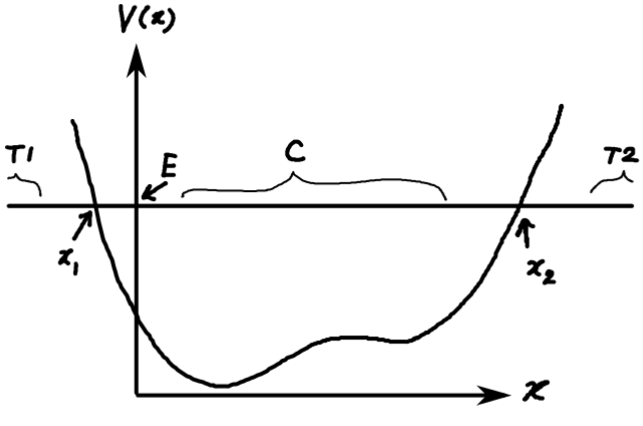
# Notes for Lecture 11

# WKB, cont.

We discuss two extremely important results of the WKB approximation: the Bohr-Sommerfeld quantization rule and the tunneling formula.

## 11.1 WKB and the Bohr-Sommerfeld rule



Consider a problem as depicted above, with energy $E$, and two turning points $x_1$ and $x_2$. The classical region (C) and the tunneling regions (T1, T2) of $x$ values are marked approximately. We assume that the potential energy $V(x)$ keeps going up for $x > x_2$ and $x < x_1$ so that there are no more turning points and no more classical regions than the one shown in the above diagram. The two turning points $x_1$ and $x_2$ are precisely the kinds for which the connection formulae Eqs. 10.15–10.18 apply.

Under these assumptions, in $T1$ we should not have any term that diverges as $x \to -\infty$, since the wave function would not be normalizable otherwise. So, in this region the WKB wave function is given by (from Eq. 10.13)[1]

$$\psi(x) = \frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int_x^{x_1} dx\, \kappa(x)\right) \qquad \text{in region T1} \qquad (11.1)$$

Similarly, for $T2$, we get

$$\psi(x) = \frac{B}{\sqrt{\kappa(x)}} \exp\left(-\int_{x_2}^{x} dx\, \kappa(x)\right) \qquad \text{in region T2} \qquad (11.2)$$

In $C$, we expect a sinusoidal wave function 10.11. We shall use the connection formulae, to write it down.

For connecting the wave function of Eq. 11.1 from the left through $x_1$, Eq. 10.15 applies, and we get

$$\psi(x) = \frac{2A}{\sqrt{k(x)}} \sin\left(\int_{x_1}^{x} dx\, k(x) + \frac{\pi}{4}\right) \qquad \text{in region C} \qquad (11.3)$$

On the other hand, we can also connect the wave function of Eq. 11.2 from the right through $x_2$, using Eq. 10.17. Then, we get

$$\psi(x) = \frac{2B}{\sqrt{k(x)}} \sin\left(\int_{x}^{x_2} dx\, k(x) + \frac{\pi}{4}\right) \qquad \text{in region C} \qquad (11.4)$$

These two different expressions of the wave function must be equal to each other. Define $\alpha \equiv \int_{x_1}^{x_2} dx\, k(x)$, $X \equiv \int_{x}^{x_2} dx\, k(x) + \frac{\pi}{4}$, and note that

$$\begin{aligned}
\sin\left(\int_{x_1}^{x} dx\, k(x) + \frac{\pi}{4}\right) &= \sin\left(\int_{x_1}^{x_2} dx\, k(x) + \int_{x_2}^{x} dx\, k(x) + \frac{\pi}{4}\right) \\
&= \sin\left(\alpha - X + \frac{\pi}{2}\right) \\
&= \cos(\alpha - X) \\
&= \cos\alpha\, \cos X + \sin\alpha\, \sin X
\end{aligned}$$

Therefore, the equality of the two expressions for the wave function in region C means that

$$A\left(\cos\alpha\, \cos X + \sin\alpha\, \sin X\right) = B \sin X$$

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[1] Please do not be alarmed that the upper limit of the integral in the exponent is taken to be $x_1$, the value of $x$ for which this wave function is *not* applicable. All we need to ensure for the WKB wave function in region C is that $x$ is not too close to any turning point. The fixed limit of the integral in the exponent can be taken to be *any* mathematically allowed value, since it contributes to just a constant. However, we are making a judicious choice of the fixed limit here, and for the next wave function, anticipating the use of the connection formulae.

for any value of $X$. This is possibly only if $\cos\alpha = 0$, or

$$\alpha = \int_{x_1}^{x_2} dx\, k(x) \;=\; n\pi + \frac{\pi}{2} \qquad\qquad n = 0, 1, 2, \ldots \tag{11.5}$$

where $n$ starts from 0, since $\alpha$ must be positive by definition. This is the energy quantization condition within the WKB approximation for a potential well with finite slopes. At the same time, we get

$$A(-1)^n \;=\; B \tag{11.6}$$

It is instructive to write the quantization condition in terms of the integral over $p$, by multiplying $\alpha$ by $\hbar$

$$\int_{x_1}^{x_2} dx\, p(x) \;=\; \left(n + \frac{1}{2}\right)\frac{h}{2} \tag{11.7}$$

The integral here is the integral of $p$ over the motion going from $x_1$ to $x_2$. $p(x) = \sqrt{2m(E - V(x))}$ is the *classical* momentum during this motion. Noticing that the classical motion is necessarily a periodic motion, we can ask "what is the corresponding integral in the second half of the motion going from $x_2$ back to $x_1$?" In the second half, we can recognize that the corresponding integral is given by $\int_{x_2}^{x_1} dx\,(-p(x))$, since clearly the momentum must be reversed for the second half[2]. But, this integral is equal in its value to $\int_{x_1}^{x_2} dx\, p(x)$. Thus, we conclude

$$\int_{x_1}^{x_2} dx\, p(x) \;=\; \frac{1}{2}\oint dx\, p(x)$$

where the integral $\oint$ is over one period of the classical motion. Therefore, we obtain the standard form of **the WKB quantization condition** for motion in a potential well whose walls have finite slopes,

$$\oint dx\, p(x) \;=\; \left(n + \frac{1}{2}\right) h \qquad\qquad n = 0, 1, 2, \ldots \text{ but} \gg 1 \tag{11.8}$$

This is a very useful result. This result has close resemblance to the original Bohr-Sommerfeld quantization rule

$$\oint dq\, p_q \;=\; nh \qquad\qquad n = 0, 1, 2, \ldots \text{ but} \gg 1 \tag{11.9}$$

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[2] That this is true for the second half of the motion comes from the time reversal symmetry of the problem. Here, we are *merely* talking about the classical time reversal symmetry, although the same symmetry argument applies, as it should, to the quantum Hamiltonian as well. $H = \frac{p^2}{2m} + V(x)$. Upon time reversal ($t \to -t$), $p \to -p$, but $H \to H$, and so the system is time-reversal invariant. In classical mechanics, this means that that, for a given motion, its time reversed motion (think a movie played backwards) is also a physical motion. What this means for the current problem is that the time reversed motion must be indeed the second half of the motion, due to the uniqueness of the solution to Newton's second law given the same initial conditions.

where $q$ is a generalized coordinate and $p_q$ is its canonical conjugate momentum.

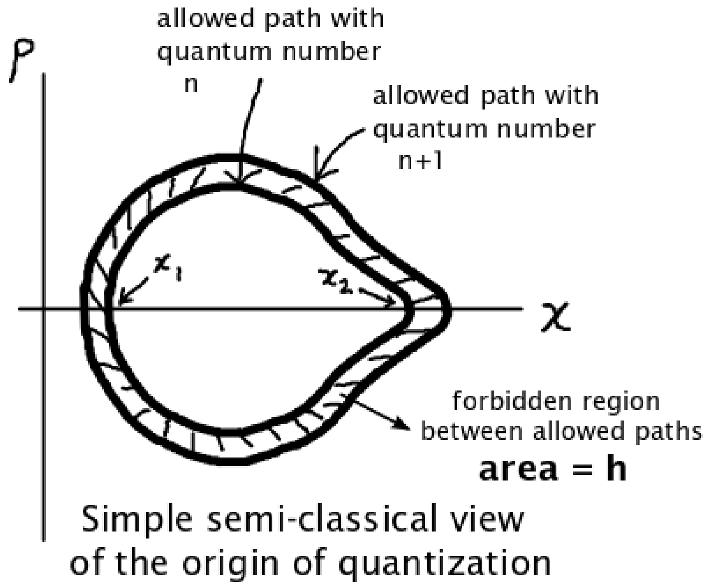
The only difference to be noticed is the offset $\frac{1}{2}$ in the WKB condition. However, this offset should not be taken too seriously. Recall from Section 10.3 that the WKB approximation is valid only when $\hbar/|\int dx p(x)| \ll 1$. We left the exact nature of the integral a bit vague in that section, but now it is quite clear. For a periodic motion inside a potential well, we can take the integral to be $\oint dx\, p(x)$. Then, then condition for $\hbar/|\int dx p(x)| \ll 1$ is simply that $n \gg 1$. But, we knew this from the beginning (cf. the discussion point 1 of page 2 of LN 10)! This self-consistency of the theory is reassuring and pleasing. It also means that $n + \frac{1}{2} \approx n$, and so the offset $\frac{1}{2}$ can be ignored. So, in this sense, the WKB quantization condition and the Bohr-Sommerfeld rule can be viewed as identical.

This is why it is explicitly noted in the above two equations that $n = 0, 1, 2, \ldots$ "but $\gg 1$." You might wonder why we do not write just "$n \gg 1$," since, for example, 0 or 1 is obviously not greater than 1, not to mention much greater than 1. The reason we do not quite let go of these low quantum numbers is explained in Section 11.3. For now, we will be quite aware that the theory that we are doing is valid only for large $n$ values, but we will also keep our knowledge of low $n$ values *from a purely mathematical point of view.*

In the literature, it is customary to write **the Bohr-Sommerfeld quantization rule** as

$$\oint dq\, p_q = (n + \gamma)\, h \qquad n = 0, 1, 2, \ldots \text{ but} \gg 1 \tag{11.10}$$

where $\gamma$ is a constant that depends on the Hamiltonian (see the next section).



The geometrical meaning of the above quantization rule is that the area enclosed by the allowed path of the motion in the phase space is quantized as $(n+\gamma)h$. Then, regardless of the value of $\gamma$, it is clear that the result above implies that the classical orbits in the phase space are quantized in such a way that the area enclosed by the orbit increases by $h$ from one orbit to the next bigger orbit, as shown in the diagram above. This quantization of orbits in the phase space is very important in classical statistical mechanics – without taking it into consideration, the entropy function is ill-defined, or defined only up to an arbitrary constant, in classical statistical mechanics.

## 11.2 $\gamma$ values

The value of $\gamma$ depends on a given one dimensional problem. For the potential considered in the previous section, we obtained $\gamma = \frac{1}{2}$. This is not the only possible value. For instance, for a potential well with two infinite vertical walls (Example T8.1), $\gamma = 0$, and for a potential well with one infinite vertical wall and a sloped wall on the other side (Example T8.3), $\gamma = \frac{3}{4}$. Please read these textbook examples to learn the derivation. When you do, please keep in mind that the $\gamma$ value above is defined with the convention of $n$ starting from 0, while in the textbook, $n$ starts from 1.

Here, let us consider another simple problem and compute the $\gamma$ value for it. Consider a particle moving in one dimension. However, we assume that the one dimensional space is on a circle of radius $R$ as in Section 5.1. In this case, the Hamiltonian is given by

$$\hat{H} = \frac{\hat{L}_\phi^2}{2mR^2} + \hat{V} \doteq -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\phi^2} + V(\phi) \tag{11.11}$$

where we use $\phi$ for the angular coordinate. We require that $V(\phi) = V(\phi + 2\pi)$. Let us assume that the potential $V(\phi)$ has a finite maximum value and $E$ is greater than that maximum value. Then, the WKB wave function is sinusoidal in the entire range of $\phi$, and is given by

$$\psi(\phi) = \frac{A}{\sqrt{p_\phi}}\exp\left(\frac{i}{\hbar}\int_0^\phi d\phi\, p_\phi\right) + \frac{B}{\sqrt{p_\phi}}\exp\left(-\frac{i}{\hbar}\int_0^\phi d\phi\, p_\phi\right) \tag{11.12}$$

$$p_\phi \equiv \sqrt{2mR^2(E - V(\phi))} \tag{11.13}$$

where $p_\phi$ is the magnitude of the classical angular momentum due to the motion along the circle[3], and the integrals in the exponents have been made definite integrals by choosing zero as the lower limit of the integral.

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[3] Since we defined $p_\phi$ to be positive, it corresponds to $|\hat{L}_\phi|$ of quantum mechanics.

The only condition that we need to impose in this case is that the wave function be single-valued, i.e. it has the period of $2\pi$.

$$\psi(\phi + 2\pi) = \psi(\phi) \tag{11.14}$$

By the periodicity of $V(\phi)$, the coefficients of exponentials already have the correct periodicity. Then, the condition $\psi(\phi + 2\pi) = \psi(\phi)$ becomes

$$\begin{aligned} & A \exp\left(\frac{i}{\hbar}\int_0^\phi d\phi\, p_\phi\right) + B \exp\left(-\frac{i}{\hbar}\int_0^\phi d\phi\, p_\phi\right) \\ & \qquad = A \exp\left(\frac{i}{\hbar}\int_0^{\phi+2\pi} d\phi\, p_\phi\right) + B \exp\left(-\frac{i}{\hbar}\int_0^{\phi+2\pi} d\phi\, p_\phi\right) \end{aligned}$$

After splitting the integrals on the right hand side, $\int_0^{\phi+2\pi} = \int_0^\phi + \int_\phi^{\phi+2\pi}$, and then defining $\star \equiv \frac{1}{\hbar}\int_0^\phi d\phi\, p_\phi$, and

$$I \equiv \int_\phi^{\phi+2\pi} d\phi\, p_\phi = \int_0^{2\pi} d\phi\, p_\phi = \oint d\phi\, p_\phi \tag{11.15}$$

the above condition becomes

$$A \exp(i\star) + B \exp(-i\star) = A \exp(i\star)\exp(iI/\hbar) + B \exp(-i\star)\exp(-iI/\hbar)$$

where $\star$ is the only variable quantity in this equation. Multiplying this equation by $\exp(i\star)$, we get

$$A \exp(2i\star) + B = A \exp(2i\star)\exp(iI/\hbar) + B \exp(-iI/\hbar)$$

For this equation to hold for any value of $\star$, we must require that $I/\hbar = 2\pi j$ where $j$ is an integer, i.e., $I = jh$. Keeping in mind that $p_\phi$ is positive, we get the WKB quantization condition

$$\oint d\phi\, p_\phi = (n+1)h \qquad\qquad n = 0, 1, 2, \ldots \text{ but } \gg 1 \tag{11.16}$$

So, in this case, $\gamma = 1$.

Note that the original Bohr-Sommerfeld picture is based on the constructive interference of the wave. In this picture, the value of $\gamma$ can be thought of as accounting for the phase shifts at the boundaries.

## 11.3 Bohr-Sommerfeld rule

Generally, a "rule" in physics means something not quite rigorous, but quite useful in general nevertheless. So, it is a rather subtle thing, and much care must be taken when using a rule.

So, in what sense, is the quantization rule that we described above a “rule”?

You may find this a bit strange, since we really *have proved* the above rule in the semi-classical regime ($n \gg 1$). From this point of view, it is more appropriate to call it “principle,” “law,” or ”theorem,” rather than “rule.” But, we do not. Before we go on, however, let us mention that there *is* a principle that is quite closely related to this Bohr-Sommerfeld quantization rule: Bohr’s correspondence principle, which we shall derive in Section 11.4.

The reason that we call the above quantization rule a “rule” is because, often, this rule is used even when $n$ is very small! Like the minimum small ($n = 0$)! Clearly, we *have not proved* the above rule for small values of $n$, which is truly a quantum regime. But, why would people do such a reckless thing as applying the semi-classical theory to the strictly quantum regime? The answer is simple: because it tends to work *for certain purposes* even in the quantum regime!

This is why we wrote the strange expression “$n = 0, 1, 2, ...$ but $\gg 1$” in the above discussions. The part “$\gg 1$” is worth a principle, but the part “$n = 0, 1, 2, ...$” is worth only a rule, if it so happens, as it does, that the quantization condition is valid in some ways even for these low quantum numbers.

Perhaps the best illustration is the two most important problems of quantum mechanics: the Hydrogen problem and the simple harmonic oscillator (SHO) problem. In both problems, the energy eigenvalues are obtained exactly for all quantum numbers, if $\gamma$ values derived above for each case (1 for the Hydrogen problem, and 1/2 for the SHO problem) are used. Also, an exact solution for the energy is obtained for the infinite square well problem using this approach ($\gamma = 0$; Example T8.1). The SHO problem from this approach is done in a homework problem. Here, we look at the Hydrogen problem.

For the hydrogen problem, defined by Eq. 6.12, we will simply take note of the fact that $\hat{H}$ commutes with $\hat{L}_\phi$, and thus with $\hat{L}_\phi^2$. We shall ignore other components of the angular momentum, and the non-circular motions[4]. That is, we are following the original Bohr model, and considering the semi-classical quantization of the $\phi$ motion only. The eigenvalue problem for $\hat{L}_\phi^2$ is a meaningful one to solve, since energy eigenstates can be written as $\hat{L}_\phi^2$ eigenstates. Therefore, what we did in the previous section is applicable here with $V(\phi) \equiv 0$, since basically what we did in the previous section becomes solving the eigenvalue equation for $\hat{L}_\phi^2$ within the WKB approximation, if we set $V(\phi) = 0$.

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[4] It is possible to treat these things in semi-classical model as well. Then, the energy eigenvalues come out somewhat differently in the quantum limit.

## Values and limits of the Bohr-Sommerfeld rule

When is Eq. 11.10 good?

1. Good as gold in the semi-classical limit ($n \gg 1$).
2. In the quantum limit, it *might* get some energies correct. It may not. Even if it does not, the *qualitative* fact that energy values are quantized is gotten correct by the rule!

   Ask yourself the following question. In quantum mechanics, the energy levels of extended states are not quantized, but those of bound states are quantized – why is this? Extended states correspond to classical motions with one or zero turning points. Bound states have two turning points. Therefore, for extended states, there is no Bohr-Sommerfeld quantization rule (please prove this statement yourself, following the logic of Section 11.1), but, for bound states, there is such a rule. This is a simple and effective answer, while, of course, there is a better, but much more complicated, quantum mechanical answer (which you already (should) know from the first course of quantum mechanics).
3. Even when the rule gets energies correct in the quantum limit, do not be misled into believing that everything is fine. It is not. Bohr model has problems as discussed in LN 7. The concept of the forbidden region and the quantization of orbits in the phase space (diagram in page 4) is cute, but it is correct only in an average sense in the quantum limit. In quantum mechanics, all points in the phase space are occupied by the wave function of an energy eigenstate. Still, the concept of quantized orbit in the phase space is intuitively very catchy. For instance, the ladder operator $\hat{a}$ (or $\hat{a}^\dagger$) in a SHO problem can be thought of as representing, approximately, the radius of a "quantized" circular motion in the properly scaled (cf. Eq. T2.47) phase space, viewed as a complex plane.

So, let us look at the quantization condition

$$\oint d\phi \, p_\phi = nh \qquad\qquad n = 1, 2, \ldots \tag{11.17}$$

where we shifted $n$ by 1, and got rid of $\gamma$. In the semi-classical framework, let us consider a classical circular motion only, for which the speed $v$ and the radius $r$ are constant. In that case, $p_\phi$ is constant $= mvr$. And so, the above quantization condition trivially becomes the Bohr quantization condition $mvr = n\hbar$. From the

Bohr condition, the energy eigenvalues of the Hydrogen problem can be calculated (the result is Eq. 7.10; read the discussions preceding that equation to learn more about the semi-classical calculation, if necessary), and they happen to be exact even in the quantum limit.

## 11.4 Bohr's correspondence principle

Consider two adjacent orbits in the phase space allowed by the Bohr-Sommerfeld quantization rule. In the semi-classical limit, we are allowed to consider each orbit as a classical orbit. The energy difference between the two orbits is small, compared to the energy of each orbit. Let the first orbit be characterized with energy $E$ and period $T$, while the second orbit be characterized with energy $E + dE$ and period $T + dT$, where $dE$ is finite but $dT$ can be zero (for a SHO). In any case, note that the integral

$$I = \oint dq\, p_q \tag{11.18}$$

is a function of $E$, since $p_q = \sqrt{2m(E - V(q))}$. We see that

$$\frac{dI}{dE} = \oint dq \frac{p_q}{2(E - V(q))} = \oint dq \sqrt{\frac{m}{2(E - V(q))}} \tag{11.19}$$

The last expression is equal to $T$, a well-known fact from classical mechanics (e.g. see page 10 of `https://griffin.ucsc.edu/ph105-11/Lecture%2B?action=AttachFile&do=get&target=L05-Conservations-1D-Motion.pdf`).

Since $dI = h$ due to the Bohr-Sommerfeld quantization rule, we get

$$dE = \frac{h}{T} = h\nu = \hbar\omega \tag{11.20}$$

which is the correspondence principle, where $T, \nu = 1/T, \omega = 2\pi\nu$ are all classical quantities, and $dE$ is the energy spacing of quantum levels for high quantum numbers.

This principle can be re-written as

$$\frac{dE}{\hbar} = \omega \tag{11.21}$$

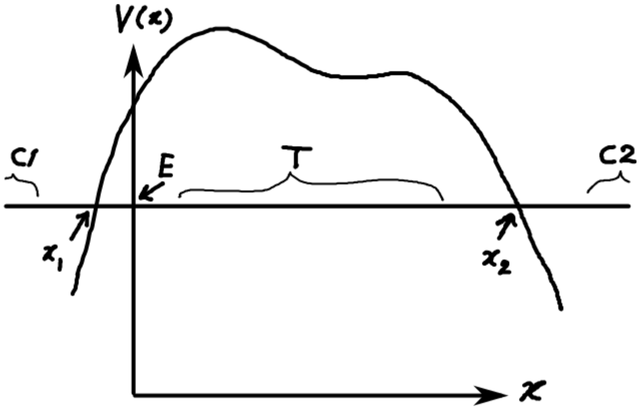
where the LHS is all quantum (i.e. quantum radiation law involving a quantum transition) and the RHS is all classical (i.e. classical radiation law involving an oscillator emitting radiation). That they should agree at high quantum number is a matter of consistency of the two theories (quantum and classical), and for this reason Bohr's correspondence principle can be taken as the fundamental corner stone in all discussions in this lecture and the previous one.

## 11.5 Tunneling

Take the potential of page 1, and flip the potential vertically with respect to the horizontal line at $E$. Then, you have a tunneling problem. In other words, in a tunneling problem, you have a classical region on the left, and then a tunneling region, and then a classical region on the right.

In such a case, one can ask – what is the probability that a particle that is shot from the left will make it to the right side. This is the tunneling probability, an important quantity related to many experiments.

The treatment of this problem is very analogous to what we did above in Section 11.1. One writes down WKB wave functions and apply the connection formulae. This is left for a homework problem (HW5.6). Here, we will use the high/broad barrier limit (or the weak tunneling limit) to obtain a simple solution.



The main observation is that if the barrier potential is high or broad, then the WKB wave function inside the barrier is approximately

$$\psi(x) \approx \frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int_{x_1}^{x} dx\, \kappa(x)\right) \tag{11.22}$$

as the term that exponentially grows must vanish in the limit of high/broad barrier. The dominating contribution for the tunneling amplitude is then given by the exponential function part, which means that the tunneling amplitude $\approx \exp\left(-\int_{x_1}^{x_2} dx\, \kappa(x)\right)$. Then, the tunneling probability, $T$, is given by its square

$$T \approx \exp\left(-2\int_{x_1}^{x_2} dx\, \kappa(x)\right) \tag{11.23}$$

This simple result is very important. Here, symbol $T$ is used for the probability, since it is also what we refer to as the "transmission coefficient" in quantum mechanics or optics.

So far we have been considering a tunneling problem from left to right, where the tunneling barrier starts at $x = x_1$ and ends at $x = x_2$ (for a given energy). Now, suppose that the potential is infinite at $x = x_1 - a$, in addition, and suppose that we put a particle between $x_1 - a$ and $x_1$. This situation is depicted in the diagram below. The particle will go through a periodic motion between $x_1 - a$ and $x_1$. Let the average speed of the particle for this periodic motion be $v$ such that the period is given as $2a/v$. This means that the frequency at which the particle "knocks on the potential barrier at $x_1$" is given by $v/(2a)$. The rate at which the particle succeeds in escaping the potential well is then given by $Tv/(2a)$. The inverse of this number is **the lifetime** of the state in which the particle trapped inside the potential well. If this problem is applied to the alpha decay phenomenon, then this is the lifetime of the nucleus going through an alpha decay, and the particle that we are considering is an alpha particle trapped inside the nucleus. Calling this $\tau$, we get

$$\tau = \frac{2a}{v}\frac{1}{T} = \frac{2a}{v}\exp\left(2\int_{x_1}^{x_2} dx\, \kappa(x)\right) \tag{11.24}$$

This is the basic theory of the $\alpha$ decay. Note that for the alpha decay problem the infinite potential at $x_1 - a$ is unnecessary. The radial equation of the Schrödinger equation naturally limits the value of $r$ to be positive, and so $r \le 0$ is forbidden (so $x_1 - a = 0$, and $x_1 = a$ is the range of the attractive nuclear force). Read Example T8.2 for more details.