Phase Waves in Finite Potentials: the Harmonic Oscillator and the Hydrogen Atom

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Abstract

Louis de Broglie’s concept of particles as sources of phase is extended to the analysis of systems in which the potential is not constant. The treatment assumes that the phase information propagates as waves according to classical electrodynamics including reflection with phase changes from potential energy barriers. The energies and weighting functions in such cases are obtained by comparison of the phase of the accelerated particle relative to the phases of reflections from the change in potential. Application to the chemically interesting systems of the harmonic oscillator and hydrogen atom are considered using the time evolution of the relative phases of the reflected de Broglie phase waves, whereby the weighting functions are obtained from the distance dependence of the phase differences between the reflections and the source. This is accomplished conveniently by taking time derivatives of the relative de Broglie phases and considering the periodicity of the motion. Optimum trajectories are determined by minimization of the action integral $2i(mv^2 - eV/\partial r)/\hbar$ which depends on the potential $V$ and the velocity $v$. The treatment leads to the Newtonian force law for circular orbits and affords the same energies as derived using the Schrödinger equation.

Keywords: De Broglie phase waves; Feynman action; Harmonic oscillator; Hydrogen atom.

1 Introduction

A previous article [1] applied de Broglie’s concept associating frequency with mass [2, 3] to describe particles as sources of phase waves which obey classical electrodynamics principles. Reflection of the phase waves was proposed to occur at potential energy boundaries resulting in interference effects which through coherence with the source established preferred trajectories. This model was shown to afford the same result for the energies and nodal pattern as the Schrödinger equation for a particle in a box [1]. Here this analysis is extended to systems with nonzero internal potentials, and by taking derivatives rather than integrals affords the weighting functions, energy spectra, and action for the harmonic oscillator and hydrogen atom.

2 Discussion

The de Broglie relation [4] (Equation 1)

$$\hbar \omega_0 = m_0 c^2$$

associates a frequency $\omega_0$ with the mass $m_0$ of a particle by Planck’s constant $\hbar = 2\pi \hbar$ and the speed of light $c$. We interpret this to describe an internal periodic oscillation of the particle as a source of phase which can transmit phase information and consider such phase waves to propagate following classical electrodynamic principles [5, 6]. Previously we described how reflection of such waves from infinite potential boundaries allows phase information to be carried back to the source in zero potential [1]. The reflections produce interference which may be considered as the superposition of two waves traveling in opposite directions. The time ($t$) evolution of one of these, produced by an even number of reflections,

$$\psi_{even} = R_{even} \exp \left[ i \frac{\omega}{\gamma} \left( \frac{t - \frac{z}{c}}{c} \right) \right] \cos \frac{\alpha}{\gamma^2} (vt - z)$$

(2)

describes a wave traveling with phase velocity $c^2/\gamma v$ and amplitude (group) velocity $+v$ in the $z$-direction and corresponds to a de Broglie wave. Here $\gamma$ and $\omega$ are defined in terms of a potential $V$ as
\[ \gamma \equiv (1 - v^2 / c^2)^{1/2} \]

\[ \omega = \omega_0 + V / h \]  

so that \(\omega/\gamma\) and the apparent mass \(m\) are constant for a conservative energy \(E\)

\[ E / c^2 = (m_0 + V / c^2)(1 - v^2 / c^2)^{-1/2} = m \]  

The phase in the exponential follows a Lorentz transform for the time and the amplitude follows the transform for the spatial coordinate. The other wave

\[ \psi_{\text{odd}} = -R_{\text{odd}} \exp \left[ i \frac{\omega}{\gamma} \left( t - \frac{v}{c} \frac{z}{c} \right) \right] \cos \left( \frac{\omega}{\gamma} (v + z) \right) \]  

is produced by an odd number of reflections and corresponds to the inverse transforms. Equation 5 describes a wave with phase velocity \(-c^2/\gamma v\) and group velocity \(-v\). The negative sign in Equation 5 is included due to the change of phase by \(-\pi\) occurring for each reflection from a ‘hard’ boundary using Euler’s formula, \(\exp(-i\pi) = -1\). An even number of such changes occur for the even-integer reflections, restoring the original sign in Equation 2. The even-integer reflections were shown to quantize the momentum \(p\) of the source

\[ p = mv = \hbar l(2L) \]

where \(l\) is an integer and \(L\) is the separation between the reflective surfaces, whereas the odd-integer reflections give rise to the nodal structure of the system [1].

The amplitude in Equation 2 will remain constant at the source, but for a change in position \(\Delta x = v \Delta t\) the amplitude in Equation 5 will oscillate rapidly with distance as \(\Delta x = 2c \Delta t \omega = \hbar / 2mc\). This corresponds to one-half Compton wavelength, contributing a low frequency ‘zitterbewegung’ [7] to the motion of the source for \(n < c / \sqrt{2}\). This behavior will not be treated further here, although it should be noted that reversal of the velocity would lead to a matching of the change of the source phase with Equation 5 so that a particle may locally inhabit regions where the phase relationship is partially maintained (perhaps by emission of a photon or virtual photon, or by interaction with the boundaries) [1].

The example of a particle in a constant nonzero potential is closely related. Since electromagnetic waves are unaffected by traveling through static electric or magnetic fields in a vacuum [8], de Broglie waves likewise should be unaffected by the presence of a static potential \(V\). The principal difference concerns the effect of the potential on the apparent mass \(m\) [9], defined by \(E/c^2\) according to Equation 4, which will not change the momentum and can be ignored for small potentials. This is in accord with the predictions of quantum mechanics using the Schrödinger equation, the solutions of which rely on the constant difference \(E-V\) which admits no change in the momentum or energy states [10]. Then the presence of the potential should not directly affect the behavior of the phase waves themselves, the only consequence arising through changes in the motion of the particle.

### 2.1 Harmonic Oscillator

The potential for a one-dimensional harmonic oscillator with \(z\)-displacement is \(V \equiv k z^2 / 2\). The composite behavior of waves reflected from this type of barrier is described as in Equation 2 and Equation 5 but with a phase shift of \(\pi/2\) at each ‘soft’ barrier [8, 11]. Using Euler’s equation, the phases of the odd \((\psi_{\text{op}})\) and even \((\psi_{\text{ep}})\) reflections would be

\[ \psi_{\text{op}} = -\exp \left[ i \frac{\omega}{\gamma} \left( t - \frac{v}{c} \frac{z}{c^2} \right) \right] \]

\[ \psi_{\text{ep}} = i \exp \left[ i \frac{\omega}{\gamma} \left( t + \frac{v}{c} \frac{z}{c} \right) \right] \]

The negative and imaginary pre-exponential signify that these two sets of reflections will be out of phase with one another by \(\pi/2\), but due to the different transit distances and times there will be occasions on which they both will be coherent with the source.

#### 2.1.1 Weighting Function

Away from the center, the velocity will decrease with increasing potential, and the phase encountered by the particle will depend on position. Insofar as the harmonic oscillator resembles a particle in a box, for which the even-integer reflections quantized the momentum, examination of the phases of these reflections (Equation 7, top) relative to that of the particle \((\psi_0)\)
reveals that the evolution of the phase of the particle would occur as \( d \psi / dt \). For a constant \( \omega / \gamma \) and a velocity which is not constant,

\[
\frac{d \psi_0}{dt} = \frac{d}{dt} \exp \left( i \frac{\omega}{\gamma} t \right) = i \frac{\omega}{\gamma} \left( 1 - \frac{v^2}{c^2} - 2 \frac{vat}{c^2} \right) \phi_0
\]

(9)

The phase of the even reflections would evolve as

\[
\frac{d \psi_{2p}}{d \psi_{2p}} \frac{dt}{dt} = i \frac{\omega}{\gamma} \left( 1 - \frac{v^2}{c^2} - \frac{az}{c^2} \right)
\]

(10)

where \( a = dv/dt \) is the acceleration. The phase of the source with respect to the even-integer reflections, which preferentially would travel a half-integer number of periods, corresponds to the exponential of the difference

\[
\frac{d \phi_{2p}}{d \phi_{2p}} \frac{dt}{dt} \equiv \frac{d \psi_0}{d \psi_0} \frac{dt}{dt} - \frac{d \psi_{2p}}{d \psi_{2p} dt} = i \frac{\omega}{\gamma} \left( 1 - \frac{v^2}{c^2} - 2 \frac{vat}{c^2} \right) - i \frac{\omega}{\gamma} \left( 1 - \frac{v^2}{c^2} - \frac{az}{c^2} \right) = i \frac{ma}{h} (z - 2vt)
\]

(11)

When the velocity is constant, as for a particle in a box, \( a = 0 \) and the particle could encounter the even reflections in phase everywhere. For the oscillator, however,

\[
a = -\partial V / \partial z = -kz
\]

(12)

and the phase of the wave will drift with distance and time from that of the particle. To determine the relative space dependence of the phase, \( \Delta \phi_{2p} \), the final term containing the time can be ignored for a standing wave. The remaining term in Equation 11 containing \( z \) should otherwise have no dependence on the time. With Equation 1 and Equation 12, integration of this term over one phase cycle \( \Delta T \) affords

\[
ima \zeta / h = -i k \zeta^2 \Delta T / h
\]

(13)

where \( z \) is taken to be the distance from the origin where the potential is constant. It is appropriate to consider an interval \( \Delta T \) for a single transit of the particle across the oscillator, which would occur in \( \frac{1}{2} \) period \( 1/\Omega = (m/k)^{1/2} \). Then the relative change in phase would be

\[
\Delta \phi_{2p} = -i k \zeta^2 / 2 \Omega h = -i k \zeta^2 / (2h \sqrt{m/k}) = -i \sqrt{k m \zeta^2} / (2h)
\]

(14)

That is, the particle would dephase with the reflections as \( \exp[-i \sqrt{k m \zeta^2} / (2h)] \), the negative sign signifying that the phase of the wave advances with increasing \( |z| \) relative to that of the particle due to an acceleration in the direction of the origin.

2.1.2 Action. The singly reflected wave also will drift from its initial phasing with respect to the particle according to

\[
\frac{d \psi_{1p}}{d \psi_{1p} dt} = i \frac{\omega}{\gamma} \left( 1 + \frac{v^2 + az}{c^2} \right)
\]

(15)

For this wave, the relative phase evolution \( \Delta \phi_{1p} \) corresponds to the difference

\[
\frac{d \phi_{1p}}{d \phi_{1p} dt} \equiv \frac{d \psi_0}{d \psi_0} \frac{dt}{dt} - \frac{d \psi_{1p}}{d \psi_{1p} dt} = i \frac{\omega}{\gamma} \left( 1 + \frac{v^2 + az}{c^2} \right) - i \frac{\omega}{\gamma} \left( 1 + \frac{v^2}{c^2} + \frac{az}{c^2} \right) = -i \frac{\omega}{\gamma} \left( 2 \frac{v^2}{c^2} + 2 \frac{vat + az}{c^2} \right)
\]

(16)

Ideally, the phase of the wave would match that of the particle which occurs maximally when the phase mismatches described by Equation 11 and Equation 16 are both zero. Substitution for the time \( t = \zeta / 2v \) from the zero of Equation 11 and for the acceleration (Equation 12) into Equation 16 affords for the optimum trajectory

\[
-2i m (v^2 + az) / h = -2im (v^2 - k \zeta^2 / m) / h = -4i(K - V) / h = 0
\]

(17)
Expressed in terms of the phase behavior, this relation has the form of action [12-14], where \( K \) is the kinetic energy and \( V \) is the potential energy, and the optimum trajectory minimizes the difference \( K - V \). This is essentially the same as Feynman’s principle of least action [15] where the (imaginary) action \( S \) at low velocities

\[
4\delta S = -4\int_l^t dt (K - V) / \hbar
\]  

(18)

is minimized over the trajectory in space. Evaluation of the integral over the path of the particle determines the cumulative phase difference in an interval \( \Delta T \), which would be minimal along the preferred trajectories [14, 15]. The smaller the phase difference, the more likely it would be for the particle to travel along that path.

Equation 17 implicitly associates momentum and force. Minimizing the relative phase change and with \( ma = -\partial V / \partial z \)

\[
mv^2 / z = -\partial V / \partial z
\]  

(19)

affords the force law for circulation in a central potential. Such motion is not possible in a one-dimensional oscillator, but it could occur in a circular or spherical oscillator, and then uniform transverse movement would be expected.

2.1.3 Energy Spectrum. The difference in time \( \Delta t \) for the two (forward and reverse) even-reflected waves to return in phase would have the condition

\[
\Delta t = (l + 1/2)2\pi / \omega = 2Lv / (c^2 \gamma^2)
\]  

(20)

The equation allows only differences resulting in half-integer values, rather than integer values as found for a particle in an infinite square well potential [1], because of the phase shift of \( 1/2 \) period so that the reflected waves return in phase not only with one another but also with their source. Optimally, the source must advance (or be delayed) by an additional half period before re-encountering the even reflections, which will differ in phase from one another by an even integer number of periods.

A phase change of \( 1/4 \) wavelength at each boundary can be conceived to occur by the phase wave penetrating the barrier by \( 1/8 \) wavelength to produce the phase change of \( 1/4 \) wavelength or \( \pi/2 \) upon each reflection. Since each even reflection is reflected twice before returning, the total distance traveled on average is taken to be \( 2L = \pi/2 \zeta_{0} \). Substituting for the frequency (Equation 1) in Equation 20 and rearranging affords the maximum velocity \( v_0 \) in terms of the maximum displacement \( z_0 \)

\[
v_0 = (l + 1/2)\hbar / (2mL) = (l + 1/2)\hbar / (\pi m z_0) = (l + 1/2)2\hbar / (m z_0)
\]  

(21)

For small potentials and velocities, this result differs from a particle in a box by the inclusion of half-integer values and the value of \( L \) describing where in the barrier reflection occurs. By conservation of energy, the oscillator frequency \( \Omega \) and the acceleration \( a \) are found classically to be

\[
\Omega \approx v_0 / z_0 \approx (k / m)^{1/2}
\]

\[
am \approx -kz
\]  

(22)

Since the period does not depend on the ratio of the maximum velocity to the maximum displacement, it is possible to find the maximum displacement using Equation 21

\[
\Omega \approx v_0 / z_0 = (l + 1/2)2\hbar / (m z_0^2)
\]

\[
z_0^2 \approx (l + 1/2)2\hbar / (m \Omega) = (l + 1/2)(m / k)^{1/2} 2\hbar / m = (l + 1/2)2\hbar / \sqrt{km}
\]  

(23)

The associated energy is

\[
kz_0^2 / 2 \approx (l + 1/2)2\hbar / (2\sqrt{km}) \approx (l + 1/2)\hbar (k / m)^{1/2} = (l + 1/2)\hbar \Omega
\]  

(24)

Behavior away from the center is complicated, but at the center of a linear oscillator the even reflections would return in phase for an advance of the particle by \( l+1/2 \) periods, and the nodal properties would be the same as those for the particle in a box, as expected due to \( a = 0 \) in that location.

2.1.4 Quantum Mechanics. The energies of the Schrödinger solution are found to be as given in Equation 24 and the eigenfunctions include a common weighting function containing \( \Omega / \hbar \) in the exponent

\[
\exp[-m\Omega Z^2 / (2\hbar)] = \exp[-m(k / m)^{1/2} z^2 / (2\hbar)] = \exp[-(km)^{1/2} z^2 / (2\hbar)]
\]  

(25)
2.2 Hydrogen Atom. Reflections in this case are assumed to occur due to the distance dependence of the Coulomb potential \( V = -e^2/4\pi\varepsilon_0 r \), where \( e \) is the fundamental unit of charge, \( \varepsilon_0 \) is the permittivity of free space, and \( r \) is the distance of the electron from the nucleus.

2.2.1 Energy Spectrum. We will proceed from Equation 6 using the framework developed for the harmonic oscillator with an optical pathlength \( 2L = 2\pi r \) following Bohr’s quantization condition for angular momentum [21],

\[
p = l\hbar / (2L) = l\hbar / (2\pi r)
\]

For purely transverse motion, the situation corresponds to the proposition by Bohr that the angular momentum is quantized in units of \( \hbar \), since \( V \) does not change with time. Equation 26, however, refers to quantization of the momentum of a particle due to an effective reflective distance \( L \). The relationship between radial and transverse motion through Equation 26 is supported by the complete degeneracy of the Kepler problem for a spherical central potential [22,23]. The energy levels [12] are obtained using \( K = -Vl2 \) (vide infra)

\[
E \approx -me^4 / (8l^2 \varepsilon_0^2 \hbar^2)
\]

2.2.2 Weighting Function. The distance dependence of the phase relationship \( mar\Delta T/lh \) (Equation 13) in the presence of a Coulomb potential is

\[
ma = -\partial V / \partial r = -e^2 / (4\pi\varepsilon_0 r^2)
\]

\[
mar\Delta T / \hbar = -\Delta T e^2 / (4\pi\varepsilon_0 \hbar r)
\]

where the distance \( r \) is used as the radial coordinate. The periodicity in this case can be associated with Equation 26, expressed as

\[
rmr^2 \Omega = l\hbar
\]

\[
rmr^2 / l\hbar = 1 / \Omega = \Delta T
\]

Then from Equation 28

\[
-\frac{e^2}{4\pi\varepsilon_0 \hbar} mr^2 / l\hbar = -\frac{1}{l} \frac{me^2}{4\pi\varepsilon_0 \hbar^2}r
\]

and dephasing will occur with distance following the (imaginary) exponential of Equation 30, \( \text{viz.} \exp \left( -\frac{i}{l} \frac{me^2}{4\pi\varepsilon_0 \hbar^2}r \right) \)

As previously mentioned, Equation 29 has the appearance of angular momentum which, due to degeneracy, couples the period for radial motion with the angular motion, describing the time to complete one Bohr orbit. For a Coulomb potential, Equation 19 and Equation 28 (with \( r = z \) in this context) produce

\[
2K = mv^2 = -mar = (e^2 / 4\pi\varepsilon_0 r^2) r = e^2 / 4\pi\varepsilon_0 r = -V
\]

Equation 31 expresses the centripetal acceleration \( a = v^2 / r \) and the relationship between kinetic and potential energy used to derive Equation 27, giving the energy for purely transverse motion from classical mechanics and revealing the reason for the success of Bohr’s approach.

2.2.3 Action. Equation 31 affords an integrand for the action

\[
-2im(v^2 + ar) / \hbar = -2i(mv^2 + V) / \hbar = -4i[(mv^2 / 2) + V / 2] / \hbar = -4i(K + V / 2) / \hbar = 0
\]

which differs from that for the harmonic oscillator in Equation 17. A path integral solution for the hydrogen atom curiously required an imaginary time transformation [24-28]. The substitution of \( i\hbar \) for \( dt \) in \( v^2 \) reverses the sign of the kinetic energy term in Equation 18. This solution subsequently transformed the radial potential into one resembling the
harmonic oscillator, $\frac{1}{2}(am^2r^2$, thereby introducing a factor of $\frac{1}{2}$ into the potential and reversing the sign of the potential energy as well. Since the acceleration for a harmonic oscillator is $a = -\omega^2 r$, the action in imaginary time can be written $-\frac{1}{2}m\omega^2 r^2 + \frac{1}{2}mar$, matching in form Equation 32.

2.2.4 Quantum Mechanics. The Schrödinger equation is solved by assuming that the variables in spherical coordinates can be separated and decomposed into radial and angular parts [12]. The radial function is a constant related to the total angular momentum [29-31], formally associating radial and transverse behavior, resembling the treatment of the Kepler problem in deriving Equation 29. Solutions include the exponential

$$\Psi_n = A_n \exp[-(m_e^2/4n\pi\hbar^2) r]$$

(33)

where $n$ is an integer representing the principal quantum number and matches the integer $l$ in Equation 26 and Equation 27. Equation 33 thus corresponds to the difference in phase as determined in Equation 30. The relative favorability of interaction with the fields is defined by coherence in the phases of the particle and the reflections. Equation 32 serves to minimize the phase difference between a particle and its reflected phase and supplies a formal connection between radial and angular motion. Transverse motion can occur uniformly, consistent with Equation 31. Interestingly, restricting the motion to a plane affords a quantum mechanical result associating the energies with half-integer rather than integer quantum numbers [10, 29-31], suggesting that the overall phase change of the reflections reencountering the source differs by $\pi$ from the unrestricted condition.

3 Conclusions

The essential features of the behavior of systems with finite potential energies $V$ can be described by considering particles to be sources of de Broglie phase waves which propagate following classical electrodynamic principles and reflect from potential energy barriers. Algebraic treatment for constant potentials was shown previously to afford the energies and nodal structure of a particle in an infinite square well box [1]. The harmonic oscillator and hydrogen atom, for which the potentials depend on distance, are better handled by evaluation of the relative phases of the de Broglie phase waves which are reflected from the potential boundaries. By taking time derivatives rather than integrals, the Wick-rotated weighting functions are obtained from the distance dependence and periodicity of the motion, with the optimum trajectories determined by minimization of the integrand of the action, found to be $- 4i(K - r\partial V/2\partial r)/\hbar$.

This treatment leads to the Newtonian force law for circular orbits and affords the same energies as derived using the Schrödinger equation.

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References


