(x) = 0, \quad |x| > 25 \quad (7) \]

Substituting \( p_x^{(\alpha)} / \alpha \) for \( p_x \) into Eq.3, we have the normalized momentum wave function

\[ \Theta(p_x^{(\alpha)}) = \frac{1}{\sqrt{2\pi \hbar}} \int \exp\left(-\frac{ip_x^{(\alpha)} x}{\alpha \hbar}\right) \Psi(x) \, dx \quad (8) \]

and the normalized momentum distribution of the nanoparticle:

\[ P(p_x^{(\alpha)}) = \frac{|\Theta(p_x^{(\alpha)})|^2}{\int |\Theta(p_x^{(\alpha)})|^2 \, dp_x^{(\alpha)}} \quad (9) \]

Taking \( \hbar = 1 \) in the natural unit, the distributions \( P(p_x^{(\alpha)}) \) with different values of \( \alpha \) are shown in Fig.3. We see the width of the distribution decreases to its classical limit as \( \alpha \to 0 \), instead of wrong \( \hbar \to 0 \).

### 2.2 Interference of nanoparticles from a double slit

Likewise, as shown in Fig.2(b), the normalized function of the double slit is

\[ \Psi(x) = \frac{1}{\sqrt{100}}, \quad -75 < x < -25, \quad 25 < x < 75 \quad (10) \]

\[ \Psi(x) = 0, \quad |x| > 75, \quad |x| < 25 \quad (11) \]

The normalized momentum distributions of the nanoparticle with different values of \( \alpha \) in the double slit interference are calculated in the same way as above for the single slit. The distributions \( P(p_x^{(\alpha)}) \) are shown in Fig.4. We see the width of the distribution decreases to its classical limit as \( \alpha \to 0 \). Clearly, the diffraction of nanoparticles from a grating can be calculated in the same way.
Figure 3: The normalized momentum distributions $P(p_x^{(\alpha)})$ of the nanoparticle in the single slit diffraction with different effective screening mass parameters $\alpha$.

Figure 4: The normalized momentum distribution $P(p_x^{(\alpha)})$ of the nanoparticle in the double slit interference with different effective screening mass parameters $\alpha$. 
The patterns of the single slit diffraction and double slit interference can be calculated from the momentum distributions if the momentum \((mv)\) of the nanoparticle and the distance between the slit screen and the detector screen are given.

3 Nanoparticle inside an infinite square potential well

Consider an infinite square potential well of width \(L\), that is, the potential function

\[ V(x) = 0, \quad 0 < x < L \]

and

\[ V(x) = \infty, \quad x \leq 0, \quad x \geq L \]

As seen in any quantum mechanics textbooks, the quantized energy and normalized wave function of a particle of mass \(m\) in the well are

\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \ldots \]

\[ \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \]

The Fourier transformation of Eq.15 yields the momentum wave functions

\[ \phi_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left(-\frac{ipx}{\hbar}\right)\psi_n(x)dx \]

Now, for a nanoparticle with the ESMP \(\alpha\), let \(p'\) denote the momentum of the effective screening layer. Substituting \(p'/\alpha\) for \(p\) into Eq.16 yields

\[ \Theta_n(p', \alpha) = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left(-\frac{i\alpha p'x}{\hbar}\right)\psi_n(x)dx \]

Thus, we have the normalized momentum distribution

\[ Q_n(p', \alpha) = \frac{|\Theta_n(p', \alpha)|^2}{\int |\Theta_n(p', \alpha)|^2 dp'} \]

The total momentum \(p\) of the nanoparticle consists of the quantum part \(p'\) and classical part \(\pm (1 - \alpha)n\pi\hbar/L\), that is,

\[ p = p' + \left(\frac{p'}{|p'|}\right)(1 - \alpha)n\pi\hbar/L \]
Let $Q^{(\alpha)}(p)$ denote the normalized momentum distribution of the nanoparticle with respect to $p$. It can be obtained from $Q_n(p',\alpha)$ by making use of the translation $p' \rightarrow p$. As an illustration example, taking $\hbar = 1$ in the natural unit and $L = 1$, the momentum distributions $Q^{(\alpha)}_2(p)$ are calculated and shown in Fig.5. We see the distribution approaches to the classical limit $p \rightarrow \pm 2\pi \hbar / L$ as $\alpha \rightarrow 0$.

![Figure 5: The normalized momentum distributions $Q^{(\alpha)}_2(p)$ of the nanoparticle inside the infinite square potential well with different effective screening mass parameters $\alpha$.](image)

### 4 Tunnelling of nanoparticles

With regard to tunnelling effects, we consider a particle with momentum $Mv$ and kinetic energy $E = Mv^2/2$ passing through or over a one-dimensional square potential barrier of height $U_0$ and thickness $L$. According to quantum mechanics, its wave function can be split into three parts:

$$\psi(x) = \exp(ikx) + \sqrt{\rho_0} \exp(-ikx), \quad x < 0, \quad k = \frac{\sqrt{2ME}}{\hbar} (20)$$

$$\psi(x) = A \exp(i\kappa x) + B \exp(-i\kappa x), \quad 0 \leq x \leq L, \quad \kappa = \frac{\sqrt{2M(E-U_0)}}{\hbar} (21)$$
\[ \psi(x) = \sqrt{\tau} \exp(ik), \quad x > L \]  

(22)

As seen in any quantum mechanics textbooks, for the case where \( E > U_0 \), the transmission coefficient is

\[ \tau = [1 + \frac{U_0^2}{4E(E-U_0)} \sin^2\left(\sqrt{\frac{2M(E-U_0)L}{\hbar}}\right)]^{-1} \]  

(23)

and for \( E < U_0 \), substituting \( ik \) for \( \kappa \) into Eq.21, the transmission coefficient is

\[ \tau = [1 + \frac{U_0^2}{4E(U_0-E)} \sinh^2\left(\sqrt{\frac{2M(U_0-E)L}{\hbar}}\right)]^{-1} \]  

(24)

The reflection coefficient is

\[ \rho = 1 - \tau \]  

(25)

Now we are going to calculate the transmission coefficient and reflection coefficients of a nanoparticle with the ESMP \( \alpha \). Since the momentum of the effective screening layer is \( k^{(\alpha)}\hbar = \alpha k\hbar \) outside the barrier and \( \kappa^{(\alpha)}\hbar = \alpha \kappa\hbar \) inside the barrier, we have to substitute \( k^{(\alpha)}/\alpha \) for \( k \) and \( \kappa^{(\alpha)}/\alpha \) for \( \kappa \) into the wave functions. Clearly the substitution is equivalent to substituting \( \alpha \hbar \) for \( \hbar \). So, for the case where \( E > U_0 \), we obtain the transmission coefficient

\[ \tau_\alpha = [1 + \frac{U_0^2}{4E(E-U_0)} \sin^2\left(\sqrt{\frac{2M(E-U_0)L}{\alpha \hbar}}\right)]^{-1} \]  

(26)

and for \( E < U_0 \), similarly, we have

\[ \tau_\alpha = [1 + \frac{U_0^2}{4E(U_0-E)} \sinh^2\left(\sqrt{\frac{2M(U_0-E)L}{\alpha \hbar}}\right)]^{-1} \]  

(27)

The reflection coefficient is

\[ \rho_\alpha = 1 - \tau_\alpha \]  

(28)

For example, for the case where \( E = 1 \) and \( U_0 = 2 \), taking \( L = 1 \) and \( M = 0.1, 0.5, 1.0 \), the transmission coefficient curves \( \tau(\alpha, M) \) are shown in Fig.6(a). If taking \( M = 1.0 \) and \( L = 0.1, 0.5, 1.0 \), the curves \( \tau(\alpha, L) \) are shown in Fig.6(b). Here we have taken \( \hbar = 1 \) in the natural unit. We see the transmission coefficients approach to their classical limits as \( \alpha \to 0 \).
Figure 6: Transmission coefficients of the nanoparticle dependent on $\alpha$ for the case where $E < U_0$: (a) the curves $\tau(\alpha, M)$ with different values of $M$, (b) the curves $\tau(\alpha, L)$ with different values of $L$.

5 Uncertainty relations for nanoparticles

In 1927, Heisenberg stated: “the more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa.” [6] This rule is known as Heisenberg uncertainty principle. Its physical reasoning has been offered in Ref.[2]. The principle is basically formulated by the relation

$$\triangle p_x \triangle x \geq \frac{\hbar}{2}$$

(29)

Now, for a nanoparticle with the ESMP $\alpha$, since $\triangle p_x^{(\alpha)} = \alpha \triangle p_x$ as seen from Fig.1(b), the Heisenberg relation becomes

$$\triangle p_x^{(\alpha)} \triangle x = \triangle p_x \alpha \triangle x \geq \frac{\alpha \hbar}{2}$$

(30)

Figs.3-6 illustrate the momentum uncertainty of nanoparticles, which decreases with decreasing $\alpha$. We would have similar energy-time, angle momentum-angle and other uncertainty relations. Thus the Heisenberg uncertainty principle is in some degree dependent on $\alpha$ applicable to nanoparticles and completely unapplicable to macroscopic objects. The fact that the momentum and position are exactly measurable in classical physics reflects the limit $\alpha \to 0$, instead of wrong limit $\hbar \to 0$. It is a logical mistake to regard $\hbar$ as a variable instead of a definite constant.
6 Conclusion

We have calculated the momentum distributions of nanoparticles in diffraction and interference dependent on the effective screening mass parameter or size parameter and presented the calculations for a nanoparticle inside an infinite square potential well and for a tunnelling nanoparticle through a square potential barrier. These results display the transition from quantum to classical mechanics and the simultaneous wave-particle duality of nanoparticles. The concept that the effective screening effect increases with increasing size of an object paves way for development of nanomechanics and nanotechnology.

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