Q3)

Function to expand g = -∇Φ upto nth order

In[208]:= `gn[a_, q_, p_, n_] := Series[g[q + 1/2 p a h], {h, 0, n}]`

First step

Δt = a h

In[209]:= `q1 = q + p a h + 1/2 a^2 h^2 gn[a, q, p, 2]`

Out[209]= $q + a\,p\,h + \frac{1}{2} a^2 g[q]\,h^2 + \frac{1}{4} a^3 p\,g'[q]\,h^3 + \frac{1}{16} a^4 p^2 g''[q]\,h^4 + O[h]^5$

In[210]:= `p1 = p + a h gn[a, q, p, 3]`

Out[210]= $p + a\,g[q]\,h + \frac{1}{2} a^2 p\,g'[q]\,h^2 + \frac{1}{8} a^3 p^2 g''[q]\,h^3 + \frac{1}{48} a^4 p^3 g^{(3)}[q]\,h^4 + O[h]^5$

Second step

Δt = b h

In[211]:= `q2 = q1 + p1 b h + 1/2 b^2 h^2 gn[b, q1, p1, 4] // Simplify`

Out[211]= $q + (a+b)\,p\,h + \frac{1}{2}(a+b)^2 g[q]\,h^2 + \frac{1}{4}\left(a^3 + 2 a^2 b + 2 a b^2 + b^3\right) p\,g'[q]\,h^3 + \frac{1}{16}(a+b)\left(4 a b^2 g[q]\,g'[q] + \left(a^3 + a^2 b + 3 a b^2 + b^3\right) p^2 g''[q]\right) h^4 + O[h]^5$

In[212]:= `p2 = p1 + b h gn[b, q1, p1, 5] // Simplify`

Out[212]= $p + (a+b)\,g[q]\,h + \frac{1}{2}(a+b)^2 p\,g'[q]\,h^2 + \frac{1}{8}(a+b)\left(4 a b\,g[q]\,g'[q] + \left(a^2 + 3 a b + b^2\right) p^2 g''[q]\right) h^3 + \frac{1}{48}(a+b)\,p\left(12 a^2 b\,g'[q]^2 + 12 a b\,(2a+b)\,g[q]\,g''[q] + \left(a^3 + 7 a^2 b + 5 a b^2 + b^3\right) p^2 g^{(3)}[q]\right) h^4 + O[h]^5$

Third step

$\Delta t = a\ h$

In[213]:=
```
q3 = q2 + p2 a h + 1/2 a^2 h^2 gn[a, q2, p2, 4] // Simplify
```

Out[213]= $q + (2a+b)\,p\,h + \frac{1}{2}(2a+b)^2 g[q]\,h^2 + \frac{1}{4}\left(6a^3+8a^2b+4ab^2+b^3\right) p\,g'[q]\,h^3 + \frac{1}{16}(2a+b)\left(4a(a+b)^2 g[q]\,g'[q] + \left(6a^3+8a^2b+4ab^2+b^3\right) p^2 g''[q]\right) h^4 + O[h]^5$

In[214]:=
```
p3 = p2 + a h gn[a, q2, p2, 5] // Simplify
```

Out[214]= $p + (2a+b)\,g[q]\,h + \frac{1}{2}(2a+b)^2 p\,g'[q]\,h^2 + \left(a(a+b)^2 g[q]\,g'[q] + \frac{1}{8}\left(10a^3+16a^2b+8ab^2+b^3\right) p^2 g''[q]\right) h^3 + \frac{1}{48}(2a+b)\,p\left(12a(a+b)^2 g'[q]^2 + 36a(a+b)^2 g[q]\,g''[q] + \left(14a^3+24a^2b+12ab^2+b^3\right) p^2 g^{(3)}[q]\right) h^4 + O[h]^5$

Taylor expansions of q and p

Substitutions for q'', q''' etc. in terms of g, g', etc.

In[215]:=
```
sq = Table[D[q[t], {t, n}] -> D[g[q[t]], {t, n - 2}], {n, 2, 5}]
```

Out[215]= $\{q''[t] \to g[q[t]],\ q^{(3)}[t] \to g'[q[t]]\,q'[t],\ q^{(4)}[t] \to q'[t]^2 g''[q[t]] + g'[q[t]]\,q''[t],\ q^{(5)}[t] \to 3q'[t]\,g''[q[t]]\,q''[t] + q'[t]^3 g^{(3)}[q[t]] + g'[q[t]]\,q^{(3)}[t]\}$

Substitutions for p', p'' etc. in terms of g, g', etc.

In[216]:=
```
sp = Table[D[p[t], {t, n}] -> D[g[q[t]], {t, n - 1}], {n, 1, 5}]
```

Out[216]= $\{p'[t] \to g[q[t]],\ p''[t] \to g'[q[t]]\,q'[t],\ p^{(3)}[t] \to q'[t]^2 g''[q[t]] + g'[q[t]]\,q''[t],\ p^{(4)}[t] \to 3q'[t]\,g''[q[t]]\,q''[t] + q'[t]^3 g^{(3)}[q[t]] + g'[q[t]]\,q^{(3)}[t],\ p^{(5)}[t] \to 3g''[q[t]]\,q''[t]^2 + 6q'[t]^2 q''[t]\,g^{(3)}[q[t]] + 4q'[t]\,g''[q[t]]\,q^{(3)}[t] + q'[t]^4 g^{(4)}[q[t]] + g'[q[t]]\,q^{(4)}[t]\}$

Expansion of q(t+h)

In[217]:=
```
qh = Series[q[t + h], {h, 0, 4}] //. sq /. {q[t] → q, q'[t] → p} // Simplify
```

Out[217]= $q + p\,h + \frac{1}{2} g[q]\,h^2 + \frac{1}{6} p\,g'[q]\,h^3 + \frac{1}{24}\left(g[q]\,g'[q] + p^2 g''[q]\right) h^4 + O[h]^5$

Expansion of p(t+h)

In[218]:=
```
ph =
  Series[p[t+h], {h, 0, 4}] /. sp /. sq /. {q[t] → q, q'[t] → p, p[t] → p} // Simplify
```

Out[218]= $p + g[q]\, h + \frac{1}{2} p\, g'[q]\, h^2 + \frac{1}{6} \left(g[q]\, g'[q] + p^2 g''[q]\right) h^3 + \frac{1}{24} p \left(g'[q]^2 + 3\, g[q]\, g''[q] + p^2 g^{(3)}[q]\right) h^4 + O[h]^5$

Matching coefficients of expansion for q

Coefficients of powers of h in the taylor expansion for q should match with the corresponding coefficients of q3

In[219]:=
```
s = Solve[q3 == qh, {a, b}]
```

Out[219]= $\left\{\left\{a \to \frac{1}{3}\left(2 + \frac{1}{2^{1/3}} + 2^{1/3}\right),\ b \to \frac{1}{3}\left(-1 - 2 * 2^{1/3} - 2^{2/3}\right)\right\},\right.$
$\left\{a \to \frac{2}{3} - \frac{1 - i\sqrt{3}}{6 * 2^{1/3}} - \frac{1 + i\sqrt{3}}{3 * 2^{2/3}},\ b \to -\frac{1}{3} + \frac{1}{3 * 2^{1/3}} + \frac{2^{1/3}}{3} - \frac{i}{2^{1/3}\sqrt{3}} + \frac{i\, 2^{1/3}}{\sqrt{3}}\right\},$
$\left.\left\{a \to \frac{2}{3} - \frac{1 - i\sqrt{3}}{3 * 2^{2/3}} - \frac{1 + i\sqrt{3}}{6 * 2^{1/3}},\ b \to -\frac{1}{3} + \frac{1}{3 * 2^{1/3}} + \frac{2^{1/3}}{3} + \frac{i}{2^{1/3}\sqrt{3}} - \frac{i\, 2^{1/3}}{\sqrt{3}}\right\}\right\}$

Taking only the real solutions for a and b

In[220]:=
```
s1 = s[[1]]
```

Out[220]= $\left\{a \to \frac{1}{3}\left(2 + \frac{1}{2^{1/3}} + 2^{1/3}\right),\ b \to \frac{1}{3}\left(-1 - 2 * 2^{1/3} - 2^{2/3}\right)\right\}$

Substituting back values back to check

In[221]:=
```
q3 /. s1 // Simplify
```

Out[221]= $q + p\, h + \frac{1}{2} g[q]\, h^2 + \frac{1}{6} p\, g'[q]\, h^3 + \frac{1}{24}\left(g[q]\, g'[q] + p^2 g''[q]\right) h^4 + O[h]^5$

In[222]:=
```
qh
```

Out[222]= $q + p\, h + \frac{1}{2} g[q]\, h^2 + \frac{1}{6} p\, g'[q]\, h^3 + \frac{1}{24}\left(g[q]\, g'[q] + p^2 g''[q]\right) h^4 + O[h]^5$

Matching coefficients of expansion for p

Coefficients of powers of h in the taylor expansion for p should match with

the corresponding coefficients of p3

In[223]:= `s = Solve[p3 == ph, {a, b}]`

Out[223]=
$$\left\{\left\{a \to \frac{1}{3}\left(2 + \frac{1}{2^{1/3}} + 2^{1/3}\right),\ b \to \frac{1}{3}\left(-1 - 2 * 2^{1/3} - 2^{2/3}\right)\right\},\right.$$
$$\left\{a \to \frac{2}{3} - \frac{1 - i\sqrt{3}}{6 * 2^{1/3}} - \frac{1 + i\sqrt{3}}{3 * 2^{2/3}},\ b \to -\frac{1}{3} + \frac{1}{3 * 2^{1/3}} + \frac{2^{1/3}}{3} - \frac{i}{2^{1/3}\sqrt{3}} + \frac{i\, 2^{1/3}}{\sqrt{3}}\right\},$$
$$\left.\left\{a \to \frac{2}{3} - \frac{1 - i\sqrt{3}}{3 * 2^{2/3}} - \frac{1 + i\sqrt{3}}{6 * 2^{1/3}},\ b \to -\frac{1}{3} + \frac{1}{3 * 2^{1/3}} + \frac{2^{1/3}}{3} + \frac{i}{2^{1/3}\sqrt{3}} - \frac{i\, 2^{1/3}}{\sqrt{3}}\right\}\right\}$$

Taking only the real solutions for a and b

In[224]:= `s2 = s[[1]]`

Out[224]=
$$\left\{a \to \frac{1}{3}\left(2 + \frac{1}{2^{1/3}} + 2^{1/3}\right),\ b \to \frac{1}{3}\left(-1 - 2 * 2^{1/3} - 2^{2/3}\right)\right\}$$

Substituting back values back to check

In[225]:= `p3 /. s2 // Simplify`

Out[225]=
$$p + g[q]\, h + \frac{1}{2} p\, g'[q]\, h^2 + \frac{1}{6}\left(g[q]\, g'[q] + p^2 g''[q]\right) h^3 + \frac{1}{24} p\left(g'[q]^2 + 3\, g[q]\, g''[q] + p^2 g^{(3)}[q]\right) h^4 + O[h]^5$$

In[226]:= `ph`

Out[226]=
$$p + g[q]\, h + \frac{1}{2} p\, g'[q]\, h^2 + \frac{1}{6}\left(g[q]\, g'[q] + p^2 g''[q]\right) h^3 + \frac{1}{24} p\left(g'[q]^2 + 3\, g[q]\, g''[q] + p^2 g^{(3)}[q]\right) h^4 + O[h]^5$$

Showing that both solutions are equal

In[227]:= `s2 == s1`

Out[227]= `True`

Final solution for a and b

In[228]:= `s1`

Out[228]=
$$\left\{\mathbf{a} \to \frac{1}{3}\left(2 + \frac{1}{2^{1/3}} + 2^{1/3}\right),\ \mathbf{b} \to \frac{1}{3}\left(-1 - 2 * 2^{1/3} - 2^{2/3}\right)\right\}$$