In[◦]:=

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TABLE I. Parameter values for a two-soliton solution that describe the entire 1YRF protein with accuracy 0.72 Å. We also present parameters for soliton-1 that describes the first loop (sites 2–13) with accuracy 0.75 Å, and t corresponding values for soliton-2 that describes the second loop (sites 14–33) with accuracy 0.28 Å.

parameter	b	c	d	e	q	m_1	m_2
1st set	$-3.070816340e-04$	$4.461893869e-01$	$1.142581922e-02$	$7.675000601e-04$	$-3.704049149e-03$	1.423206983	1.616099122
2nd set	$-1.095208557e-04$	1.172495797	$5.811514400e-04$	$2.013501270e-04$	$-2.880826898e-04$	1.520126333	1.540139296
soliton-1	$1.800314201e-04$	0.4222887366	$7.02765265e-03$	$4.663610215e-04$	$-2.190120515e-03$	1.444455611	1.565166201
soliton-2	$-2.22159366e-04$	1.088046084	$1.308858509e-03$	$3.94423507e-04$	$-6.4844084e-04$	1.518466566	1.543914339

;

In[◦]:=

$$U[\kappa] = -\left(\frac{bd - eq}{2b}\right)^2 \frac{1}{e + b\kappa^2} - \left(\frac{q^2 + 8bcm^2}{4b}\right)\kappa^2 + c\kappa^4. \; ;$$

In[3]:=

```
ClearAll["Global`*"]
```

In[4]:=

```
U = -((b d - e q) / (2 b))^2 / (e + b k^2) - (q^2 + 8 b c m^2) / (4 b) k^2 + c k^4;
D[U, k] /. k → u[i][t]
```

Out[4]=

$$-\frac{\left(8\,b\,c\,m^2 + q^2\right)\,u[i][t]}{2\,b} + 4\,c\,u[i][t]^3 + \frac{(b\,d - e\,q)^2\,u[i][t]}{2\,b\,\left(e + b\,u[i][t]^2\right)^2}$$

In[45]:=
```
a = Pi / 2
j = 2;
L = 200;
b = -0.000222159366;
c = 1.088046084;
d = 0.001308858509;
e = 0.000394423507;
q = -0.00064844084;
m = 1.518466566;
delta = 0.7;
h = 2;
grid = Range[-L / 2, L / 2, h]
k = Length[grid]
deltaHat = h * delta
var = Table[u[i][t], {i, k}];

eqs = Table[u[i]''[t] - (u[i + 1][t] + u[i - 1][t] - 2 * u[i][t]) + deltaHat * u[i]'[t] -
    (8 b c m^2 + q^2) u[i][t] / (2 b) + 4 c u[i][t]^3 + (b d - e q)^2 u[i][t] / (2 b (e + b u[i][t]^2)^2) == 0, {i, 2, k - 1}];

bc = {u[1][t] == 0, u[k][t] == 0};
ic = Join[Thread[var == a * Sin[j * Pi * h * grid / L]] /. t → 0,
   Table[u[i]'[0] == 0, {i, 2, k - 1}]];
```

Out[45]=

$\frac{\pi}{2}$

Out[56]=

{-100, -98, -96, -94, -92, -90, -88, -86, -84, -82, -80, -78, -76, -74, -72,
 -70, -68, -66, -64, -62, -60, -58, -56, -54, -52, -50, -48, -46, -44,
 -42, -40, -38, -36, -34, -32, -30, -28, -26, -24, -22, -20, -18, -16,
 -14, -12, -10, -8, -6, -4, -2, 0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24,
 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62,
 64, 66, 68, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90, 92, 94, 96, 98, 100}

Out[57]=

101

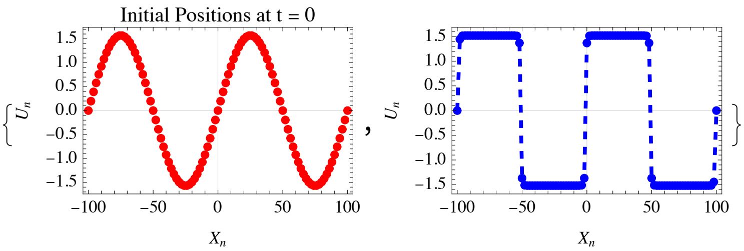
Out[58]=

1.4

In[63]:=
```
tmax = 3000;
sol = NDSolve[Join[eqs, {u[1]'[t] == 0, u[k]'[t] == 0}, ic], var, {t, 0, tmax},
  Method → {"LinearlyImplicitEuler"}, StartingStepSize → 0.01];
```

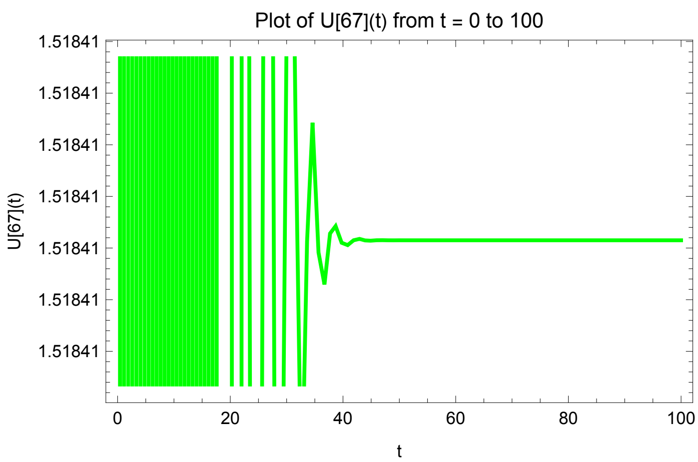
In[64]:=
```
{ListPlot[Transpose[{grid, var /. sol[[1]] /. t → 0}],
   FrameLabel → {"\!\(\*SubscriptBox[\(X\), \(n\)]\)",
     "\!\(\*SubscriptBox[\(U\), \(n\)]\)"},
   PlotLabel → "Initial Positions at t = 0", PlotTheme → "Scientific",
   PlotStyle → {Red, PointSize[Medium]}],
  Show[ListPlot[Transpose[{grid, var /. sol[[1]] /. t → tmax}],
    FrameLabel → {"\!\(\*SubscriptBox[\(X\), \(n\)]\)",
      "\!\(\*SubscriptBox[\(U\), \(n\)]\)"}, PlotLabel → "",
    PlotTheme → "Scientific", PlotStyle → {Blue, PointSize[Medium]}],
   ListLinePlot[Transpose[{grid, var /. sol[[1]] /. t → tmax}],
    {PlotStyle → {Blue, Dashed}}]]}
```

Out[64]=



In[65]:=
```
(*Plotting U[67](t) from t=0 to t=100*)
Plot[Evaluate[u[67][t] /. sol], {t, 0, 100},
 PlotStyle → Green, Frame → True, FrameLabel → {"t", "U[67](t)"},
 PlotLabel → "Plot of U[67](t) from t = 0 to 100"]
```

Out[65]=



In[66]:=
```
(*Extract the interpolation function and evaluate at t=3.0 for U[100]*)
u100Value = With[{uFunc = u[100][t] /. sol[[1]]}, uFunc /. t → 3.0]
```

Out[66]=

```
-1.52993
```