

Continue



































tunneling is of molecular hydrogen, water (ice) and the prebiotic important formaldehyde.[27]Tunnelling of molecular hydrogen has been observed in the lab.[32]Quantum tunnelling is among the most non-trivial quantum effects in quantum biology.[33] Here it is important both as electron tunnelling and proton tunnelling. Electron tunnelling is a key factor in many biochemical redox reactions (photosynthesis, cellular respiration) as well as enzymatic catalysis. Proton tunnelling is a key factor in spontaneous DNA mutation.[27]Spontaneous DNA mutation occurs when normal DNA replication takes place after a particularly significant proton has tunneled.[34] A hydrogen bond joins DNA base pairs. A double well potential along a hydrogen bond separates a potential energy barrier. It is believed that the double well potential is asymmetric, with one well deeper than the other such that the proton normally rests in the deeper well. For a mutation to occur, the proton must have tunneled into the shallower well. The proton's movement from its regular position is called a tautomeric transition. If DNA replication takes place in this state, the base pairing rule for DNA may be jeopardized, causing a mutation.[35] Per-Olov Lowdin was the first to develop this theory of spontaneous mutation within the double helix. Other instances of quantum tunnelling-induced mutations in biology are believed to be a cause of aging and cancer.[36]Quantum tunnelling through a barrier. The energy of the tunneled particle is the same but the probability amplitude is decreased. The time-independent Schrödinger equation for one particle in one dimension can be written as 



2
m
d

2


x
2


(
x
)
+
V
(
x
)
(
x
)
=
E
(
x
)


{\displaystyle -{\frac {\hbar ^{2}}{2m}}{\frac {d^{2}}{dx^{2}}}\Psi (x)+V(x)\Psi (x)=E\Psi (x)}

 or 



d

2


x
2


(
x
)
=
2
m
2


(
V
(
x
)
E
)
2
m
2


M
(
x
)
(
x
)
,


{\displaystyle {\frac {d^{2}}{dx^{2}}}\Psi (x)={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)\Psi (x)\equiv {\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)M(x)\Psi (x),}

 where 



M
(
x
)


{\displaystyle M(x)}

 is the reduced Planck constant,m is the particle mass,x represents distance measured in the direction of motion of the particle, is the Schrödinger wave function,V is the potential energy of the particle (measured relative to any convenient reference level),E is the energy of the particle that is associated with motion in the x-axis (measured relative to V),M(x) is a quantity defined by V(x)E, which has no accepted name in physics. The solutions of the Schrödinger equation take different forms for different values of x, depending on whether M(x) is positive or negative. When M(x) is constant and negative, then the Schrödinger equation can be written in the form 



d

2


x
2


(
x
)
=
2
m
2


M
(
x
)
(
x
)
=
k
2


x
(
x
)
,


{\displaystyle {\frac {d^{2}}{dx^{2}}}\Psi (x)={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)\Psi (x)=-k^{2}\Psi (x),}

 where 



k
2


=
2
m
2


M
(
x
)
.


{\displaystyle k^{2}=2m^{2}M(x).}

 The solutions of this equation represent travelling waves, with phase-constant +k or k. Alternatively, if M(x) is constant and positive, then the Schrödinger equation can be written in the form 



d

2


x
2


(
x
)
=
2
m
2


M
(
x
)
(
x
)
=
2
(
x
)
,


{\displaystyle {\frac {d^{2}}{dx^{2}}}\Psi (x)={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)\Psi (x)=\kappaappa ^{2}\Psi (x),\quad (\text{where})\;\kappa\kappa ^{2}={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)M(x).}

 The solutions of this equation are rising and falling exponentials in the form of evanescent waves. When M(x) varies with position, the same difference in behaviour occurs, depending on whether M(x) is negative or positive. It follows that the sign of M(x) determines the nature of the medium, with negative M(x) corresponding to medium A and positive M(x) corresponding to medium B. It thus follows that evanescent wave coupling can occur if a region of positive M(x) is sandwiched between two regions of negative M(x), hence creating a potential barrier. The mathematics of dealing with the situation where M(x) varies with x is difficult, except in special cases that usually do not correspond to physical reality. A full mathematical treatment appears in the 1965 monograph by Frman and Frman. Their ideas have not been incorporated into physics textbooks, but their corrections have little quantitative effect.Main article: WKB approximationThe wave function is expressed as the exponential of a function: 



(
x
)
=
e
(
x
)
,


{\displaystyle \Psi (x)=e^{\Phi (x)},}

 where 



(
x
)
+
(
x
)
=
2
m
2


(
V
(
x
)
E
)
.


{\displaystyle \Phi '(x)+\Phi ''(x)={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right).}

 (x) (displaystyle \Phi '(x)) is then separated into real and imaginary parts: 



(
x
)
=
A
(
x
)
+
i
B
(
x
)
,


{\displaystyle \Phi '(x)=A(x)+iB(x),}

 where A(x) and B(x) are real-valued functions.Substituting the second equation into the first and using the fact that the imaginary part needs to be 0 results in: 



A
(
x
)
+
A
(
x
)
2
B
(
x
)
2
=
2
m
2


(
V
(
x
)
E
)
,


{\displaystyle A'(x)+A(x)^{2}-B(x)^{2}={\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right).}

 Quantum tunneling in the phase space formulation of quantum mechanics. Wigner function for tunneling through the potential barrier 



U
(
x
)
=
8
e
.
025
x
2


{\displaystyle U(x)=8e^{0.25x^{2}}}

 in atomic units (a.u.). The solid lines represent the level set of the Hamiltonian 



H
(
x
,
p
)
=
p

2


/
2
+
U
(
x
)


{\displaystyle H(x,p)=p^{2}/2+U(x)}

. To solve this equation using the semiclassical approximation, each function must be expanded as a power series in (displaystyle \hbar ). From the equations, the power series must start with at least an order of 1 (displaystyle \hbar ^{-1}) to satisfy the real part of the equation; for a good classical limit starting with the highest power of the Planck constant possible is preferable, which leads to 



A
(
x
)
=
1
k
=
0
k
A
k
(
x
)


{\displaystyle A(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}A\_{k}(x)}

 and 



B
(
x
)
=
1
k
=
0
k
B
k
(
x
)
,


{\displaystyle B(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}B\_{k}(x),}

 with the following constraints on the lowest order terms, 



A
0
(
x
)
2
B
0
(
x
)
2
=
2
m
(
V
(
x
)
E
)


{\displaystyle A\_{0}(x)^{2}-B\_{0}(x)^{2}=2m\left(V(x)-E\right)}

 and 



A
0
(
x
)
B
0
(
x
)
=
0.


{\displaystyle A\_{0}(x)B\_{0}(x)=0.}

 At this point two extreme cases can be considered.Case 1If the amplitude varies slowly as compared to the phase 



A
0
(
x
)
=
0


{\displaystyle A\_{0}(x)=0}

 and 



B
0
(
x
)
=
2
m
(
E
V
(
x
)
)


{\displaystyle B\_{0}(x)=\pm {\sqrt {2m\left(E-V(x)\right)}}}

 which corresponds to classical motion. Resolving the next order of expansion yields 



(
x
)
C
e
i
d
x
2
m
2


(
V
(
x
)
)
+
2
m
2


(
E
V
(
x
)
)
4


{\displaystyle \Psi (x)\approx C\left(e^{i\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)}}+\theta }\right)\left({\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)\right)^{-1/2}}

 Case 2If the phase varies slowly as compared to the amplitude, 



B
0
(
x
)
=
0


{\displaystyle B\_{0}(x)=0}

 and 



A
0
(
x
)
=
2
m
(
V
(
x
)
E
)


{\displaystyle A\_{0}(x)=\pm {\sqrt {2m\left(V(x)-E\right)}}}

 which corresponds to tunneling. Resolving the next order of the expansion yields 



(
x
)
C
e
+
e
+
d
x
2
m
2


(
V
(
x
)
E
)
+
C
e
d
x
2
m
2


(
V
(
x
)
E
)
2
m
2


(
V
(
x
)
E
)
4


{\displaystyle \Psi (x)\approx {\frac {C}{+e^{+\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}+C}}e^{-\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}}}

 (displaystyle \Psi (x)) in atomic units (a.u.). The solid lines represent the level set of the Hamiltonian 



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A
(
x
)
=
1
k
=
0
k
A
k
(
x
)


{\displaystyle A(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}A\_{k}(x)}

 and 



B
(
x
)
=
1
k
=
0
k
B
k
(
x
)
,


{\displaystyle B(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}B\_{k}(x),}

 with the following constraints on the lowest order terms, 



A
0
(
x
)
2
B
0
(
x
)
2
=
2
m
(
V
(
x
)
E
)


{\displaystyle A\_{0}(x)^{2}-B\_{0}(x)^{2}=2m\left(V(x)-E\right)}

 and 



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 which corresponds to classical motion. Resolving the next order of expansion yields 



(
x
)
C
e
i
d
x
2
m
2


(
V
(
x
)
)
+
2
m
2


(
E
V
(
x
)
)
4


{\displaystyle \Psi (x)\approx C\left(e^{i\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)}}+\theta }\right)\left({\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)\right)^{-1/2}}

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(
x
)
C
e
+
e
+
d
x
2
m
2


(
V
(
x
)
E
)
+
C
e
d
x
2
m
2


(
V
(
x
)
E
)
2
m
2


(
V
(
x
)
E
)
4


{\displaystyle \Psi (x)\approx {\frac {C}{+e^{+\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}+C}}e^{-\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}}}

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(
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)
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1
k
=
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k
A
k
(
x
)


{\displaystyle A(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}A\_{k}(x)}

 and 



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(
x
)
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1
k
=
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B
k
(
x
)
,


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 with the following constraints on the lowest order terms, 



A
0
(
x
)
2
B
0
(
x
)
2
=
2
m
(
V
(
x
)
E
)


{\displaystyle A\_{0}(x)^{2}-B\_{0}(x)^{2}=2m\left(V(x)-E\right)}

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 which corresponds to classical motion. Resolving the next order of expansion yields 



(
x
)
C
e
i
d
x
2
m
2


(
V
(
x
)
)
+
2
m
2


(
E
V
(
x
)
)
4


{\displaystyle \Psi (x)\approx C\left(e^{i\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)}}+\theta }\right)\left({\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)\right)^{-1/2}}

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0
(
x
)
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)
E
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e
d
x
2
m
2


(
V
(
x
)
E
)
2
m
2


(
V
(
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k
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k
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{\displaystyle A(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}A\_{k}(x)}

 and 



B
(
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)
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1
k
=
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k
B
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(
x
)
,


{\displaystyle B(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}B\_{k}(x),}

 with the following constraints on the lowest order terms, 



A
0
(
x
)
2
B
0
(
x
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2
=
2
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(
x
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)


{\displaystyle A\_{0}(x)^{2}-B\_{0}(x)^{2}=2m\left(V(x)-E\right)}

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(
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0
(
x
)
2
B
0
(
x
)
2
=
2
m
(
V
(
x
)
E
)


{\displaystyle A\_{0}(x)^{2}-B\_{0}(x)^{2}=2m\left(V(x)-E\right)}

 and 



A
0
(
x
)
B
0
(
x
)
=
0.


{\displaystyle A\_{0}(x)B\_{0}(x)=0.}

 At this point two extreme cases can be considered.Case 1If the amplitude varies slowly as compared to the phase 



A
0
(
x
)
=
0


{\displaystyle A\_{0}(x)=0}

 and 



B
0
(
x
)
=
2
m
(
E
V
(
x
)
)


{\displaystyle B\_{0}(x)=\pm {\sqrt {2m\left(E-V(x)\right)}}}

 which corresponds to classical motion. Resolving the next order of expansion yields 



(
x
)
C
e
i
d
x
2
m
2


(
V
(
x
)
)
+
2
m
2


(
E
V
(
x
)
)
4


{\displaystyle \Psi (x)\approx C\left(e^{i\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)}}+\theta }\right)\left({\frac {2m}{\hbar ^{2}}}\left(E-V(x)\right)\right)^{-1/2}}

 Case 2If the phase varies slowly as compared to the amplitude, 



B
0
(
x
)
=
0


{\displaystyle B\_{0}(x)=0}

 and 



A
0
(
x
)
=
2
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(
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(
V
(
x
)
E
)
+
C
e
d
x
2
m
2


(
V
(
x
)
E
)
2
m
2


(
V
(
x
)
E
)
4


{\displaystyle \Psi (x)\approx {\frac {C}{+e^{+\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}+C}}e^{-\int dx{\sqrt {{\frac {2m}{\hbar ^{2}}}\left(V(x)-E\right)}}}}

 (displaystyle \Psi (x)) in atomic units (a.u.). The solid lines represent the level set of the Hamiltonian 



H
(
x
,
p
)
=
p

2


/
2
+
U
(
x
)


{\displaystyle H(x,p)=p^{2}/2+U(x)}

. To solve this equation using the semiclassical approximation, each function must be expanded as a power series in (displaystyle \hbar ). From the equations, the power series must start with at least an order of 1 (displaystyle \hbar ^{-1}) to satisfy the real part of the equation; for a good classical limit starting with the highest power of the Planck constant possible is preferable, which leads to 



A
(
x
)
=
1
k
=
0
k
A
k
(
x
)


{\displaystyle A(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}A\_{k}(x)}

 and 



B
(
x
)
=
1
k
=
0
k
B
k
(
x
)
,


{\displaystyle B(x)={\frac {1}{\hbar }}\sum \_{k=0}^{\infty }\hbar ^{-k}B\_{k}(x),}

 with the following constraints on the lowest order terms, 



A
0
(
x
)
2
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0
(
x
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2
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2
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e
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x
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=
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