Universal Formula for the Expectation Value of the Radial Operator under the Aharonov-Bohm Flux and the Coulomb Field

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A useful and universal formula for the expectation value of the radial operator in the presence of the Aharonov-Bohm flux and the Coulomb field is established. We find that the expectation value \( \langle r^\lambda \rangle \) \((-\infty \leq \lambda \leq \infty\) is greatly affected due to the non-local effect of the magnetic flux although the Aharonov-Bohm flux does not have any dynamical significance in classical mechanics. In particular, the quantum fluctuation increases in the presence of the magnetic flux due to the Aharonov-Bohm effect. In addition, the Virial theory in quantum mechanics is also constructed for the spherically symmetric system under the Aharonov-Bohm effect.

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I. INTRODUCTION

The calculation of the expectation values \( \langle r^\lambda \rangle \) with different power \( \lambda \) of the radial operator \( \hat{r} \) is important in the Hellmann-Feynman theory \( [2] \), the interactions of the molecular theory \( [3] \), and the quantum chemistry \( [4,5,6,7] \). On the other hand, the Aharonov-Bohm (AB) effect, a topological non-local physical significance at the quantum level, has shed light on the understanding of the phenomenon of the fractional quantum Hall effect \( [8,9,10,11] \), the superconductivity \( [11,12] \), and the repulsive Bose gases \( [13] \) in the last 20 years. It is known that the global influence of the AB effect affects all charged particle’s systems \( [14] \). In this paper, we will derive a recurrence formula for the expectation value \( \langle r^\lambda \rangle \) \((-\infty \leq \lambda \leq \infty\) of the radial operator \( \hat{r} \) in the presence of the Coulomb field under the Aharonov-Bohm effect (ABC). Moreover, the Virial theory in quantum mechanics will also be generalized to the system with spherical symmetry under the AB flux. The general effect of the AB flux to the expectation value will also be discussed in this paper.

The fixed-energy bare Green’s function \( G_0(r,r';E) \) for a charged particle with mass \( m \) propagating from \( r' \) to \( r \) satisfies the Schrödinger equation

\[
\left[ E - \hat{H}_0(r, \frac{\hbar}{i} \nabla) \right] G_0(r, r'; E) = \delta^3(r - r').
\] (1.1)

Here the Hamiltonian of the system is given by \( \hat{H}_0 = -\hbar^2\nabla^2/2m + V(r) \). The angular decomposition of the Green’s function can be written as

\[
G_0(r, r'; E) = \sum_{l=0}^{\infty} \sum_{k=-l}^{l} G^0_l(r, r'; E) Y_lk(\theta, \varphi) Y_{lk}(\theta', \varphi'),
\] (1.2)

in the spherically symmetric system with \( Y_lk \) the well-known spherical harmonics. Hence the left hand side of the Eq. (1.1) can be reduced to the following form:

\[
\left\{ E - \sum_{l=0}^{\infty} \sum_{k=-l}^{l} \left[ \frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2mr^2} \right] - V(r) \right\} \times G^0_l(r, r'; E) Y_lk(\theta, \varphi) Y_{lk}(\theta', \varphi').
\] (1.3)

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II. RADIAL WAVE EQUATION FOR A CHARGED PARTICLE IN A MAGNETIC FIELD

For a charged particle in a magnetic field, the charged Green’s function \( G \) is related to the bare Green’s function \( G^0 \) by the following equation:

\[
G(\mathbf{r}, \mathbf{r}'; E) = G^0(\mathbf{r}, \mathbf{r}'; E)e^{\frac{i\pi}{2}\int_{\mathbf{r}'} A(\mathbf{r})d\mathbf{r}},
\]

(2.1)

with a globally path-dependent nonintegrable phase factor \( A(\mathbf{r}) \) given above. Here the vector potential \( A(\mathbf{r}) \) is used to represent the contribution from the magnetic field. For the Aharonov-Bohm magnetic flux under consideration, the vector potential can be written as

\[
A(\mathbf{x}) = \begin{cases} \frac{1}{2} B \rho \hat{e}_\varphi & (\rho < \epsilon) \\ \frac{1}{2} B \rho^2 \hat{e}_\varphi = \frac{\varphi}{2\pi\rho} \hat{e}_\varphi & (\rho > \epsilon) \end{cases}.
\]

(2.2)

Here the two-dimensional radial length square is defined as \( \rho^2 = x^2 + y^2 \). Moreover, \( \hat{e}_\varphi \) is the unit vector of the coordinate \( \varphi \) and \( \epsilon \) is the radius of region where the magnetic field exists. Hence the total magnetic flux is given by \( \Phi = \pi \epsilon^2 B \). Note that the associated magnetic field lines are confined inside a tube, with radius \( \epsilon \), along the \( z \)-axis. Along the region free of the magnetic field, the path-dependent nonintegrable phase factor is given by \( \exp\{-i\mu_0 \int_{\mathbf{r}'} d\mathbf{r}' \varphi(\mathbf{r}')\} \).

Here we have used the subscript \( k \) to represent the path-dependent nature of the phase factor. In addition, we have denoted \( \varphi(\mathbf{r}') = d\varphi/d\mathbf{r}' \). Moreover, \( \mu_0 = -2eg/\hbar c \) is a dimensionless numerical factor defined by \( \Phi = 4\pi \epsilon \). The minus sign we adopted is a matter of convention. According to the discussion in Ref. [16], only phase factors with closed-loop contour are considered where the description of electromagnetic phenomena are complete. Hence, we have

\[
n = \frac{1}{2\pi} \int_{\mathbf{r}'} d\mathbf{r}' \varphi(\mathbf{r}'),
\]

(2.3)

with integer values \( n \) corresponding to the winding number. The magnetic interaction is therefore a purely topological phenomenon. Therefore the nonintegrable phase factor becomes \( \exp\{ -i\mu_0 (2\pi n) \} \). With the help of equality between the associated Legendre polynomial \( P^m_n(z) \) and the Jacobi function \( P_n^{(\alpha,\beta)}(z) \) \([17,18]\), we find that

\[
P^k(\cos \theta) = (-1)^k \frac{\Gamma(l+k+1)}{\Gamma(l+1)} \left( \cos \frac{\theta}{2} \sin \frac{\theta}{2} \right)^k P^{(k,k)}_{l-k}(\cos \theta).
\]

(2.4)

Therefore the angular part of the Green’s function in the expression (2.3) can be shown to be

\[
\sum_{k=-l}^{l} Y_{ik}(\theta, \varphi)Y_{ik}^{*}(\theta', \varphi') = \sum_{k=-l}^{l} \frac{2l+1 \Gamma(l-k+1)}{4\pi \Gamma(l+k+1)} P^k_l(\cos \theta) P^k_l(\cos \theta') e^{ik(\varphi - \varphi')}
\]

\[
= \sum_{k=-l}^{l} \left[ \frac{2l+1 \Gamma(l-k+1) \Gamma(l+k+1)}{4\pi \Gamma^2(l+1)} \right] \left( \cos \frac{\theta}{2} \cos \frac{\theta'}{2} \sin \frac{\theta}{2} \sin \frac{\theta'}{2} \right)^k \times P^{(k,k)}_{l-k}(\cos \theta) P^{(k,k)}_{l-k}(\cos \theta') e^{ik(\varphi - \varphi')}.
\]

(2.5)

To include the nonintegrable phase factor due to the AB effect, we can rename the index \( l \) into \( q \) related by the relation \( l - k = q \). As a result, Eq. (2.3) can be written as

\[
\left\{ E - \sum_{q=0}^{\infty} \sum_{k=-q}^{q} \left[ -\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{(q+k)(q+k+1)\hbar^2}{2mr^2} \right] - V(r) \right\}
\]

\[
\times G^0_{q+k}(r, r'; E) \left[ \frac{2(q+k)+1 \Gamma(q+1) \Gamma(q+2k+1)}{4\pi \Gamma^2(q+k+1)} \left( \cos \frac{\theta}{2} \cos \frac{\theta'}{2} \sin \frac{\theta}{2} \sin \frac{\theta'}{2} \right)^k \right]
\]

(2.6)
Hence, the corresponding radial wave equation reads

\[ \times P_q^{(k,k)}(\cos \theta) P_q^{(k,k)}(\cos \theta') e^{i k (\varphi - \varphi')} . \]  

(2.6)

In addition, the nonintegrable phase factor \( \exp \{ -i \mu_0 (2n\pi) \} \) can thus be included with the help of the Poisson’s summation formula (p.124, \[15\])

\[ \sum_{k=-\infty}^{\infty} \sum_{q=0}^{\infty} \frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{(q + |k + \mu_0|)(q + |k + \mu_0| + 1)\hbar^2}{2mr^2} \right] - V(r) \right\}

\times G_{q+\frac{1}{2}}(r',r'; E) \left[ \frac{2(q + |k + \mu_0| + 1) \Gamma (q + 1) \Gamma (2|k + \mu_0| + q + 1)}{4\pi \Gamma^2 (|k + \mu_0| + q + 1)} \right] \right) \right] e^{i k (\varphi - \varphi')} \]

\times (\cos \theta/2 \cos \theta'/2 \sin \theta/2 \sin \theta'/2) |^{k+\mu_0} P_q^{(k+\mu_0,|k+\mu_0|)}(\cos \theta) P_q^{(k+\mu_0,|k+\mu_0|)}(\cos \theta') .  

(2.8)

\[ \delta (\Omega - \Omega') = \sum_{l=0}^{\infty} \sum_{k=-l}^{l} Y_{lk}(\theta, \varphi) Y_{lk}^*(\theta', \varphi') . \]

(2.10)

Therefore, for the set of the fixed quantum numbers \((q, k)\) one can show that the radial Green’s function satisfies

\[ \left\{ E - \left[ \frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{(q + |k + \mu_0|)(q + |k + \mu_0| + 1)\hbar^2}{2mr^2} \right] - V(r) \right\}

\times G_{q+\frac{1}{2}}(r',r'; E) = \delta (r-r') . \]

(2.11)

Hence, the corresponding radial wave equation reads

\[ \frac{\hbar^2}{2m} \frac{d^2}{dr^2} u_\alpha (r) + \left[ E - \left( V(r) + \frac{\hbar^2}{2m} \frac{\alpha (\alpha + 1)}{r^2} \right) \right] u_\alpha (r) = 0 , \]

(2.12)

where we have set \( \alpha = q + |k + \mu_0| \), and \( u_\alpha (r) = r R_\alpha (r) \). It is clear that \( R_\alpha \) satisfies the spherical Bessel equation

\[ \left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left( \kappa^2 - U(r) - \frac{\alpha (\alpha + 1)}{r^2} \right) \right] R_\alpha (r) = 0 \]

(2.13)
with the definition \( \kappa = \sqrt{2mE/\hbar^2} \) and the reduced potential \( U(r) = 2mV(r)/\hbar^2 \). For simplicity, we have written \( R_{n\alpha}(r) \) instead of \( R_{n,q,k}(r) \) in which each set \((n,q,k)\) denote a quantum state. Hence the AB effect reflects itself by the coupling to the angular momentum in the radial Green’s function, which turns the integer quantum number to a fractional one.

In order to derive the expectation value \( \langle r^\lambda \rangle \) in an arbitrary quantum state \((n,q,k)\) of the ABC system, one notes that the attractive potential of the Coulomb field is given by \( V(r) = -Ze^2/r \) in which \( Ze \) is the total charge at the center of source and \(-e\) representing the charge of the electron. One can show that the exact solution of the energy spectra in this case is given by \[20,23\]

\[
E_{n,q,k} = -\frac{Z^2e^2}{2a_0[n + q + |k + \mu_0| + 1]^2},
\]

(2.14)

where \( a_0 = \hbar^2/me^2 \) is the Bohr radius, and the ranges of the quantum number are \( n, q = 0, 1, 2, \ldots \), and \(-\infty < k < \infty \). With the help of the result, Eq. (2.12) can be brought to the following form:

\[
\frac{d^2}{dr^2}u(r) + \left[ \frac{2Z}{a_0r} - \frac{\alpha(\alpha + 1)}{r^2} - \left( \frac{Z}{\hbar a_0} \right)^2 \right] u(r) = 0.
\]

(2.15)

### III. Recurrence Formula for the Expectation Value of the Radial Operator of the Aharonov-Bohm-Coulomb System

For simplicity, we have written \( u(r) \) instead of \( u_n(r) \), and \( \tilde{n} = [n + q + |k + \mu_0| + 1] \). For our purpose of calculating the diagonal matrix element, we will multiply \( r^\lambda u \) to both sides of the above equation. Integrating this equation with respect to \( r, \int_0^\infty \cdots dr \), one derives

\[
\int_0^\infty r^\lambda u \left( \frac{d^2}{dr^2}u \right) dr - \alpha(\alpha + 1) \langle r^{\lambda-2} \rangle + \frac{2Z}{a_0} \langle r^{\lambda-1} \rangle - \left( \frac{Z}{\tilde{n}a_0} \right)^2 \langle r^\lambda \rangle = 0.
\]

(3.1)

With the help of integration by part, the first term yields

\[
\int_0^\infty r^\lambda u \left( \frac{d^2}{dr^2}u \right) dr = r^\lambda u \left( \frac{d}{dr}u \right)_0^\infty - \int_0^\infty \left( r^\lambda \frac{d}{dr}u + \lambda r^{\lambda-1}u \right) \left( \frac{d}{dr}u \right) dr
\]

\[
= \left[ r^\lambda u \left( \frac{d}{dr}u \right) - \frac{\lambda}{2} r^{\lambda-1}u \right]_0^\infty + \frac{\lambda(\lambda - 1)}{2} \langle r^{\lambda-2} \rangle - \int_0^\infty r^\lambda \left( \frac{d}{dr}u \right)^2 dr.
\]

(3.2)

One can show that the asymptotic behavior of the wave function is given by \[18,22\]

\[
r \to 0, \quad u \sim r^{\alpha+1} \]

\[
r \to \infty, \quad u \sim \tilde{n} e^{-Zr/\tilde{n}a_0}
\]

(3.3)

directly from the asymptotic wave equation. Therefore, one has the necessary and sufficient condition to guarantee the vanishing of the first part of the Eq. (3.2)

\[
r^\lambda u \left( \frac{d}{dr}u \right)_0^\infty = 0, \quad r^{\lambda-1} u_0^\infty = 0,
\]

(3.4)

as long as \( \lambda > -(2\alpha + 1) \). Therefore

\[
\left[ \frac{\lambda(\lambda - 1)}{2} - \alpha(\alpha + 1) \right] \langle r^{\lambda-2} \rangle + \frac{2Z}{a_0} \langle r^{\lambda-1} \rangle - \left( \frac{Z}{\tilde{n}a_0} \right)^2 \langle r^\lambda \rangle = \int_0^\infty r^\lambda \left( \frac{d}{dr}u \right)^2 dr.
\]

(3.5)

Similarly, let’s multiply \( 2r^{\lambda+1} du/dr \) to the both sides of the Eq. (2.15) and then integrate over \( \int_0^\infty \cdots dr \). One can thus derive the following equations:
\[
\int_0^\infty 2r^{\lambda+1} \left( \frac{d}{dr}u \right) \left( \frac{d^2}{dr^2}u \right) dr = r^{\lambda+1} \left( \frac{d}{dr}u \right)^2 \bigg|_0^\infty - \int_0^\infty (\lambda + 1)r^\lambda \left( \frac{d}{dr}u \right)^2 dr, \tag{3.6}
\]
\[
\int_0^\infty 2r^{\lambda+1}u \left( \frac{d}{dr}u \right) dr = r^{\lambda+1}u^2\bigg|_0^\infty - (\lambda + 1) \langle r^\lambda \rangle. \tag{3.7}
\]

One can also derive similar equations with the power factor \(\lambda + 1\) replaced by \(\lambda\) or \(\lambda - 1\) in above equation. According to the equation (3.4), the first terms in the rhs of the Eq.s (3.6)-(3.7) all vanishes. Hence, we obtain

\[
(\lambda - 1)\alpha(\alpha + 1) \langle r^{\lambda-2} \rangle - 2\lambda \frac{Z}{a_0} \langle r^{\lambda-1} \rangle + (\lambda + 1) \left( \frac{Z}{\hbar a_0} \right)^2 \langle r^\lambda \rangle = (\lambda + 1) \int_0^\infty r^{\lambda} \left( \frac{d}{dr}u \right)^2 \, dr. \tag{3.8}
\]

Eliminating the term on the rhs of the above equation with the help of the equation (3.11), we finally obtain the general recurrence formula for the ABC system

\[
\frac{\lambda + 1}{n^2} \langle r^\lambda \rangle - (2\lambda + 1) \frac{a_0}{Z} \langle r^{\lambda-1} \rangle + \frac{\lambda}{4} \left( (2\alpha + 1)^2 - \lambda^2 \right) \left( \frac{a_0}{Z} \right)^2 \langle r^{\lambda-2} \rangle = 0. \tag{3.9}
\]

This formula provides a very convenient tool to calculate the expectation value of the radial operator \(\hat{r}^\lambda\) for arbitrary power \(\lambda\) in any arbitrary quantum state \((n, q, k)\) for the ABC system without facing the complication computing the wave functions directly. For example, let’s calculate a few leading terms of the expectation value of the radial operator. First of all, one can set \(\lambda = 0\) where the recurrence formula (3.9) gives

\[
\left\langle \frac{1}{r} \right\rangle_{n,q,k} = \frac{Z}{\tilde{n}^2 a_0} = \frac{Z}{(n + q + |k + \mu_0| + 1)^2 a_0}. \tag{3.10}
\]

Note that the effect of the magnetic flux leads to the decrease of the expectation value of the potential. Note that this effect has no correspondence in classical system. Moreover, if we choose \(\lambda = 1, 2\), one will instead derive

\[
\left\langle r \right\rangle_{n,q,k} = \frac{1}{2} \left[ 3\tilde{n}^2 - \alpha(\alpha + 1) \right] \frac{a_0}{Z}, \\
\left\langle r^2 \right\rangle_{n,q,k} = \frac{\tilde{n}^2}{2} \left[ 1 + 5\tilde{n}^2 - 3\alpha(\alpha + 1) \right] \left( \frac{a_0}{Z} \right)^2. \tag{3.11}
\]

These results show that the magnetic flux effect will increase the expectation of the radial operator such as the case where the quantum states given by \((n, q, k)\) = \((0, 0, 0)\). Indeed, one can show that

\[
\left\langle r \right\rangle_{0,0,0} = \frac{1}{2} \left[ 2 |\mu_0|^2 + 5 |\mu_0| + 3 \right] \frac{a_0}{Z}, \\
\left\langle r^2 \right\rangle_{0,0,0} = \frac{(|\mu_0| + 1)^2}{2} \left[ 2 |\mu_0|^2 + 7 |\mu_0| + 6 \right] \left( \frac{a_0}{Z} \right)^2. \tag{3.12}
\]

Note that these results reduce to the well-known pure Coulomb system, where \(\mu_0 = 0\), \(\left\langle r \right\rangle_{0,0,0} = 3a_0/2Z\), and \(\left\langle r^2 \right\rangle_{0,0,0} = 3(a_0/Z)^2\) where the nonlocal effect of the magnetic flux in the physical average becomes manifest in these formulæ.

According to the definition leading to the Eq. (2.13), we have \(\alpha_{\text{max}} = (q + |k + \mu_0|)_{\text{max}} = \tilde{n} - 1\) corresponding to the nodes of the wave function at \(n = 0\) for the modified circular Bohr orbit. In this case, the radial wave function reduces to [18]

\[
u_{0,q,k}(r) = r R_{0,q,k}(r) = r^{\tilde{n}} e^{-Zr/\tilde{n}a_0}. \tag{3.13}
\]

Hence we can calculate the most possible position of the radius \(r_{\text{most}}\), defined as the position where the probability function \(|u|^2\) attains its maximal, given by \(d\nu_{0,q,k}(r = r_{\text{most}})/dr = 0\). The result indicates that

\[
r_{\text{most}} = \frac{\tilde{n}^2 a_0}{Z}. \tag{3.14}
\]

for the most possible position of the radius. It is clear that the presence of the magnetic flux increases the value of the most possible position. On the other hand, Eq. (3.11) gives the following radial expectation value, when \(\alpha\) is equal to \(\alpha_{\text{max}}\).
\begin{equation}
\langle r \rangle_{0,n-1} = \left[ \tilde{n}^2 + \frac{\tilde{n}}{2} \right] \frac{a_0}{Z}
\end{equation}

Therefore quantum mechanical average (the expectation value) for the radius of the modified Bohr orbit is bigger than the most possible position of the radius. In addition, the position fluctuation is given by

\begin{equation}
(\Delta r)_{0,n-1} = \sqrt{\langle r^2 \rangle_{0,n-1} - \langle r \rangle_{0,n-1}^2} = \sqrt{\left[ \frac{\tilde{n}^3}{2} + \frac{\tilde{n}^2}{4} \right] \frac{a_0}{Z}}
\end{equation}

which implies the increase of the quantum fluctuation due to the increase of the magnetic flux. Consequently, one can derive the ratio between the fluctuation and the corresponding average

\begin{equation}
\frac{(\Delta r)_{0,n-1}}{\langle r \rangle_{0,n-1}} = \frac{1}{\sqrt{2\tilde{n} + 1}}
\end{equation}

which indicates that the quantum mechanical result tends to approach the Bohr picture of orbit quantization as \( \tilde{n} \) increases or equivalently the magnetic flux increases.

If we choose \( \lambda = -1, -2 \), the recurrence relation indicates that

\begin{align*}
\langle r^{-3} \rangle_{n,q,k} &= \frac{a_0/Z}{\alpha(\alpha + 1)(a_0/Z)^2} \langle r^{-2} \rangle_{n,q,k} = \frac{1}{\tilde{n}^3\alpha(\alpha + 1/2)(\alpha + 1)} \left( \frac{Z}{a_0} \right)^3, \\
\langle r^{-4} \rangle_{n,q,k} &= \frac{3\tilde{n}^2 - \alpha(\alpha + 1)}{2\tilde{n}^3(\alpha - 1/2)(\alpha + 1/2)(\alpha + 1)(\alpha + 3/2)} \left( \frac{Z}{a_0} \right)^3.
\end{align*}

Here we have used the result

\begin{equation}
\langle r^{-2} \rangle_{n,q,k} = \frac{1}{\tilde{n}^3(\alpha + 1/2)} \left( \frac{Z}{a_0} \right)^2,
\end{equation}

which is the only moment can not be derived from the recurrence Eq. (3.9). It can, however, be derived from the well-known Hellmann-Feynman formula

\begin{equation}
\frac{\partial E_{n,q,k}}{\partial \alpha} = \langle \Psi_{n,q,k} \left| \frac{\partial \hat{H}}{\partial \alpha} \right| \Psi_{n,q,k} \rangle,
\end{equation}

where the Hamiltonian operator is given by

\begin{equation}
\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{\alpha(\alpha + 1)}{r^2} - \frac{Ze^2}{r}.
\end{equation}

It hence follows that

\begin{equation}
\frac{\partial E_{n,q,k}}{\partial \alpha} = (\alpha + 1) \frac{\hbar^2}{m} \langle r^{-2} \rangle_{n,q,k}.
\end{equation}

With the help of the Eq. (2.14), one derives the result shown in Eq. (3.20). This result gives us the ratio information of the modified centrifugal potential in quantum mechanics, namely,

\begin{equation}
\frac{\alpha(\alpha + 1)\hbar^2}{2mr^2} \bigg|_{n,q,k} = -\frac{\alpha(\alpha + 1)}{(\alpha + 1/2)\tilde{n}} E_{\tilde{n}}.
\end{equation}

Since the total kinetic energy of the system equals \( < \hat{T} >_{n,q,k} = -E_{\tilde{n}} \) (see appendix for details), the ratio of the centrifugal potential to the total kinetic energy, \( r_c = < V_c > / < T > \), is

\begin{equation}
r_c = \alpha(\alpha + 1)/[\alpha + 1/2] \tilde{n}.
\end{equation}

This result indicates that, for fixed \( \tilde{n} \), the increase of the intensity of the magnetic flux induces the increase of the ratio \( r_c \) and thus the weight of the centrifugal potential. When \( \alpha \) is equal to \( \alpha_{\text{max}} = \tilde{n} - 1 \) corresponding to the modified Bohr orbit case, the ratio \( r_c \) become
On the other hand, the ratio of the average of the radial kinetic energy to the total kinetic energy, \( r_r = \langle \frac{p_r^2}{2m} \rangle_{0,q,k} = \frac{1}{2\tilde{n} - 1} \) \( \frac{\tilde{n} - 1/2}{\tilde{n} - 1} \), is given by
\[
(3.26)
\]

at the limit \( \alpha = \alpha_{\text{max}} \). Therefore when \( \tilde{n} \gg 1 \), the radial kinetic energy will become very small reproducing the classical result.

In addition, one can also discuss the effect of the magnetic flux in the well-known formulae introduced by J. Schwinger [21]. It was shown that
\[
\langle dV/dr \rangle = \frac{2\pi\hbar^2}{m} |\Psi(0)|^2, \quad l = 0
\]
\[
\langle dV/dr \rangle = \frac{l(l+1)\hbar^2}{m} \langle \frac{1}{r^3} \rangle, \quad l \neq 0.
\]
\[
(3.27)
\]

These results are very useful and of considerably general interest for the study of the bound states in a system with a central potential. The first identity relates the \( s \)-wave wave function at the origin to the gradient of the potential. This identity comes explicitly with the Planck constant \( \hbar \) indicating the significance of the quantum effect. Therefore there is no classical correspondence. The second identity is, however, a generalization of the quantum effect of an important classical theory
\[
\langle dV/dr \rangle_{\text{av}} = \frac{l^2}{m} \langle \frac{1}{r^3} \rangle_{\text{av}},
\]
\[
(3.28)
\]

where \( (f)_{\text{av}} \) represents the average of the periodic function \( f(t) \) over a classical period. Eq. (3.28) states that the average of a external force equals to the average of the centripetal force over the classical period.

In the presence of the magnetic flux, the Hamilton operator is given by
\[
\hat{H} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\alpha(\alpha + 1)\hbar^2}{2mr^2} + V(r).
\]
\[
(3.29)
\]

Computing the commutator of the operators \( \partial/\partial r \) and \( \hat{H} \), one has
\[
\left[ \frac{\partial}{\partial r}, \hat{H} \right] = \frac{\hbar^2}{mr^2} \frac{\partial}{\partial r} - \frac{\alpha(\alpha + 1)\hbar^2}{m r^3} + \frac{dV}{dr}.
\]
\[
(3.30)
\]

Evaluating the expectation value with respect to an arbitrary bound state which makes the contribution from the lhs vanished, we would have
\[
\langle \frac{dV}{dr} \rangle - \alpha(\alpha + 1)\hbar^2 \langle \frac{1}{r^3} \rangle = -\frac{\hbar^2}{m} \langle \frac{1}{r^3} \rangle \frac{\partial}{\partial r} \Psi
\]
\[
= -\frac{\hbar^2}{m} \int r^2 dr d\Omega \Psi^* \frac{1}{r} \frac{\partial}{\partial r} \Psi,
\]
\[
(3.31)
\]

with \( d\Omega \) the solid angle. Since the mean value in the lhs of the above equation is a real number, so does the rhs of the above equation. Hence one has
\[
\int dr \Psi^* \frac{\partial}{\partial r} \Psi = \int dr \Psi \frac{\partial}{\partial r} \Psi^* = \frac{1}{2} \int dr \frac{\partial}{\partial r} (\Psi \Psi^*) = \frac{1}{2} \Psi \Psi^* \bigg|_0^\infty = 0.
\]
\[
(3.32)
\]

In deriving the above equations, we have used the following facts: (1) the wave function of the bound state vanishes at the region \( r \to \infty \); (2) in the presence of the magnetic flux, the vanishing of the wave function \( \Psi(0) = 0 \) holds at the origin [22]. To prove the second proposition, one notes that the asymptotic form of the wave function can be shown to be [22]
The AB effect can be introduced by the similar procedure leading to the Eqs. (2.7) near the origin in the presence of the magnetic flux. Because that $u_α(r) = rR_α(r)$, one has immediately that $u_α'(r) = R_α(r) + rR_α'(r)$. Therefore we obtain $u_α'(0) = R_α(0)$. In addition, Eq. (3.33) says that $u_α'(r) = (α + 1)r^α$ implying that $u_α'(0) = 0$. This proves the second proposition that $Ψ(0) = 0$.

Accordingly, in a central force system with a magnetic flux, one can generalize the Schwinger theorem (3.27) to the following form:

$$\left\langle \frac{dV}{dr} \right\rangle_{n,q,k} = \frac{α(α + 1)\hbar^2}{m} \left\langle \frac{1}{r} \right\rangle_{n,q,k}. \quad (3.34)$$

In addition, the s-wave no longer exists in the presence of the magnetic flux, there is no corresponding generalization of the first identity in the Eq. (3.27). On the other hand, we find that the topological effect of the magnetic flux has a generalized quantum mechanical shown in Eq. (3.27) although such effect does not have any dynamical significance in classical mechanics.

IV. CONCLUSION

We have derived a general recurrence formula of the expectation value of the radial operator with different power for an Aharonov-Bohm-Coulomb system providing us a convenient method to compute the average of the radial operator in any power. With this useful recurrence formula, one can avoid tedious and complicate integration with the wave functions. The useful formulae and techniques shown in this paper have many interesting applications in the study of many physical systems in the presence of a magnetic field. For example, we have shown the generalized theorem of Schr¨odinger for bound state system under the influence of a magnetic field.

In addition, the two dimensional (2D) system is important in the fractional quantum Hall effect and the high-$T_c$ superconductivity, we will also generalize our result to the 2D system at the end of this paper. Two dimensional central force quantum system is governed by the radial Schr¨odinger equation:

$$\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} \right] - \frac{k^2}{\rho^2} + V(\rho) \right\} R_{nk} = ER_{nk}, \quad (4.1)$$

where $\rho$ is the corresponding radial length in 2D, i.e. $\rho = \sqrt{x^2 + y^2}$. The corresponding total wave functions is given by $Ψ(\rho, \varphi) = R_{nk}(\rho)e^{ik\varphi}$ with the range of the quantum number specified by $k = 0, ±1, ±2, …$. In addition, the energy spectra $E$ depends on $|k|$ and the wave function $R_{n|k|}$ corresponding to the energy level $E_{n|k|}$ satisfies the orthonormal condition

$$\int_0^∞ dp R_{n|k|}^*(\rho)R_{n'|k|}(\rho) = δ_{nn'}. \quad (4.2)$$

If we perform a transformation $R_{n|k|}(\rho) = \chi_{n|k|}(\rho)/\sqrt{\rho}$, Eq. (4.1) will reduce to

$$\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{d\rho^2} + \frac{(k - 1/2)(k + 1/2)}{\rho^2} \right] + V(\rho) \right\} \chi_{n|k|}(\rho) = E\chi_{n|k|}(\rho). \quad (4.3)$$

The AB effect can be introduced by the similar procedure leading to the Eqs. (2.7)~(2.13). The result is

$$\left\{ -\frac{\hbar^2}{2m} \left[ \frac{d^2}{d\rho^2} + \frac{1}{2}(\tilde{α} - 1/2)(\tilde{α} + 1/2) \right] + V(\rho) \right\} \chi_{n|k|}(\rho) = E\chi_{n|k|}(\rho), \quad (4.4)$$

where we have defined $\tilde{α} = |k + μ₀|$. Comparing this equation with Eq. (2.13), one finds that results derived for the 3D system can be generalized to the 2D system with the parameters $α$ and $\tilde{α}$ related by the following relation

$$α(α + 1) \leftrightarrow (\tilde{α} - 1/2)(\tilde{α} + 1/2), \quad (4.5)$$

or simply

$$α \leftrightarrow (\tilde{α} - 1/2).$$
For example, we find that the energy spectra of the 2D ABC system is given by

\[ E_{n,\tilde{\alpha}} = -\frac{Z^2 e^2}{2a_0 \left| n + |k + \mu_0| + 1/2 \right|^2} = \frac{Z^2 e^2}{2a_0 \tilde{\alpha}_0^2}. \]  

(4.6)

This exact formula agrees with the previous result obtained in Ref. [23]. In addition, one can also derive some useful and important expectation values for the 2D ABC system:

\[ \langle \frac{1}{\rho} \rangle_{n,k} = \frac{Z}{\tilde{\alpha}} a_0, \]  

(4.7)

\[ \langle \frac{1}{\rho^2} \rangle_{n,k} = \frac{1}{\tilde{\alpha} a_0} \left( \frac{Z}{a_0} \right)^2, \]  

(4.8)

\[ \langle \frac{1}{\rho^3} \rangle_{n,k} = \frac{1}{\tilde{\alpha}^2 (\tilde{\alpha} - 1/2) (\tilde{\alpha} + 1/2)} \left( \frac{Z}{a_0} \right)^3. \]  

(4.9)

Generalization to many other cases are straightforward following similar procedures.

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V. APPENDIX

In the appendix, we shall prove the Virial theorem for the spherically symmetric system under an AB magnetic flux. The Hamiltonian for the spherically symmetric system under an AB magnetic flux is given by the Eq. (2.13)

\[ \hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\alpha(\alpha + 1)\hbar^2}{2m r^2} + V(r), \]  

(5.1)

where the Hermite operator is defined as

\[ \hat{p}_r = \hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) = \hat{p}_r^\dagger. \]  

(5.2)

To obtain the Virial theorem, one notes that the Heisenberg equations of motion for the position and the momentum operators are

\[ \frac{d\mathbf{r}}{dt} = \frac{1}{i\hbar} \left[ \mathbf{r}, \hat{H} \right] = \nabla_p \hat{H} = \hat{e}_{p_r} \hat{p}_r, \]  

(5.3)

\[ \frac{d\mathbf{p}}{dt} = \frac{1}{i\hbar} \left[ \mathbf{p}, \hat{H} \right] = \nabla_r \hat{H} = \left[ \frac{\alpha(\alpha + 1)\hbar^2}{m r^3} - \frac{dV(r)}{dr} \right] \hat{e}_r, \]  

(5.4)

where \( \hat{e}_{p_r} \) is the unit vector of \( p_r \) in the momentum space. Therefore, we have

\[ \frac{d}{dt} (\mathbf{r} \cdot \mathbf{p}) = \frac{1}{i\hbar} \left[ \mathbf{r} \cdot \mathbf{p}, \hat{H} \right] \]

\[ = \frac{d\mathbf{r}}{dt} \cdot \mathbf{p} + \mathbf{r} \cdot \frac{d\mathbf{p}}{dt} = \frac{\hat{p}_r^2}{m} + \frac{\alpha(\alpha + 1)\hbar^2}{m r^2} - r \frac{dV(r)}{dr}. \]  

(5.5)

Average with respect to the wave functions, we obtain
\[ \left\langle \frac{\hat{p}_r^2}{2m} + \frac{\alpha(\alpha + 1)\hbar^2}{2mr^2} \right\rangle = \frac{1}{2} \left\langle r \frac{dV(r)}{dr} \right\rangle, \]  

(5.6)

where we have used the identity \( \left\langle [\mathbf{r} \cdot \mathbf{p}, \hat{H}] \right\rangle = 0 \). Let us define the total kinetic energy operator as

\[ \hat{T} = \frac{\hat{p}_r^2}{2m} + \frac{\alpha(\alpha + 1)\hbar^2}{2mr^2}. \]  

(5.7)

Hence one can derive the following Virial theorem for the spherically symmetric system under an AB magnetic flux

\[ 2 \left\langle \hat{T} \right\rangle = \left\langle r \frac{dV(r)}{dr} \right\rangle. \]  

(5.8)

In particular, if the potential \( V(r) \) is a homogeneous function of degree \( \nu \), namely \( V(br) = b^\nu V(r) \), the Eq. (5.8) can be shown to be

\[ 2 \left\langle \hat{T} \right\rangle = \nu \left\langle V(r) \right\rangle. \]  

(5.9)

Together with the total energy relation,

\[ \left\langle \hat{T} + V \right\rangle = E_{n,q,k}, \]  

(5.10)

it is easily to show that the relations between the averages of the kinetic and the potential energy, and hence the total energy

\[ \left\langle \hat{T} \right\rangle_{n,q,k} = \frac{\nu}{\nu + 2} E_{n,q,k}, \]  

\[ \left\langle V \right\rangle_{n,q,k} = \frac{2}{\nu + 2} E_{n,q,k}. \]  

(5.11)

For an ABC system (\( \nu = -1 \)), one has \( \left\langle \hat{T} \right\rangle_{n,q,k} = -E_{n,q,k} \), and \( \left\langle V \right\rangle_{n,q,k} = 2E_{n,q,k} \).

[1] H. Hellmann, Acta Physicochimica URSS I, 6, 913 (1935); IV, 2, 225 (1936).
[2] R.P. Feynman, Phys. Rev. 56, 340 (1935).
[3] J.C. Slater, Solid State and Molecular Theory (Wiley, New York, 1975).
[4] B.M. Deb (ed.), The Force Concept in Chemistry ( Van Nostrand Reinhold, New York, 1981).
[5] J.H. Van Vleck, Proc. Roy. Soc. A 143, 679 (1934).
[6] H.A. Bethe and E.E. Salpeter, Encyclopedia of Physics, edited by S. Flügge (Springer, Berlin, 1957, Vol. xxxv, pp. 98-104.
[7] L. Pauling and S. Goudsmit, The Structure of Line Spectra (McGraw-Hill, New York, 1930), p. 32.
[8] Z.F. Ezawa, M. Hotta, and A. Iwazaki, Phys. Rev. D 44, 3906 (1991).
[9] C.A. Trugenberger, Phys. Rev. D 45, 3807 (1992).
[10] R.B. Laughlin, Phys. Rev. B 23, 3383 (1983); F.D.M. Haldane, Phys. Rev. Lett. 51, 605 (1983); B.I. Halperin, Phys. Rev. Lett. 52, 1583 (1984).
[11] Z.F. Ezawa and A. Iwazaki, Phys. Rev. B 43, 2637 (1991).
[12] R.B. Laughlin, Phys. Rev. Lett. 60, 1057 (1988); A. Fetter, C. Hanna, and R.B. Laughlin, Phys. Rev. B 39, 9679 (1989).
[13] I.V. Barashenkov and A.O. Harin, Phys. Rev. Lett. 72, 1575 (1994); Phys. Rev. D 52, 2471 (1995).
[14] S. Nakajima, Y. Murayama, and A. Tomonura (eds.), Foundations of Quantum Mechanics ( World Scientific, Singapore, 1996).
[15] C.N. Yang, Phys. Rev. Lett, 33, 445 (1974).
[16] T.T. Wu and C.N. Yang, Phys. Rev. D12, 3845 (1975).
[17] D.H. Lin, J. Math. Phys. 41, 2723 (2000).
[18] D.H. Lin, Ann. Phys. 290, 1 (2001).
[21] J. Schwinger, *Quantum Mechanics* (Springer, New York, 2001).
[22] W.F. Kao, P.G. Luan, and D.H. Lin, Phys. Rev. A 65, 052108 (2002).
[23] D.H. Lin, J. Phys. A, 4785 (1998); J. Math. Phys. 40,1264 (1999).
[24] F. Wilczek, *Fractional Statistics and Anyon Superconductivity* (World Scientific, Singapore, 1990).
[25] J.Y. Zeng, *Quantum Mechanics* (Science Press, Beijing, 1999).