Double-valuedness of the electron wave function and rotational zero-point motion of electrons in rings

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I propose that the phase of an electron ‘s wave function changes by $\pi$ when the electron goes around a loop maintaining phase coherence. Equivalently, that the minimum orbital angular momentum of an electron in a ring is $\hbar/2$ rather than zero as generally assumed, hence that the electron in a ring has azimuthal zero point motion. This proposal provides a physical explanation for the origin of electronic ‘quantum pressure’, it implies that a spin current exists in the ground state of aromatic ring molecules, and it suggests an explanation for the ubiquity of persistent currents observed in mesoscopic rings.

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I. INTRODUCTION

Quantum mechanics teaches us that when we confine a particle to a small spatial region it acquires “zero point motion”, the more so the smaller the region. Consider an electron in the ring shown in Fig. 1(a), with an infinite potential barrier at azimuthal angle $\varphi = 0$. According to Schrödinger’s equation, its ground state wave function is given by

$$\psi(\varphi) \propto e^{i\varphi/2} - e^{-i\varphi/2}$$

as far as its azimuthal dependence is concerned, to satisfy the boundary condition

$$\psi(\varphi = 0) = \psi(\varphi = 2\pi) = 0$$

where the potential is infinite. Its azimuthal energy (kinetic energy from azimuthal degree of freedom) is

$$E_\varphi = \frac{\hbar^2 \pi^2}{2m_e P^2}$$

with $P = 2\pi r$, $r$ the (average) radius of the ring and $m_e$ the electron mass. The zero point energy Eq. (3) arises from the confinement of the electron in the perimeter length $P$, or equivalently from the confinement of the azimuthal angle $\varphi$ in the finite region

$$0 \leq \varphi \leq 2\pi$$

as ordained by the uncertainty relations $\Delta l \Delta p_l \sim \hbar$ ($l$ being the arc length, $p_l$ the associated linear momentum), or $\Delta \varphi \Delta L_z \sim \hbar$, with $L_z$ the angular momentum perpendicular to the plane of the ring.

Ordinarily an electron confined to a finite box exerts “quantum pressure” on the walls, and moving a wall outward lowers the quantum zero point energy. In Fig. 1(a) however, equal “quantum pressure” is exerted on both sides of the potential barrier so it averages to zero. This suggests that the energy will not be lowered if the barrier is removed. However, conventional quantum mechanics predicts that when the barrier is completely removed (Fig. 1(b)) the ground state wavefunction is

$$\psi(\varphi) = \text{constant}$$

with azimuthal energy

$$E_\varphi = 0,$$

hence that the energy is lowered by $\Delta E = -\hbar^2 \pi^2/(2m_e P^2)$ from the case where the barrier is completely in. One may reasonably ask, how is the electron able to exert a radial ‘force’ on the barrier to lower its energy from Eq. (3) to Eq. (6) in the geometry of figure 1?

Note also the following peculiarity of the wavefunction Eq. (1). Its average angular momentum in the $z$ direction

$$<L_z> = 0,$$

and its uncertainty is

$$\Delta L_z = \sqrt{<L_z^2> - <L_z>^2} = \frac{\hbar}{2}.$$

This suggests that a measurement of the $L_z$ angular momentum of the electron will yield half of the time $\hbar/2$, the other half of the time $-\hbar/2$. Usually in quantum mechanics when a particle is in a state which is a coherent superposition of states with well-defined quantum numbers, there is a way to ‘collapse’ the wavefunction (e.g. by doing a measurement) into one of the states with one
Thus, Eq. (9) is a better upper bound than Eq. (10)

when the barrier is almost completely out. Let

Eq. (1) is that it is double-valued, namely

Nevertheless, it is well known that variational

wavefunctions with piecewise continuous first derivatives are al-

lowed within the variational principle and yield valid up-

per bounds to the ground state energy [1]. Thus, the

energy Eq. (3) is an upper bound for the azimuthal con-

tribution to the ground state energy for any position of the

barrier in the ring.

We can find a better upper bound for the case when the

barrier is almost completely out. Let \( r_1, r_2 \) be the inner

and outer radii of the ring, and \( w = r_2 - r_1 \) the ring width.

Assume the barrier occupies the region \( r_2 - \Delta w \leq r \leq r_2 \)

for \( \varphi = 0 \). The true wavefunction goes to zero at \( r = r_1 \)

and \( r = r_2 \) for any \( \varphi \). Take as variational wavefunction

one that is confined to the radial region not occupied by

the barrier \( (r_1 < r < r_2 - \Delta w) \) and constant as function

of \( \varphi \), and identically zero in the region \( r_2 - \Delta w \leq r \leq r_2 \)

for all \( \varphi \). Its energy is

\[
E_1 = \frac{\hbar^2}{2m_e} \left( \frac{\pi^2}{(w - \Delta w)^2} \right)
\]

while the energy when the barrier is completely in, which

is also an upper bound for any position of the barrier, is

\[
E_{in} = \frac{\hbar^2}{2m_e} \left( \frac{\pi^2}{w^2} + \frac{\pi^2}{P^2} \right).\)

Thus, Eq. (9) is a better upper bound than Eq. (10)

when \( E_1 < E_{in} \), i.e.

\[
\Delta w \leq \frac{1}{2} \left( \frac{w}{P} \right)^2.
\]

According to this variational wavefunction, the electron

exerts a (nearly) constant outward force \(-\partial E_1/\partial \Delta w\) on

the barrier when the barrier is almost completely out.

To gain further insight, we solve the Schrödinger equa-
tion numerically on a discrete lattice with \( N_r \) points in

the radial direction and \( N_\varphi \) points in the azimuthal direc-
tion. The boundary conditions are

\[
\Psi(r_1, \varphi) = \Psi(r_2, \varphi) = 0 \quad \text{and} \quad \Psi(r, 0) = 0 \quad \text{for} \quad r_2 - \Delta w \leq r \leq r_2,
\]

where the barrier is fully in and out respectively.

The nearest neighbor hopping amplitudes in the \( r \) and \( \varphi \)
directions are

\[
t_r = \frac{\hbar^2 \pi}{2m_e a_r^2} = \frac{\hbar^2 (N_r + 1)^2}{2m_e u^2}\)
\]

\[
t_\varphi = \frac{\hbar^2 \pi}{2m_e a_\varphi^2} = \frac{\hbar^2 (N_\varphi + 1)^2}{2m_e P^2}\)

When the barrier is fully in, the ground state wavefunc-
tion is

\[
\Psi(i_r, i_\varphi) = f(i_r)g(i_\varphi)\)

with

\[
f(i_r) = \sqrt{\frac{2}{N_r + 1}} \sin \left( \frac{\pi i_r}{N_r + 1} \right)
\]

\[
g(i_\varphi) = \sqrt{\frac{2}{N_\varphi + 1}} \sin \left( \frac{\pi i_\varphi}{N_\varphi + 1} \right)
\]

and \( i_r, i_\varphi \) labeling the discrete lattice points in the \( r \) and \( \varphi \)
directions. When the barrier is completely out, the ground state
wavefunction is Eq. (14) with \( f(i_r) \) given by Eq. (15a) and
\( g(i_\varphi) = 1/\sqrt{N_\varphi} \). The ground state
energies are given by

\[
E_{in} = \frac{\hbar^2}{2m_e} \left( \frac{\pi^2}{w^2} + \frac{\pi^2}{P^2} \right)
\]

\[
E_{out} = \frac{\hbar^2}{2m_e} \left( \frac{\pi^2}{w^2} \right)
\]

when the barrier is fully in and out respectively.

Consider for definiteness a ring of inner and outer radii

\( r_1 = 2, r_2 = 2.5 \). Fig. 2 shows the behavior of the

fractional energy increase

\[
\Delta \epsilon = \frac{E - E_{out}}{E_{in} - E_{out}}
\]

for \( N_r = 10 \) and various values of \( N_\varphi \) as a function of

the barrier position. The horizontal axis variable \( x = \Delta w/w \)
takes 10 discrete values in this case, with 0 (1) denoting

the barrier fully out (in) respectively. It can be seen that
as \( N_\varphi \) increases the curves become increasingly flatter for large \( x \). This indicates that the electron is happy in a state very similar to Eq. (15) (equivalent to Eq. (1)) and is not exerting any ‘quantum pressure’ to push the barrier out. We conjecture that in the continuum limit \( (N_\varphi \to \infty) \) the energy will make a crossover from Eq. (16a) to Eq. (16b) in a tiny interval given approximately by the variational estimate Eq. (11), which for the parameters used here \( (r_1 = 2, r_2 = 2.5) \) corresponds to \( 0 \leq \Delta w/w \leq 1/1600 \).

For the ground state wavefunction, we find that to a very good approximation it factorizes as given by Eq. (14) with \( f(i_r) \) given by Eq. (15a) and \( g(i_r) \) interpolating between Eq. (15b) and a constant depending on the position of the barrier. Fig. 3 shows results for

\[
g \equiv \sqrt{\frac{N_\varphi + 1}{2}} \frac{\Psi(i_r, i_\varphi)}{f(i_r)}
\]

as function of \( \varphi = 2\pi i_\varphi/N_\varphi \) with \( f(i_r) \) given by Eq. (15a) and four values of the barrier position: \( x = 0 \), \( x = 0.2 \), \( x = 0.4 \) and \( x = 1 \). The \( i_r \) dependence of the results is nearly indistinguishable in Fig. 3, it can only barely be discerned near the extremes \( i_\varphi = 0 \) and \( i_\varphi = N_\varphi /2 \) where the different curves very slightly ‘fan out’. It can be seen that as \( N_\varphi \) increases the ground state wavefunction for any value of \( \Delta w/w \) except zero approaches the wavefunction for \( x = \Delta w/w = 1 \) given by Eq. (15b).

In addition the numerical results show that the wavefunction Eq. (18) as well as the ground state energy are essentially independent of the degree of lattice discretization in the \( r \) direction \( (N_r) \) provided the strength of the hopping across the barrier is properly scaled. As the extreme case we consider a 1-dimensional chain \( (N_r = 1) \) of \( N_\varphi \) sites and take the hopping between site \( N_\varphi \) and site 1 to have magnitude

\[
t'_\varphi = t_\varphi \sum f(i_r)^2
\]

with \( f(i_r) \) given by Eq. (15a), and where the sum extends over the \( i_r \) points where the barrier is absent. The numerical results from this calculation are shown in Fig. 3 as the points, and the results for the case \( N_r = 10 \) by the lines. Similarly in Fig. 2 the numerical results from this calculation are shown as the diamonds and the dashed lines. It can be seen that the agreement between the results for \( N_r = 1 \) and \( N_r = 10 \) is nearly perfect for the ring considered \( (r_1 = 2, r_2 = 2.5) \). This no longer holds for rings where the width becomes comparable or larger than the inner radius. For the single chain with one hopping \( t'_\varphi < t_\varphi \) it can be shown analytically that in the continuum limit \( (i.e. \ N_\varphi \to \infty, a_\varphi \to 0) \) the wavefunction and the energy converge to the results for the open chain \( (t'_\varphi = 0) \), no matter how small the difference between \( t'_\varphi \) and \( t_\varphi \) is.

In summary, these results indicate that the behavior of an electron in a ring predicted by conventional quantum mechanics is very peculiar. As the barrier is gradu-
ally pulled out the electron is trying very hard to remain in the state where the barrier was fully in, with phase change $\pi$ around the ring, rather than helping to push the barrier out and eliminating the phase change, except near the very end of the process where the barrier is almost out.

I argue that these predictions of conventional quantum mechanics are so highly counterintuitive that perhaps they do not describe physical reality. When the barrier is completely in, the zero-point energy Eq. (3) is non-zero because the angle $\varphi$ is confined to the finite region Eq. (4). As the barrier is pulled out, the azimuthal angle $\varphi$ remains confined to the same finite region. I propose that as a consequence “zero point motion” still has to exist and the azimuthal energy Eq. (3) will be unchanged. The wavefunction is no longer constrained to be the particular linear combination Eq. (1) in the region where the barrier is absent, thus it can be either

$$\psi_1(\varphi) = e^{i\varphi/2} \quad (20a)$$

or

$$\psi_2(\varphi) = e^{-i\varphi/2}. \quad (20b)$$

Putting the barrier back will change the wavefunction to the appropriate linear combination of (20a) and (20b) but shouldn’t cost any energy because the electron in this geometry cannot “push” radially outward. The wavefunctions Eq. (20) have angular momentum in the $z$ direction

$$L_z = \pm \hbar/2 \quad (21)$$

and I propose that this is the minimum value of orbital angular momentum for an electron in the ring without the barrier when phase coherence exists, rather than the prediction of conventional quantum mechanics $L_z = 0$ (Eq. (5)).

If an electron is in a linear box of length $L$ it oscillates back and forth with speed $v = h\pi/(m_L L)$ in its ground state. If one of the walls is not infinitely high, or is suddenly made more transparent, or is removed very quickly, the electron will tunnel out or fly out with the same speed $v = h\pi/(m_L L)$ that it had when the wall was in place. Similarly the electron in the case of 1(a) is orbiting back and forth in the ring with speed $v = \hbar^2/(2m_0 r)$, with $r$ the radius of the ring, and one might reasonably expect that the electron will keep this speed if the barrier is suddenly removed or made transparent. This is consistent with the electron having orbital angular momentum of $\hbar/2$ or $-\hbar/2$ when the barrier is no longer there, as described by the wavefunctions Eq. (20). Or, the electron could stay in the state Eq. (1) if the ‘sudden approximation’ is valid and $\Psi(t = 0^+) = \Psi(t = 0^-)$ . Note that within conventional quantum mechanics the sudden approximation has to break down for this situation because it is impossible to express the ground state of the electron in Fig. 1(a) as a linear combination of states of the electron in Fig. 1(b).

Besides the considerations above, this proposal is motivated by a prediction of the theory of hole superconductivity, proposed to describe all superconductors. It was found within that theory\(^2\) that in the superconducting state electrons move in mesoscopic orbits of radius $2\lambda_L$ ($\lambda_L$ = London penetration depth) with speed $v_0 = \hbar/(4m_0\lambda_L)$, thus carrying orbital angular momentum $\hbar/2$. Electrons in superconductors have macroscopic phase coherence. Thus it is natural to infer that the angular momentum $\hbar/2$ and associated phase change of $\pi$ when the electron traverses a closed $2\lambda_L$ orbit is an intrinsic property of the phase-coherent electron rather than a particular property of superconductors.

More generally I point out that a non-zero ground state angular momentum provides a physical argument for “quantum pressure” and the stability of matter\(^3\) that is absent in conventional quantum theory. A particle of mass $m$ rotating in a circle of radius $r$ with angular momentum $L$ has kinetic energy

$$E_{\text{kin}} = \frac{L^2}{2mr^2} \quad (22)$$

and reducing $r$ for fixed $L$ increases its kinetic energy, mimicking the kinetic energy term in Schrödinger’s equation $-(\hbar^2/2m)\nabla^2$ for $L \sim \hbar$. This argument underlies the stability of Bohr’s orbits, where the angular momentum $L = nh$ is always nonzero ($n \geq 1$). De Broglie was guided to his relation $p = \hbar/\lambda$ by the argument that a finite number of wavelengths, $n$, should fit into the $n$-th Bohr orbit $(2\pi r = n\lambda \Rightarrow L = pr = nh)$. This physics is lost in the Schrödinger equation, that allows for zero angular momentum solutions (e.g. the $l = 0$ states of hydrogen) subject to ‘quantum pressure’ of unknown origin. Thus I argue that the old Bohr-Wilson-Sommerfeld quantization rule

$$\oint \vec{p} \cdot d\vec{q} = nh \quad (23)$$

with $p$ and $q$ canonically conjugate and $n \geq 1$ has deeper physical content than the Schrödinger equation that it inspired.

The wavefunctions Eq. (20) satisfy Schrödinger’s equation with energy Eq. (3), are continuous and have continuous derivative as the Schrödinger equation requires in the absence of infinite potentials, but are not considered to be a valid description of physical reality because they are not single-valued\(^4\). When the electron goes around the ring once, it ends up in a state of opposite sign, and two rounds are needed to get back to the original state. But if the observable object is the square of the wavefunction, $P(\varphi) = |\psi(\varphi)|^2$ giving the probability of finding the electron at azimuthal angle $\varphi$, all we should require is that $P(\varphi + 2\pi) = P(\varphi)$, which the wavefunctions Eq. (20) do satisfy. Ascribing two possible values to the electron wavefunction at the same point in space may contradict our classical physical intuition, but not more so than the notion that the same electron somehow
This gives a rationale to the well-known spin-statistics relationship\[13\]. Here I propose that the (-) sign arising when one electron loops around another in a ring, thus interchanging their positions, is due to the single fermion going around the circle, whether or not the other fermion is present.

Which of the two wavefunctions Eq. (20) will the electron choose? In the absence of applied magnetic field it is natural to expect that the rotational zero point motion will be the same as that predicted for superconductors\[2\], namely $\bar{v}_\sigma \parallel (\hat{r} \times \hat{\sigma})$ for the velocity direction of the electron of spin $\sigma$ perpendicular to the plane of the ring and $\hat{r}$ pointing radially outward. In other words, an electron with spin pointing into (out of) the paper in Fig. 1(b) will rotate counterclockwise (clockwise). This is the lowest energy state dictated by spin-orbit coupling in the presence of an outward-pointing electric field. Quite generally, because electrons are lighter than protons, they tend to move outward from compensating positive charge and thus experience outward-pointing electric fields.

The conventional Bohr-Wilson-Sommerfeld quantization rule Eq. (23) needs to be modified to reflect this physics, to read

$$\int \hat{p} \cdot d\hat{q} = (n \pm \frac{1}{2})\hbar$$  \hspace{1cm} (25)

with the + (-) sign corresponding to spin orientation opposite to (the same as) the direction given by the right-hand rule in traversing the integration circuit, and $n$ an integer. It is interesting to note that Eq. (25) (with the (+) sign and $n \geq 0$) gives the correct energy for the harmonic oscillator including its zero point motion, which the conventional rule Eq. (23) does not. With respect to Bohr’s semiclassical model of hydrogen, note that it does not take into account spin. Taking the average of Eq. (25) over both spin orientations will give back the conventional rule Eq. (23) and yield the correct answers for the energy levels of hydrogen.

Imagine standing at a point in the ring watching an electron fly by. How can you tell when the electron returns after encircling the loop whether or not it has retained phase coherence? In the scenario proposed here, the electron reappearing with wavefunction of opposite sign is the telltale signature of phase coherence. Thus the “closing” of the wavefunction emphasized by A.V. Nikulov as characterizing quantum coherence\[10\] can be detected locally as opposed to the conventional scenario that requires knowledge of the entire wavefunction of the electron around the loop\[10\].

What differentiates a phase-coherent superconductor from a phase-coherent normal mesoscopic ring? In both cases the individual electron wave function changes sign in going around the loop. But in the superconductor electrons are paired, and $(-1) \times (-1) = 1$, so the Cooper pair wave function does not change sign. This allows for the establishment of macroscopic phase coherence in the superconductor by locking the phases of different Cooper pairs, and it is not possible for unpaired electrons because

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure4.png}
\caption{Interchanging the position of two identical fermions is topologically equivalent to rotating one around the other\[13\]. The two-electron wavefunction changes its sign, both according to conventional quantum mechanics and to the physics proposed here.}
\end{figure}
of random occurrence of positive and negative signs.

Consider now the states of several non-interacting electrons of the same spin in a ring of length $L$. The states Eq. (20) correspond to the electron having wavevector $k = \pm \pi / L$, as shown in Fig. 5(a). The electron with spin in the $\hat{z} \equiv \hat{r} \times \hat{\varphi}$ direction will occupy the $k = -\pi / L$ state due to the spin-orbit interaction, orbiting with angular momentum pointing in the $-\hat{z}$ direction. For two electrons of the same spin, the $k$ values shift to become the same as conventionally, as shown in Fig. 5(b). For an even number of electrons there is a state at $k = 0$, for an odd number of electrons the lowest $k$ is $\pm \pi / L$. The degeneracy in the ground states is broken by the spin-orbit interaction.

For an even number of fermions there is a state at $k = 0$, the allowed wavevectors for the electrons in a ring of length $L$ of random occurrence of positive and negative signs. The dots are spaced at distance $\Delta k = 2\pi / L$. The “tireless electrons”[17] of Fig. 5 will have a stronger tendency to move around and create persistent currents than conventional electrons, where half of the states do not carry current. There have been many experiments on persistent currents in mesoscopic rings[17–20] over the years and the field has been mired in controversy. Although it is not apparent in many of the papers written on the subject, the underlying theme is the surprisingly large persistent currents that are typically observed, larger by up to two orders of magnitude from what is theoretically expected. Within the physics proposed here, mesoscopic rings will carry a spin current in the absence of applied magnetic field, and an applied magnetic flux will simply slow down one of the components of the spin current and speed up the other thus giving rise to a charge current, rather than creating the charge current from scratch. It should be in principle possible (though experimentally challenging) to detect the spin current in the absence of applied magnetic field through the small electric field that it creates. It should be easier in superconducting rings as discussed in [2]. The physics discussed here may also be related to experimental signatures of spin currents in surface states observed in a variety of materials in recent years[21, 22]. The quantum number shift in the Bohr-Wilson-Sommerfeld quantization rule proposed here (Eq. (25)) may provide an explanation for the puzzling experimental observations of Nikulov and coworkers on asymmetric superconducting rings[23].

There is in fact no reason to restrict the physical arguments presented here to the ring topology. They suggest that quite generally the origin of electronic ‘quantum pressure’ in nature, manifest in the fact that electrons tend to expand their wavefunction radially as far as possible, is that they undergo zero-point rotational motion in the region of space that they have available, with angular momentum $\hbar / 2$, just as predicted for electrons in superconductors[2, 24]. This spinning zero-point orbital motion originates in the two-valuedness of the electron wavefunction and carries the same magnitude of angular momentum as, and opposite direction to, the intrinsic electron spin, which itself can be represented by a mass $m_e$ orbiting at speed $c$ in a circle of radius $r_0 = \hbar / (2mc)$. I do not explain here the origin of this zero-point rotational agitation, which presumably derives from the topological structure of space-time itself. Schrödinger’s equation, while undoubtedly correct for a large number of physical situations, does not describe this physics, nor does Dirac’s equation in its current form. If correct it
is evident that this physics has profound implications for the understanding of matter. In particular I discuss elsewhere\cite{25} that it leads to the expected existence of ground state spin currents in aromatic ring molecules, ubiquitous in biological matter. This physics will generally lead to less ‘inert’ structures than the conventional understanding, and may ultimately explain questions as general as the ‘elan vital’ and how the universe avoids heat death.

It is likely that the concepts discussed in this paper have connections and overlaps with a variety of concepts that have been discussed in the condensed matter and particle physics literature in recent years such as Dirac monopoles, anyons, Chern numbers, flux phases, composite fermions, TKNN invariant, quantum spin Hall effect, topological superfluids, topological insulators, fiber bundles, Berry phase, Aharonov-Casher phase, vortices, strings, dyons, skyrmions, etc. I have not elucidated these connections in detail and apologize for not citing possibly relevant references, but believe that the concrete physics proposed in this paper has not been proposed before. Connections with other related work should yield interesting insights and further progress in understanding.

**Note added:** After completion of this paper it came to my attention that the possibility of a double-valued wavefunction for the electron has been considered by various workers in the past\cite{26–28}. However the possibility that this may explain the origin of ‘quantum pressure’ has not been suggested before to my knowledge.

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