5 WKB Approximation

As an alternative solution technique that is of an asymptotic nature, here the **WKB approximation** is introduced, named after Wentzel, Kramers and Brillouin, who developed it in the context of the Schrödinger equation. It is explicitly applied to 2nd order ODEs of the form **M & W, Sec. 1-4**

$$\frac{d^2y}{dx^2} + f(x)\,y \;=\; 0 \quad , \tag{63}$$

where the coefficient $f(x)$ varies slowly with x when compared with $y(x)$.

• Observe that *any* homogeneous, 2nd order linear ODE can be cast in this form using the transformation on pp. 11-12 of Mathews and Walker (Eqs. 1-38 to 1-41). For the homogeneous ODE

$$\frac{d^2\psi}{dx^2} + p(x)\,\frac{d\psi}{dx} + q(x)\,\psi \;=\; 0 \quad . \tag{64}$$

we substitute $\psi(x) = v(x)\,y(x)$. Then the dy/dx term in the ensuing equation is identically zero for the choice

$$2\,\frac{v'(x)}{v(x)} \;=\; -p(x) \quad\Rightarrow\quad v(x) \;=\; \exp\left\{ -\frac{1}{2}\int_{x_0}^{x} p(x')\,dx' \right\} \tag{65}$$

as an effective integrating factor. Then

$$f(x) \;=\; \frac{v''(x)}{v(x)} + p(x)\,\frac{v'(x)}{v(x)} + q(x) \quad\Rightarrow\quad f(x) \;=\; q(x) - \frac{p'(x)}{2} - \frac{[p(x)]^2}{4} \quad . \tag{66}$$

For example, Bessel's equation can be converted into this form, yielding $f(x) = 1 - (n^2 - 1/4)/x^2$, which is slowly varying for $x \gg n$. Accordingly, this highlights the asymptotic character of the ensuing analysis.

• Many physics equations are already in this form. The 1-D Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\Big[E - V(x)\Big]\,\psi \;=\; 0 \tag{67}$$

satisfies the criterion if either the potential $V(x)$ is a slowly-varying function, or $E \gg V(x)$. In addition, the spatial component of the 1-D wave equation [obtained by setting $y \propto \exp(\pm i\,\omega t)$]

$$\frac{\partial^2 y}{\partial x^2} - \frac{1}{c^2}\,\frac{\partial^2 y}{\partial t^2} \;=\; 0 \quad \Rightarrow \quad \frac{d^2 y}{dx^2} + \frac{\omega^2}{c^2}\,y \;=\; 0 \tag{68}$$

is automatically of the desired form if the propagation speed c is a slowly-varying function of x.

• The basic principle of the WKB technique is elementary — it is built upon the fact that when $f(x)$ is constant (call it k^2), the solution is trivial:

$$\frac{d^2 y}{dx^2} + k^2\,y \;=\; 0 \quad \Rightarrow \quad y \;\propto\; e^{\pm i\,kx} \quad . \tag{69}$$

Extrapolating this to cases where $f(x)$ is almost, but not quite, constant, the obvious trial *ansatz* is

$$y \;=\; e^{i\,\phi(x)} \quad \Rightarrow \quad y' \;=\; i\,\phi'\,y \quad \text{and} \quad y'' \;=\; \left[i\,\phi'' - (\phi')^2\right]\,y \quad , \tag{70}$$

where $\phi(x)$ is almost, but not quite a constant times x. Substituting this into Eq. (63) gives

$$\left[i\,\phi'' - (\phi')^2 + f(x)\right]\,y \;=\; 0 \quad . \tag{71}$$

Then follows the key assumption that $|\phi''| \ll f$, a result that is guaranteed for constant f since then $\phi'' = 0$ identically. This then promotes the dropping of that term as a first approximation, to obtain:

$$\phi' \;\approx\; \pm\sqrt{f} \quad \Rightarrow \quad \phi(x) \;\approx\; \pm\int \sqrt{f(x')}\,dx' \quad . \tag{72}$$

Accordingly, with this form, $\exp\{i\,\phi(x)\}$ is the first approximation to the solution of Eq. (63).

• We now seek a refinement to this, which is obtained by iteration. Starting with Eq. (72), we can derive $\phi'' \approx \pm f'/(2\sqrt{f})$, and insert this into Eq. (71). The result can be solved for ϕ' to give

$$\begin{aligned} \phi' \;&\approx\; \pm\sqrt{f \pm \frac{i}{2}\,\frac{f'}{\sqrt{f}}} \;\approx\; \pm\sqrt{f} + \frac{i}{4}\,\frac{f'}{f} \\ \phi(x) \;&\approx\; \pm\int \sqrt{f(x')}\,dx' + \frac{i}{4}\,\log_e f(x) \quad . \end{aligned} \tag{73}$$

The second term on the second line therefore serves as our correction term. Note that the $\pm$ choice for ϕ' in Eq. (72) uniquely specifies the $\pm$ under the square root sign in Eq. (73), and they combine to yield a net positive sign for the $\log_e f$ term. The final result for the **WKB approximation** is **M & W, pp. 27-8**

$$\boxed{y(x) \;\approx\; \frac{1}{[f(x)]^{1/4}}\, \exp\left\{\pm i \int \sqrt{f(x')}\, dx'\right\} \quad .} \tag{74}$$

• Observe that in mathematical character, this is very similar to the **method of steepest descents** (to be studied later) that is used to evaluate integrals, highlighting the relationship between differential and integral equations.

• Observe that if $f(x) > 0$, the solutions are oscillatory in nature, whereas for $f(x) < 0$ they possess exponential character.

• **Example 8:** Consider the wave equation in Eq. (69), with the wavenumber given by $k = \omega/c$. Suppose the wave frequency ω is constant, but that the wave speed $c = c_0(1 - x/L)$ (for $x \ll L$) varies slowly over space on a scale of the order of the damping scale L. Then for $k_0 = \omega/c_0$,

$$f(x) \;=\; k^2 \;\approx\; k_0^2 \left(1 + \frac{2x}{L}\right) \quad\Rightarrow\quad \sqrt{f(x)} \;\approx\; k_0 \left(1 + \frac{x}{L}\right) \quad , \tag{75}$$

and the WKB approximation generates the solution

$$y(x) \;\approx\; \left(1 - \frac{x}{2L}\right) \exp\left[\pm i\, k_0 x \left(1 + \frac{x}{2L}\right)\right] \quad . \tag{76}$$

This is a propagating wave whose wavenumber slowly increases (wavelength decreases) in x, and whose amplitude decreases at the same time: this means <u>it loses energy</u>, appropriate for the interpretation of electromagnetic waves.

$*$ This highlights the coupling between real parts (propagation) and imaginary parts (damping) of the wave's phase ϕ [see Eq. (73)] that exemplify **dispersion theory** in action, in this case where the speed of wave propagation and **refractive index** are spatially-dependent.

• As a final note, with $\phi' \approx \pm\sqrt{f}$, the condition for validity of the WKB approximation becomes

$$|\phi''| \approx \frac{1}{2}\left|\frac{f'}{\sqrt{f}}\right| \ll |f| \quad . \tag{77}$$

Observe that $1/\sqrt{f} \sim 1/k$ is of the order of *one wavelength* if the solution is oscillatory, or *one e-folding length* if it is exponential (i.e., when $f < 0$). Accordingly, the approximation is valid if the fractional change in $f(x)$ is small over either the wavelength or the e-folding length, as appropriate.

6 Numerical Solutions: Euler's Method

Euler's algorithm for the numerical solution of ordinary differential equations is usually applied to first order ODEs of the form **Garcia, pp. 39-41**

$$\frac{d}{dx}\, y(x) \;=\; f(x,\, y) \quad , \tag{78}$$

with the initial condition $y(x_0) = y_0$. The form of $f(x,\, y)$ can be explicitly known, or it could be more involved such as an integral expression appearing in an integro-differential equation. In principal, a step-by-step solution may be developed to arbitrary accuracy using a Taylor series expansion

$$y(x+h) \;=\; y(x) + h\, y'(x) + \frac{h^2}{2!}\, y''(x) + \frac{h^3}{3!}\, y'''(x) + \dots \tag{79}$$

In practice, evaluating higher order derivatives can be tedious, regardless of whether they provide numerical or analytic tasks.

• Therefore, **Euler's method** truncates the Taylor expansion, and usually the compromise between expediency and precision dictates carrying calculations up to at most the 4th order derivatives. If only the linear term is kept, then one can perform a sequence of iterations **A&W Sec. 8.2**

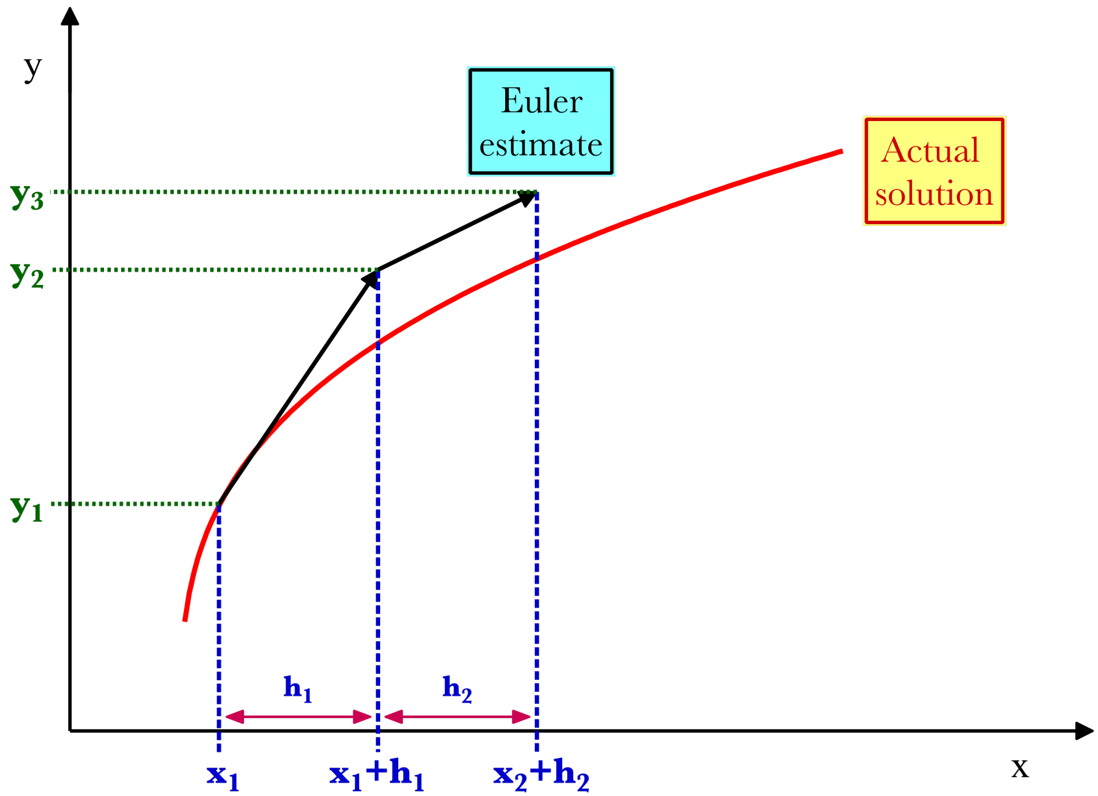
$$y_{k+1} \;= y_k + h_k\, y'_k \;=\; y_k + h_k\, f(x_k,\, y_k) \quad , \quad h_k \;=\; x_{k+1} - x_k \quad , \tag{80}$$

to cover an interval $[x_0,\, x_n]$ spanned by the set of sub-interval dividing points x_k. The point $(x_0,\, y_0)$ provides a boundary condition. The set y_k defines an approximate solution to the ODE, and for this case of retaining only linear derivatives, quickly becomes highly erroneous as k increases.

Plot: Euler's method: Fixed and Variable Steps

$*$ Normally, the sub-interval widths h_k are set to an identical value h, but this protocol does not have to followed, particularly of the variation of $y(x)$ changes considerably over the interval $[x_0,\, x_n]$, i.e. y' possesses considerable dynamic range. Then variable steps h_k can be employed to advantage.

Euler's Method for ODE Solution



Euler's method numerically solves first order ODEs of the form

$$\frac{d}{dx}y(x) = f(x,y) \quad \text{using} \quad y(x+h) = y(x) + \sum_{n=1}^{\infty} \frac{h^n}{n!} y^{(n)}(x) \quad .$$

It usually truncates the Taylor series expansion at up to four terms. When specialized to linear truncations, a sequence of iterations is performed:

$$y_{k+1} = y_k + h_k\, y'_k = y_k + h_k\, f(x_k, y_k) \quad , \quad h_k = x_{k+1} - x_k \quad .$$

$*$ Denser sampling, i.e. smaller h, usually provides greater numerical precision, provided that the function $f(x, y)$ has acceptable pathology, such as being devoid of singularities on $[x_0, x_n]$. However, to more readily achieve this, it is wiser to generalize the algorithm to include higher order derivatives.

• To extend Euler's technique to higher derivatives, one can differentiate Eq. (78) implicitly, which is quite routine using symbolic languages such as `Mathematica` or `Maple`. The sequence of differential operations d/dx automatically maps over to a sequence of algebraic evaluations:

$$\begin{aligned} \frac{d^2y}{dx^2} &= \frac{d}{dx} f(x, y(x)) = \frac{\partial}{\partial x} f(x, y(x)) + \frac{dy}{dx}\frac{\partial}{\partial y} f(x, y(x)) \\ &\equiv \frac{\partial}{\partial x} f(x, y(x)) + f(x, y(x))\frac{\partial}{\partial y} f(x, y(x)) \quad , \end{aligned} \tag{81}$$

followed by

$$\begin{aligned} \frac{d^3y}{dx^3} &= \frac{\partial}{\partial x}\left(\frac{d^2y}{dx^2}\right) + f(x, y(x))\frac{\partial}{\partial y}\left(\frac{d^2y}{dx^2}\right) \quad , \\ \frac{d^4y}{dx^4} &= \frac{\partial}{\partial x}\left(\frac{d^3y}{dx^3}\right) + f(x, y(x))\frac{\partial}{\partial y}\left(\frac{d^3y}{dx^3}\right) \quad . \end{aligned} \tag{82}$$

If the functional form of f is known, then the right hand sides of these equations assume algebraic forms that are readily computed. If it is not, then the Euler technique is more involved, requiring numerical evaluations of the derivatives at each x_k, but is of similar precision and robustness.

Plot: Example of Euler's method using `Mathematica`

• Finally, note that second order ODEs can simply be distilled into two simultaneous first order ODEs, for y and $v = dy/dx$, and the Euler technique then employed in a slightly more involved construction.

Euler's ODE Method: Mathematica Example

- Let us examine Euler's method using `Mathematica` for the solution of

$$\frac{d}{dx}y(x) = f(x,y) \quad , \quad f(x,y) = x^2 + y \quad .$$

The function on the RHS and the sequence of derivatives can be encoded

```
 f[x_, y_ ] := x^2 + y ,
f2[x_, y_ ] := Factor[ D[f[x,y],x] + D[f[x,y],y] f[x,y] ];
f3[x_, y_ ] := Factor[ D[f2[x,y],x] + D[f2[x,y],y] f[x,y] ];
f4[x_, y_ ] := Factor[ D[f3[x,y],x] + D[f3[x,y],y] f[x,y] ];
```

The iterative steps require an operator that expresses the increments of the truncated Taylor series evaluation:

```
euler4[{x_,y_}] = { x+h, y+h*f[x,y]+(h^2/2)*f2[x,y]
                         +(h^3/6)*f3[x,y]+(h^4/24)*f4[x,y] }
```

The initial conditions and interval size are specified using

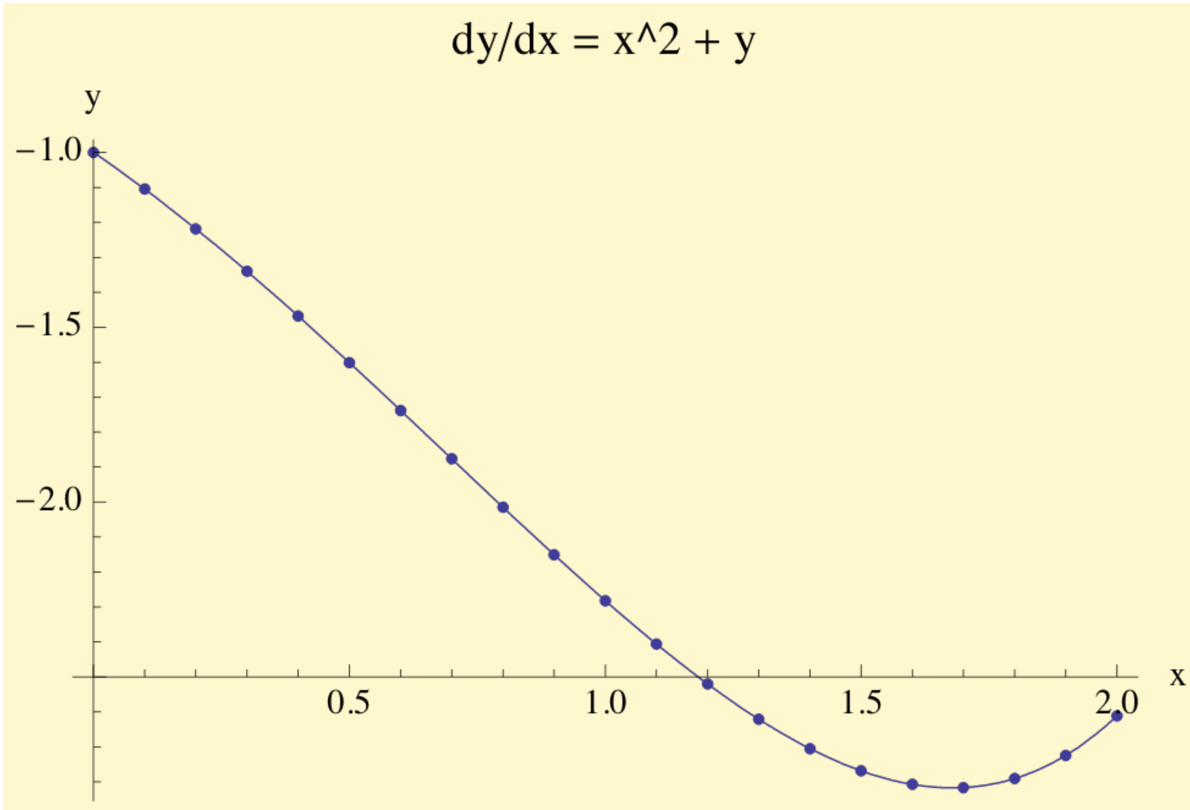
```
h = 0.1; x0 = 0.0; y0 = -1.0;
```

Then the iteration is performed using the `Nestlist[]` sequential operation to generate a data table for the numerical solution:

```
outlist = NestList[euler4, {x0,y0},20]
```

and can be compared with the exact solution obtained using `Mathematica`.

Euler's ODE Method: Solution



- Comparison of the Euler's method numerical solution (dots) to the exact solution of the ODE, $e^x - 2 - 2x - x^2$ (solid curve).
- The precision is excellent when expanding the Taylor series of derivatives to the fourth order.

7 Runge-Kutta Technique

[*Reading Assignment: This is so that you know that it exists!*]

The Euler technique effectively amounts to an iteration on the value of y and its first four derivatives. In a discrete scheme, these derivatives can be approximated by **finite difference** methods, so that information about y at a point x_k and its predecessor points $c_{k-1}\dots$ can be used to approximate the derivatives. Hence, one can devise an iterative scheme that uses such differences, and therefore is eminently suited to tackling problems where the function $f(x,\, y)$ is of a numerical nature. The **Runge-Kutta method** is just such a refinement, and computes solutions to ODEs with an error of the order of h^5. Here, we just state the iterative difference equations, without derivation, and provide an illustrative example; the reader can refer to Section 3.2 of Garcia, *Numerical Methods for Physics* for more details.

Garcia, Sec. 3.2

Fourth-order Runge-Kutta technique: Given a first order ODE of the form in Eq. (78), the relevant formulas for computing the point $(x_{n+1},\, y_{n+1})$ given all preceding points $(x_k,\, y_k)$ for $k = 0, 1 \dots n$, are

$$y_{n+1} \;=\; y_n + \frac{1}{6}\Bigl[k_0 + 2k_1 + 2k_2 + k_3\Bigr] \quad , \tag{83}$$

where

$$\begin{aligned} k_0 &= h\, f(x_n,\, y_n) \quad , \\ k_1 &= h\, f(x_n + h/2,\, y_n + k_0/2) \quad , \\ k_2 &= h\, f(x_n + h/2,\, y_n + k_1/2) \quad , \\ k_3 &= h\, f(x_n + h,\, y_n + k_2) \quad . \end{aligned} \tag{84}$$

The Runge-Kutta method is stable, meaning that small errors do not get amplified. This contrasts the Euler technique, which can be quite unstable, especially when of low order.

$*$ We shall discover in due course that the structure of this system of equations is very reminiscent of **Simpson's rule** for numerical integration, a consequence of the similar origins for the two constructions.

- **Example 10:** The Runge-Kutta scheme can be applied to the same ODE as in Example 9 using the following Mathematica coding:

```
f[x_, y_ ] := x^2 + y ;
RK[{x_,y_}] := Module[{k1,k2,k3,k4},
                k1=h*f[x,y];
                k2=h*f[x+h/2,y+k1/2];
                k3=h*f[x+h/2,y+k2/2];
                k4=h*f[x+h,y+k3];
                  {x+h, y+(1/6)*(k1+2*k2+2*k3+k4)}]

h = 0.1; x0 = 0.0; y0 = -1.0;
outlist = NestList[RK, {x0,y0},20]
```

This can then be compared with the exact solution, just as for the Euler method, and for all intensive purposes the plot is identical to that above.