2019.12.4
物性物理学C

ランジュバン方程式

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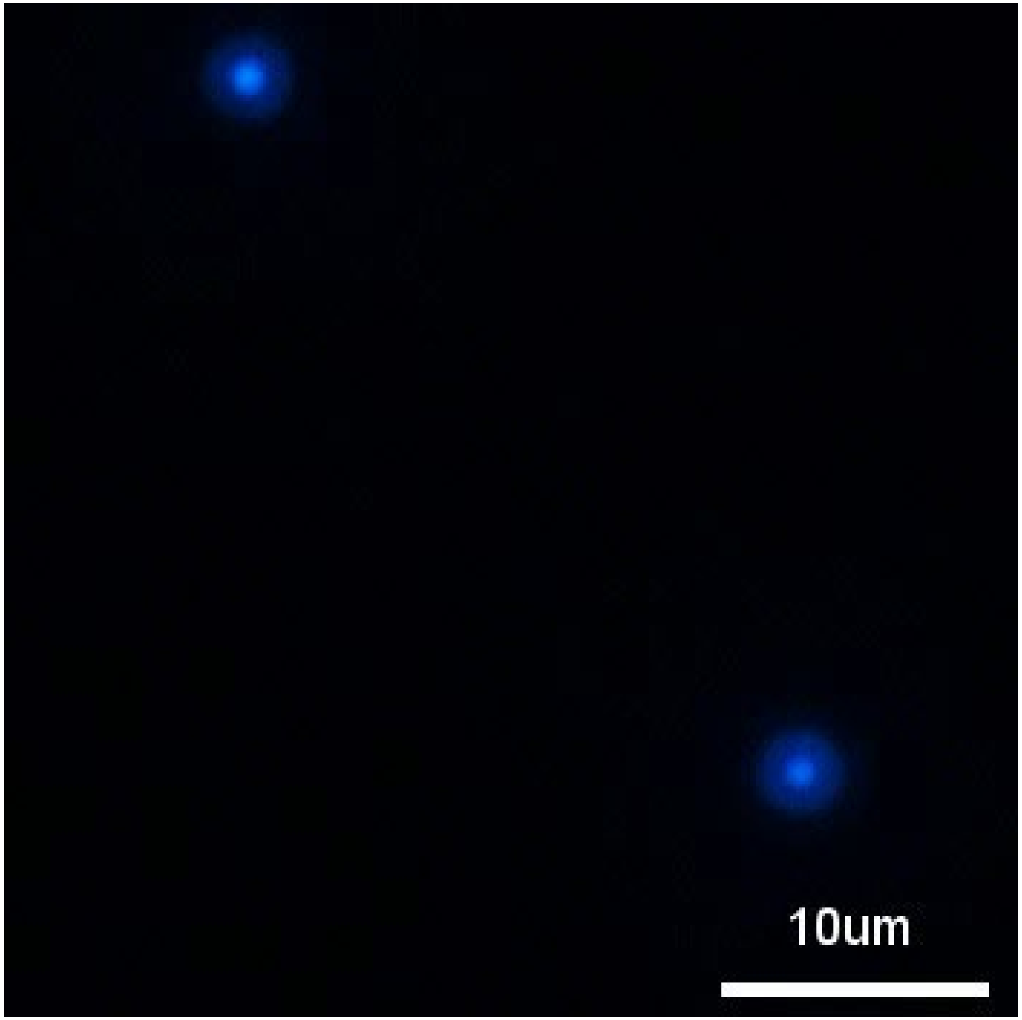
ブラウン運動

ナノ粒子



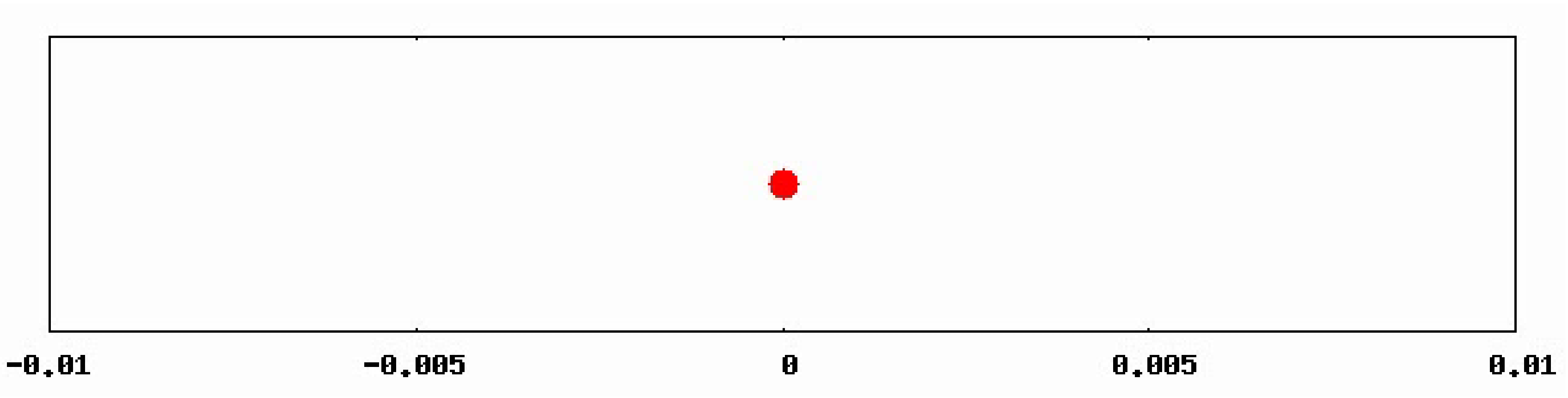
Langevin方程式

$$m\frac{\mathrm{d}^2\boldsymbol{r}}{\mathrm{d}t^2} = -\gamma\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} + \boldsymbol{\xi}(t)$$

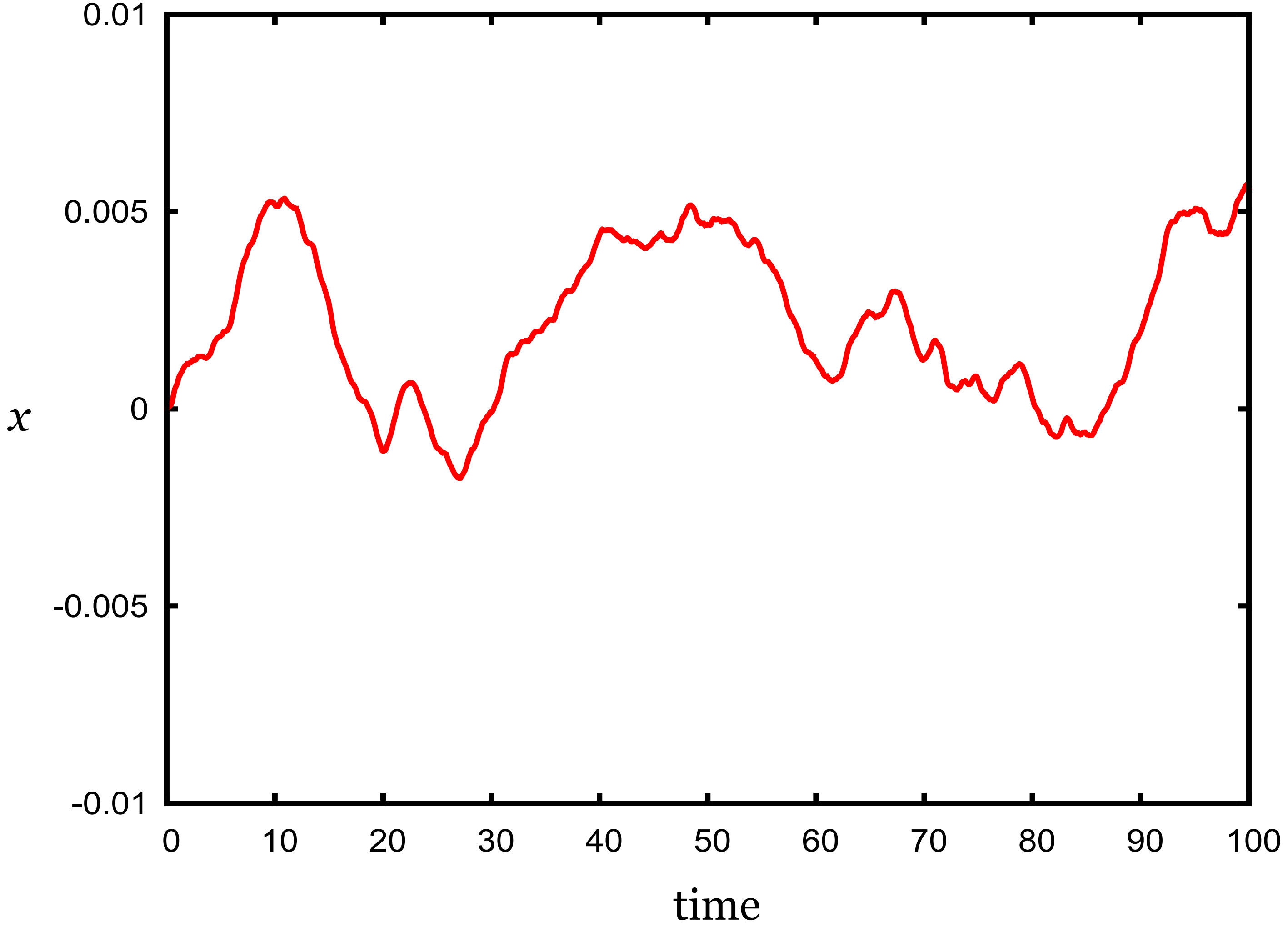
$$\left\langle \boldsymbol{\xi}(t) \right\rangle = 0$$

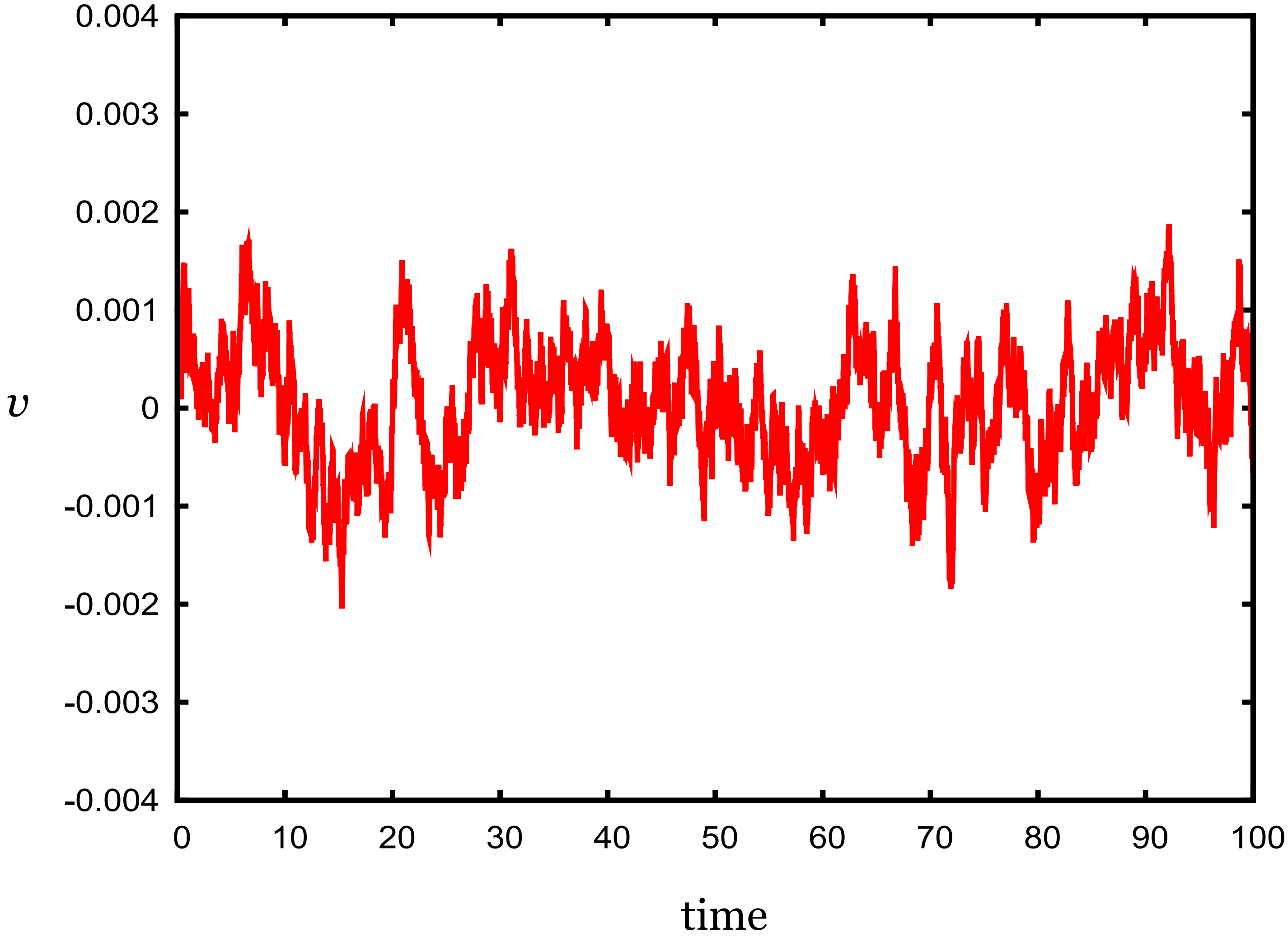
$$\left\langle \boldsymbol{\xi}(t)\cdot\boldsymbol{\xi}(s) \right\rangle = 2M\delta(t-s)$$

1次元系でのLangevin方程式による挙動

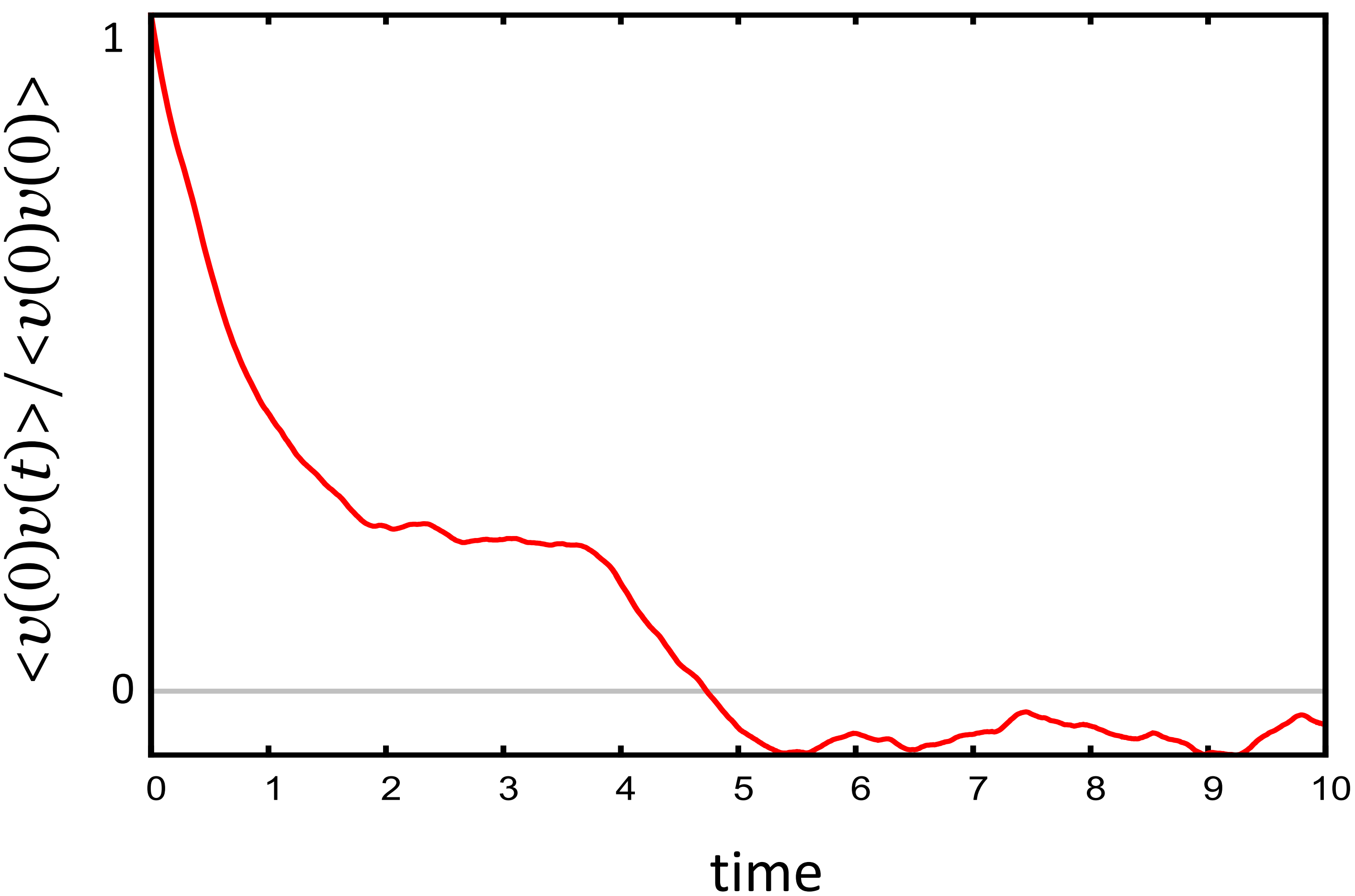


x

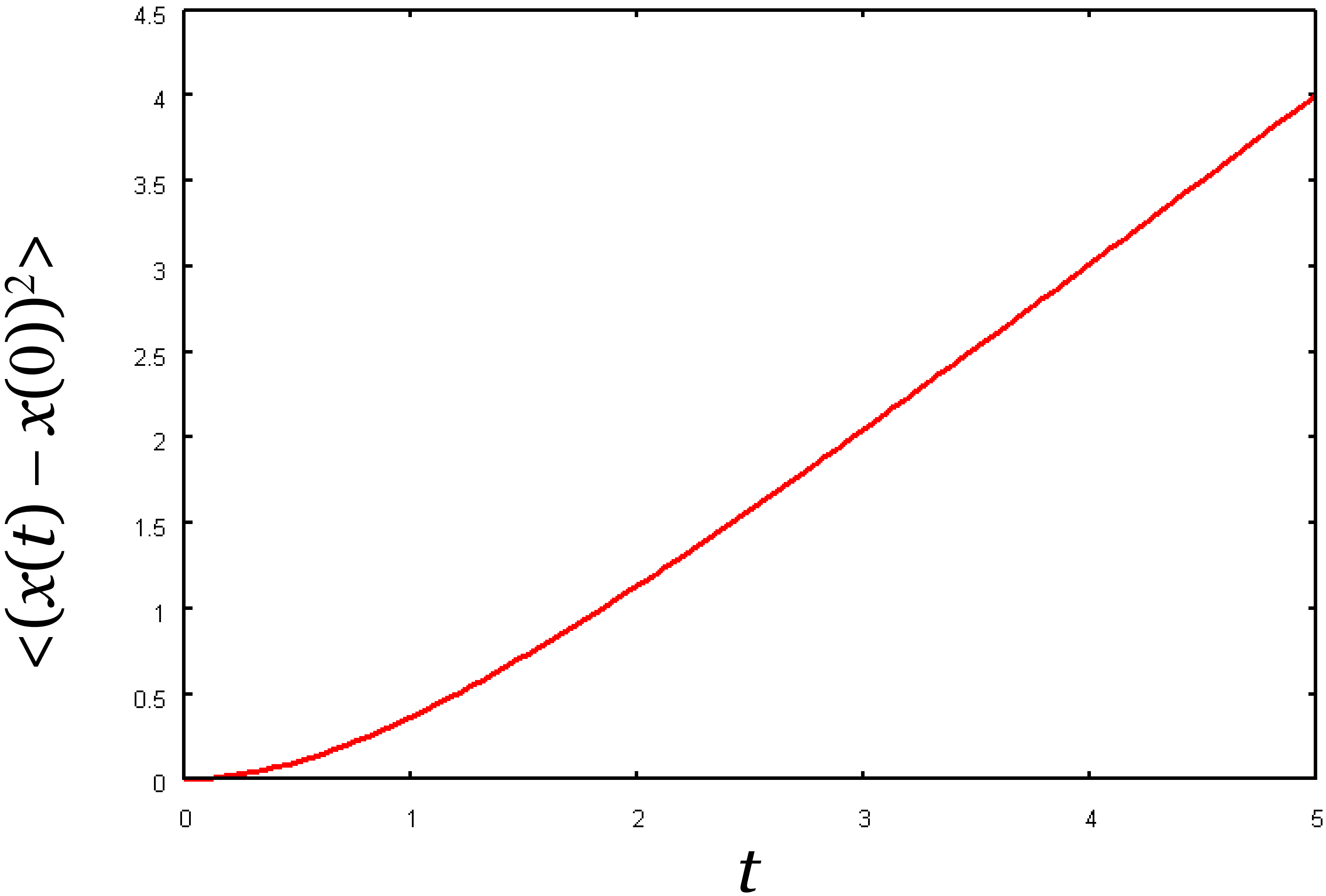

0.01
0.005
0
-0.005
-0.01
x
0
10
20
30
40
50
60
70
80
90
100
time



0.004
0.003
0.002
0.001
0
-0.001
-0.002
-0.003
-0.004
v
0
10
20
30
40
50
60
70
80
90
100
time

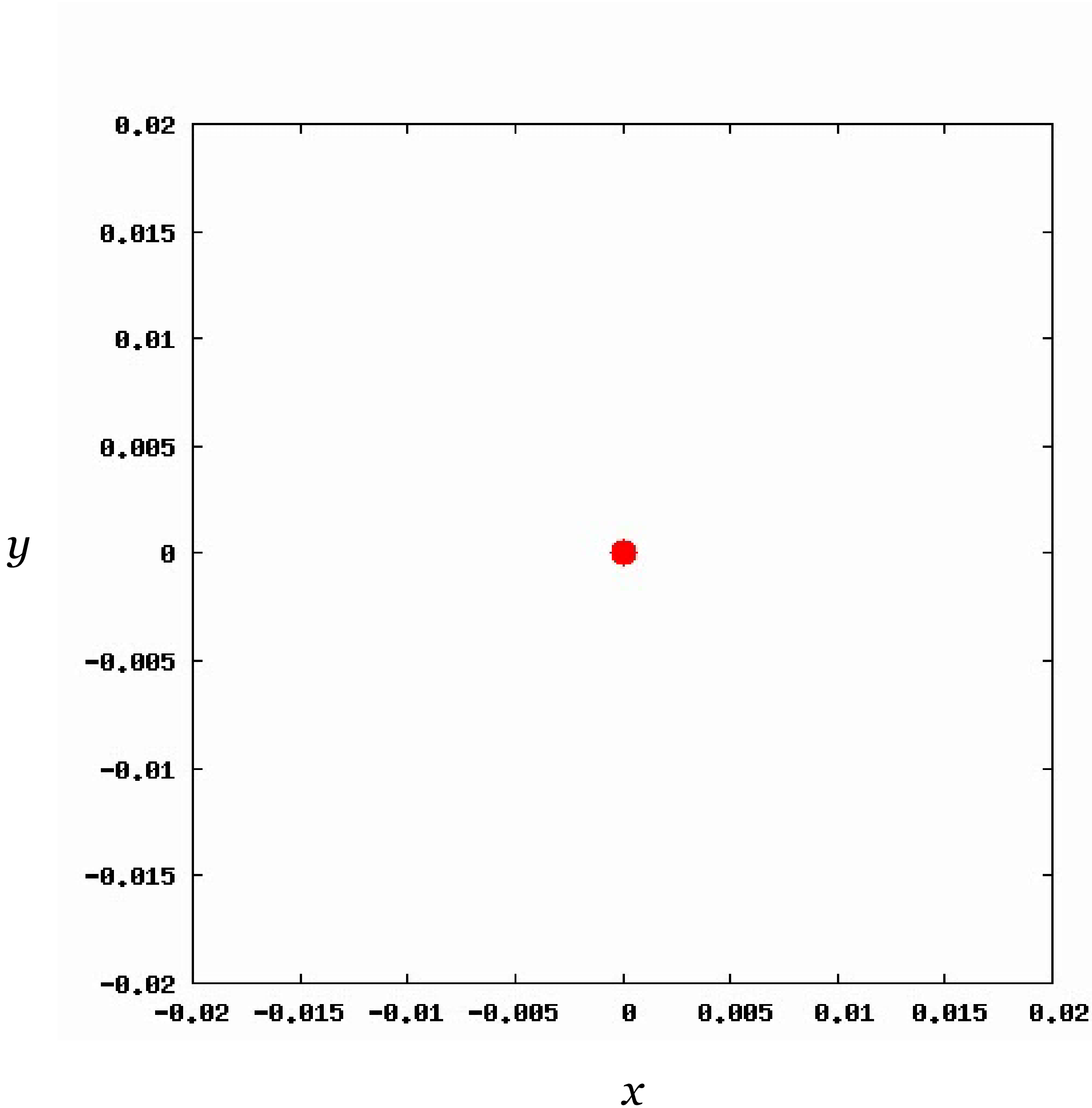


$$\langle v(0)v(t)\rangle / \langle v(0)v(0)\rangle \propto \exp(-t/\tau)$$

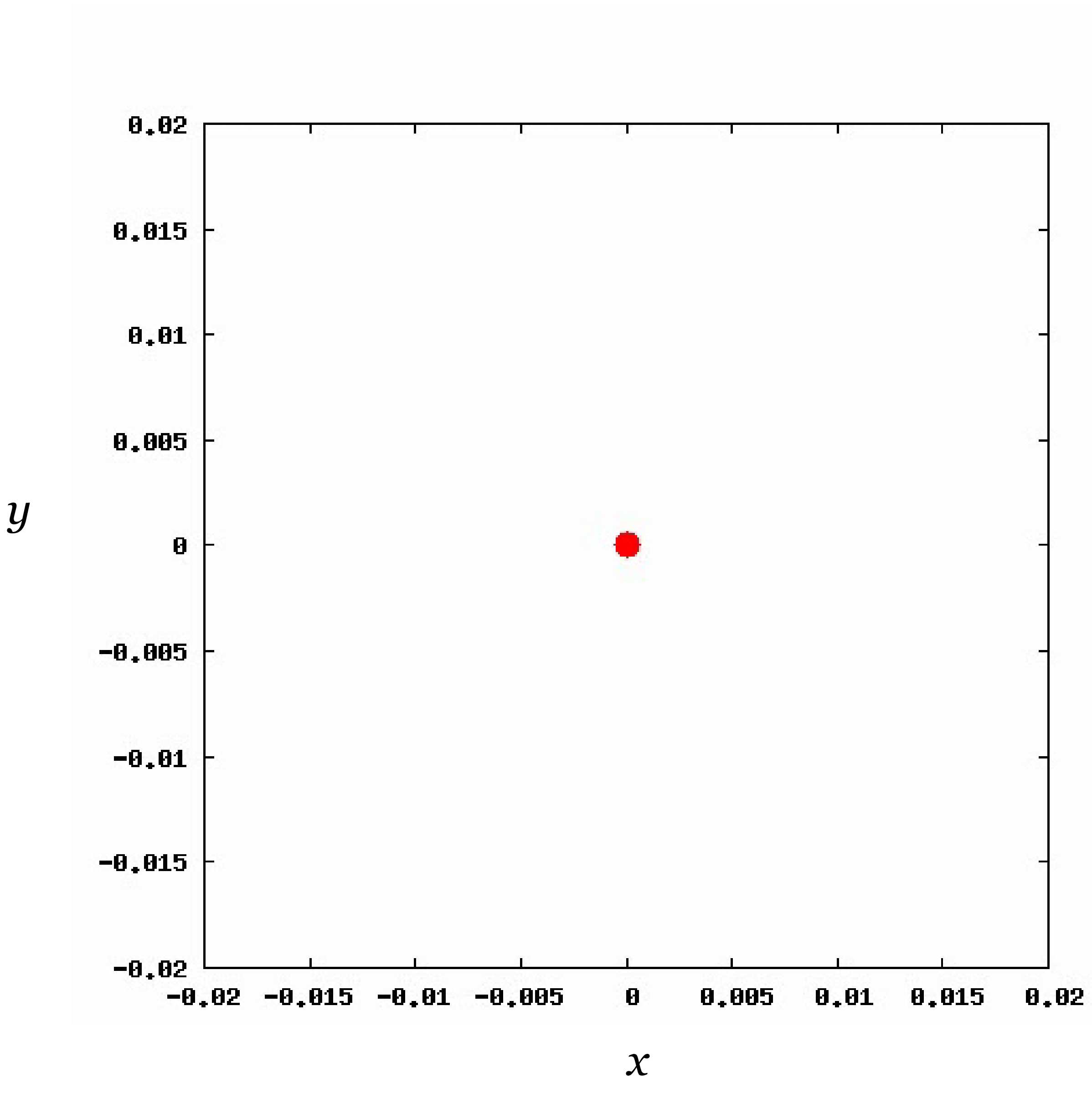


$$\left\langle \left(x(t) - x(0) \right)^2 \right\rangle = \frac{2M}{\gamma^2}\left[t + \frac{m}{\gamma}\left(e^{-\frac{\gamma}{m}t} - 1 \right) \right]$$

2次元での数値計算


0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02
y
x

軌跡を残すと

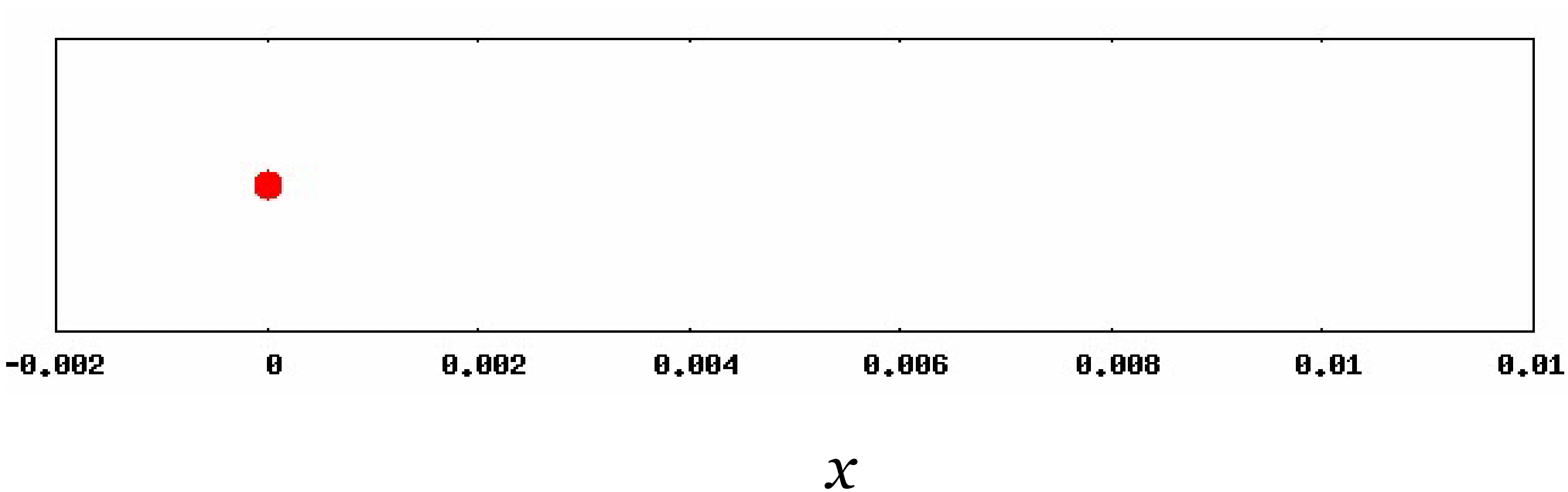

0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0.015
0.02
y
x

1次元で一定の外力の場合

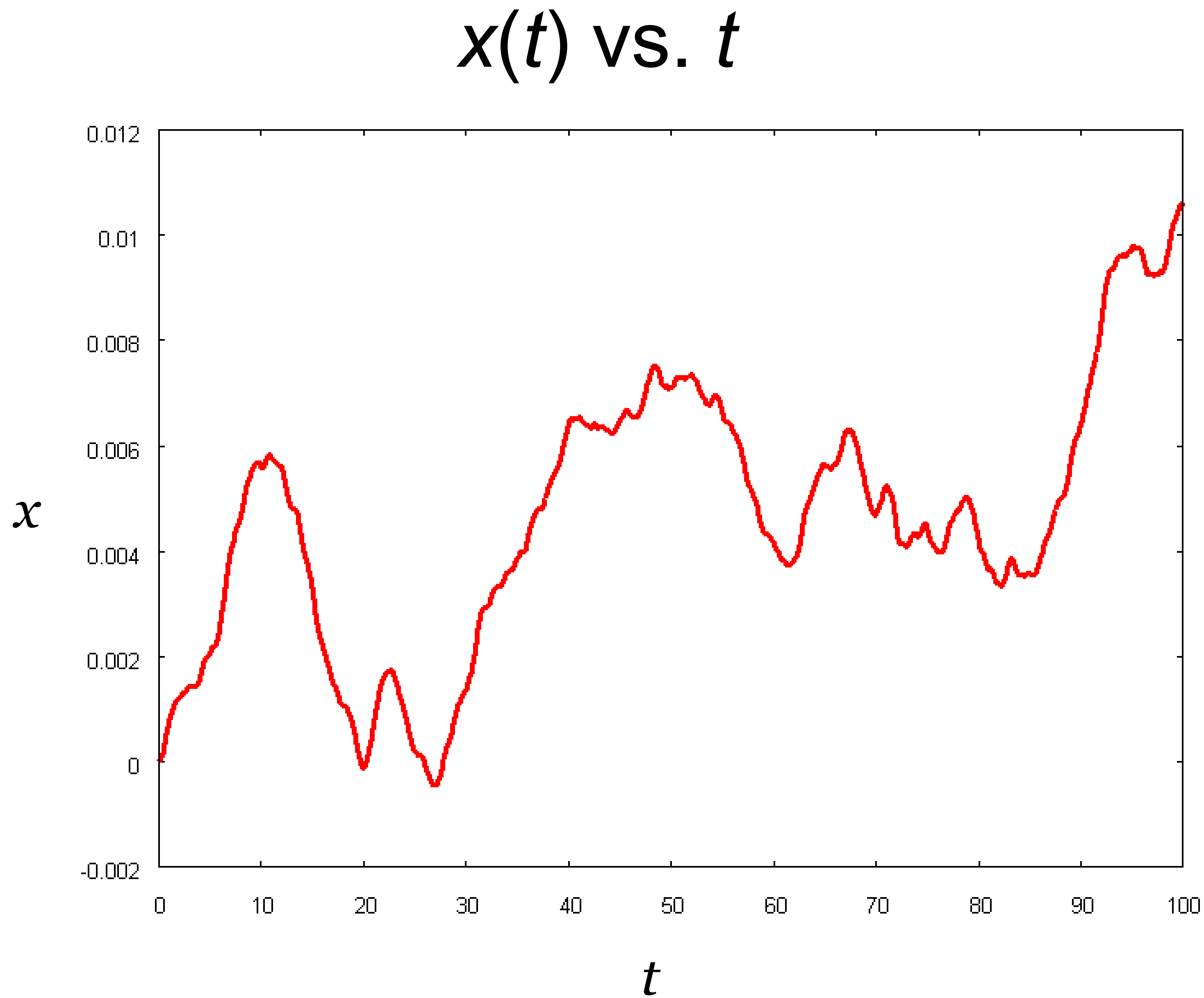
$$m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\gamma\frac{\mathrm{d}x}{\mathrm{d}t} + F + \xi(t)$$

$$\left\langle \xi(t) \right\rangle = 0$$

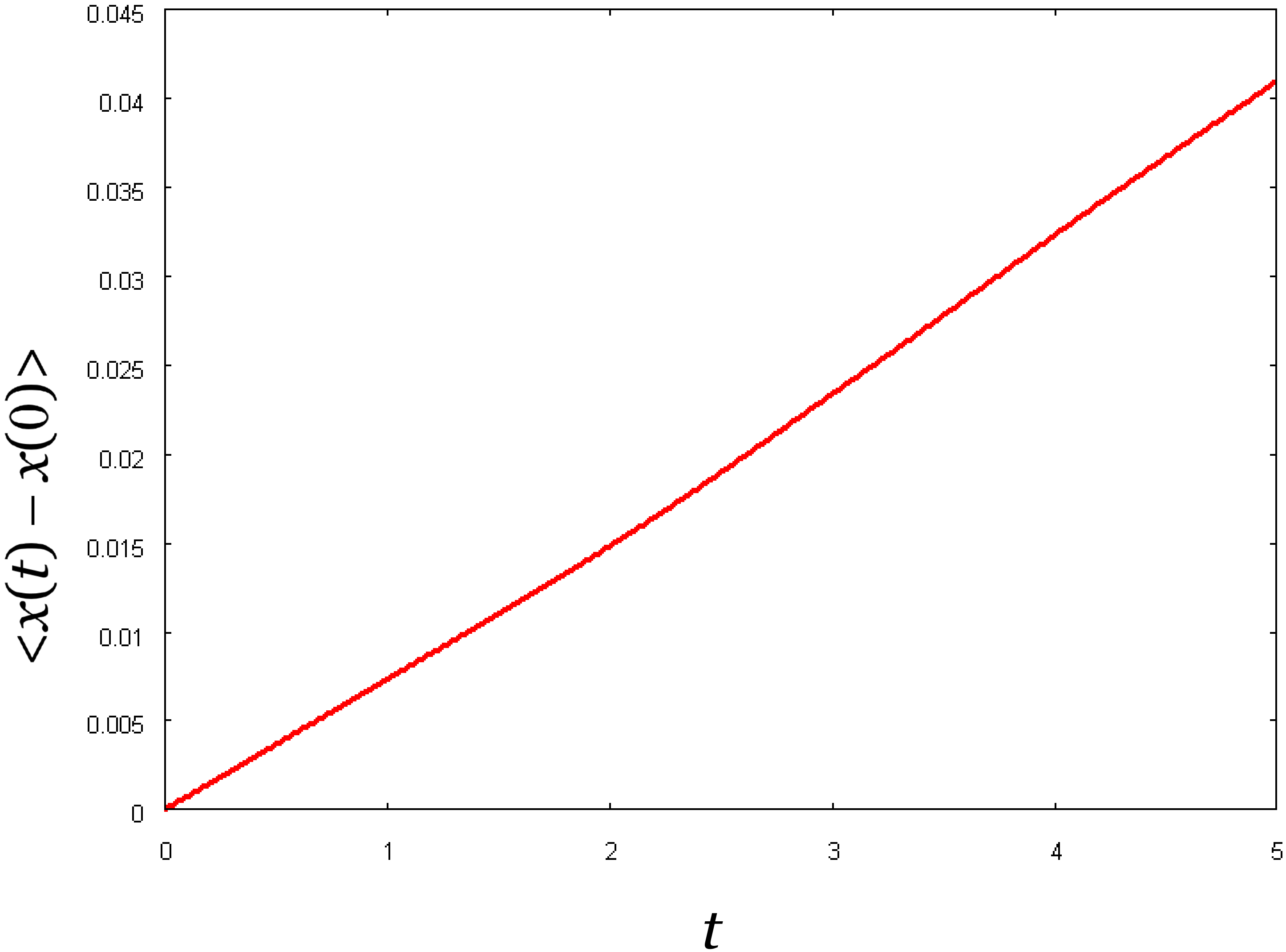
$$\left\langle \xi(t)\cdot\xi(s) \right\rangle = M\delta\left(t-s\right)$$



-0.002
0
0.002
0.004
0.006
0.008
0.01
0.01
x


x(t) vs. t
0.012
0.01
0.008
0.006
0.004
0.002
0
-0.002
x
0
10
20
30
40
50
60
70
80
90
100
t

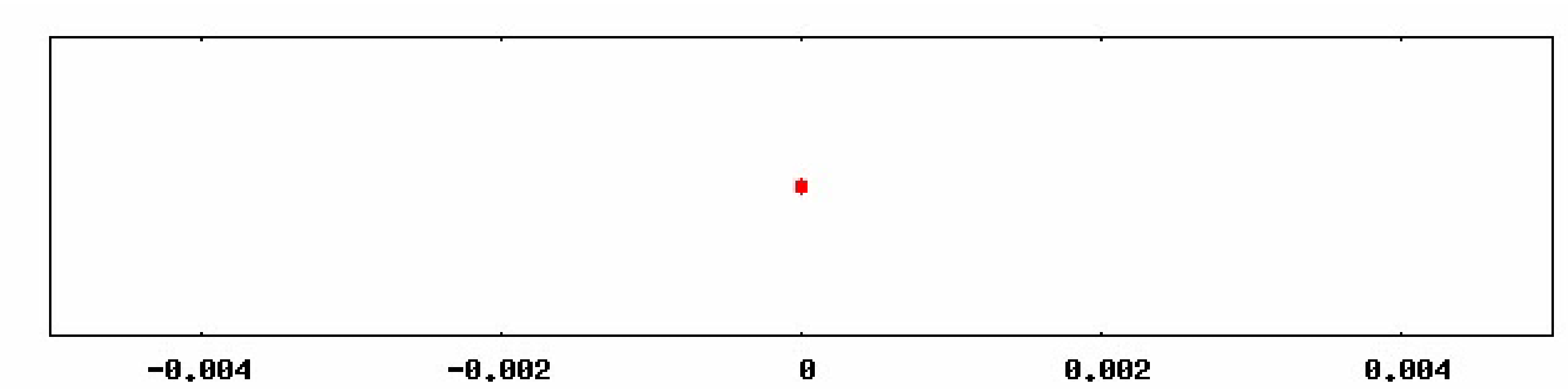
$\langle x(t) - x(0) \rangle$ vs. t



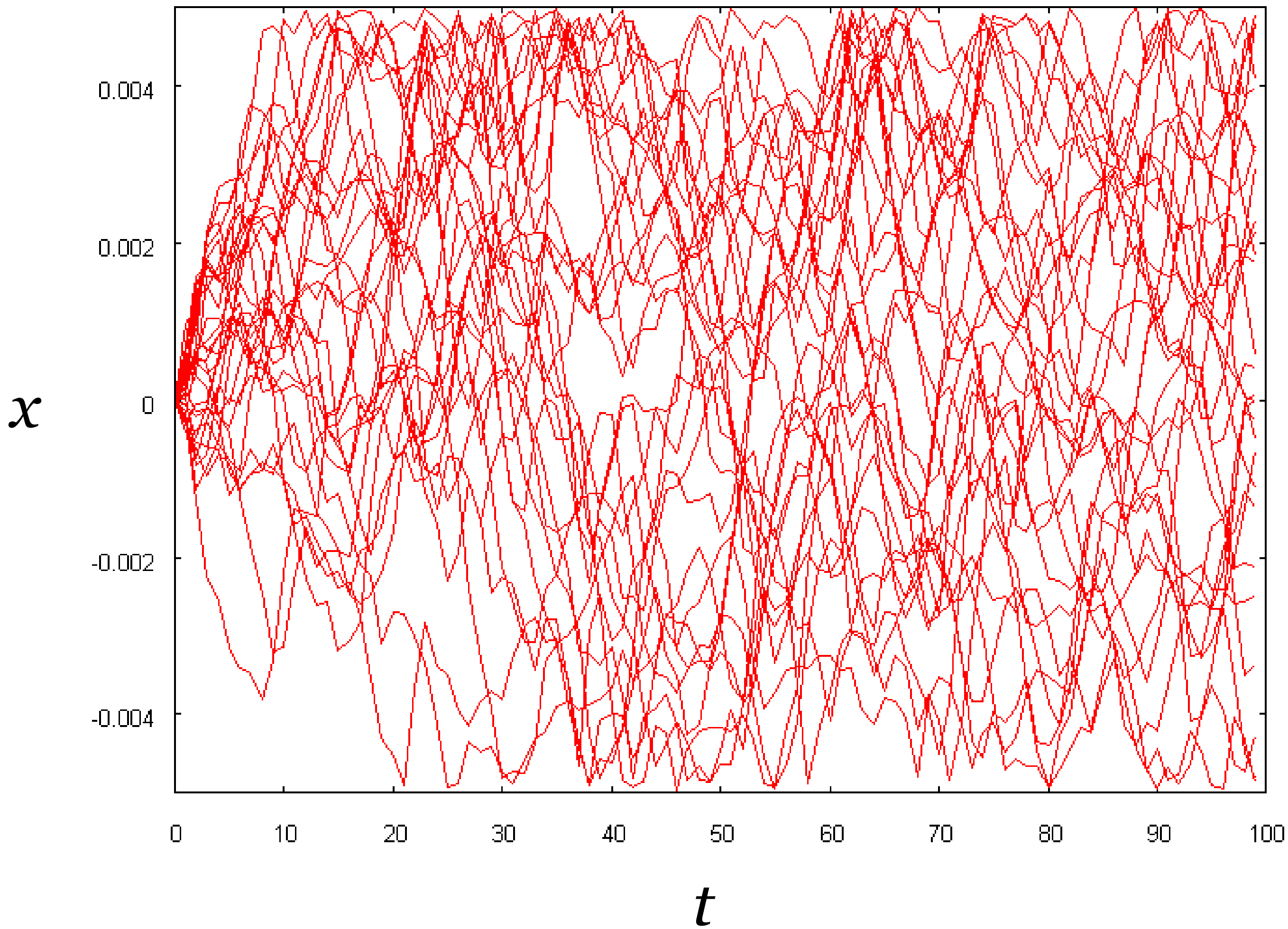
$$\langle v(t) \rangle = F / \gamma$$

1次元で一定の外力の場合

（多くの粒子を入れて、領域を区切ると･･･）

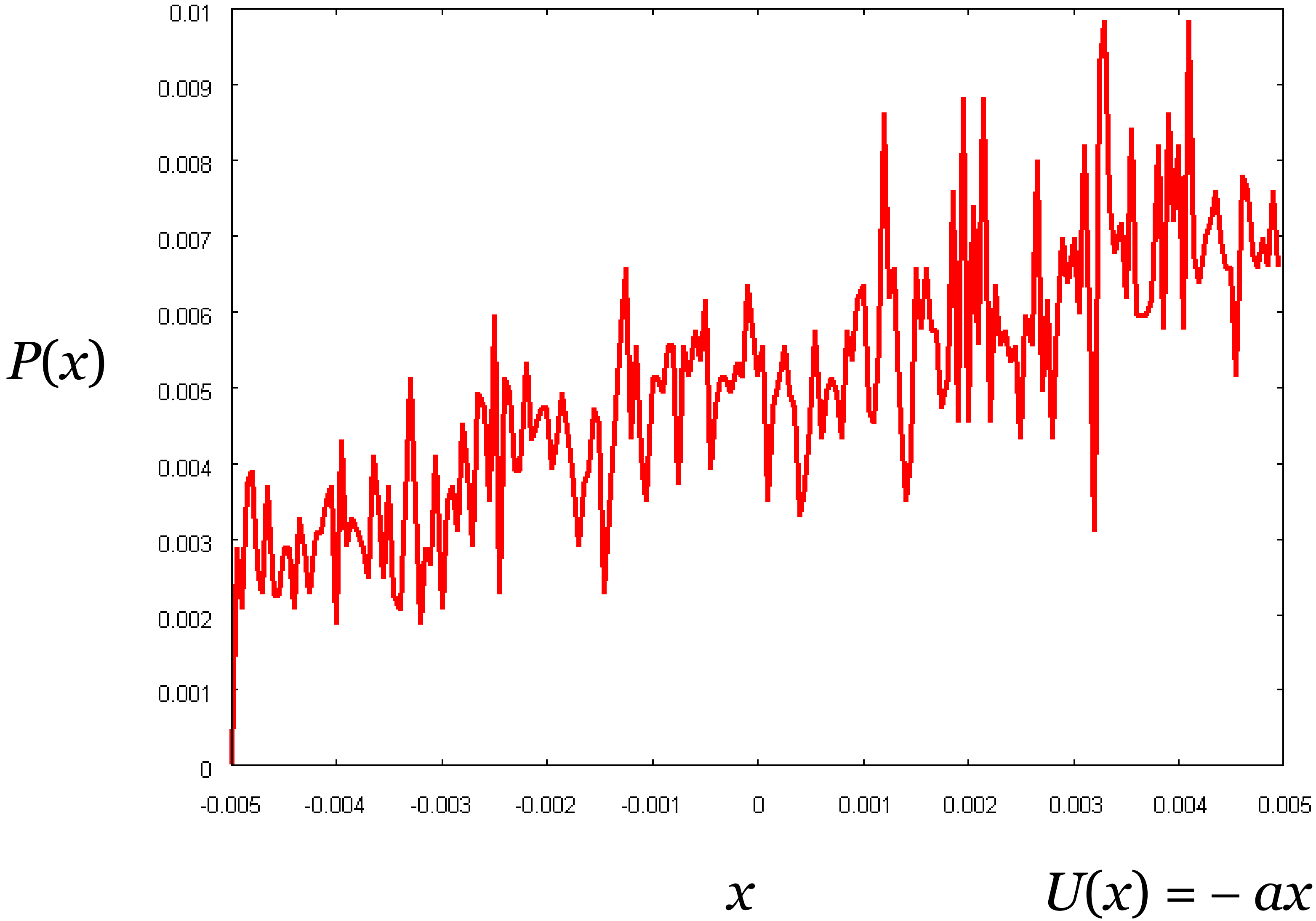


x



x
0.004
0.002
0
-0.002
-0.004
0
10
20
30
40
50
60
70
80
90
100
t

分布



$P(x)$
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
-0.005
-0.004
-0.003
-0.002
-0.001
0
0.001
0.002
0.003
0.004
0.005
x
$U(x) = -ax$

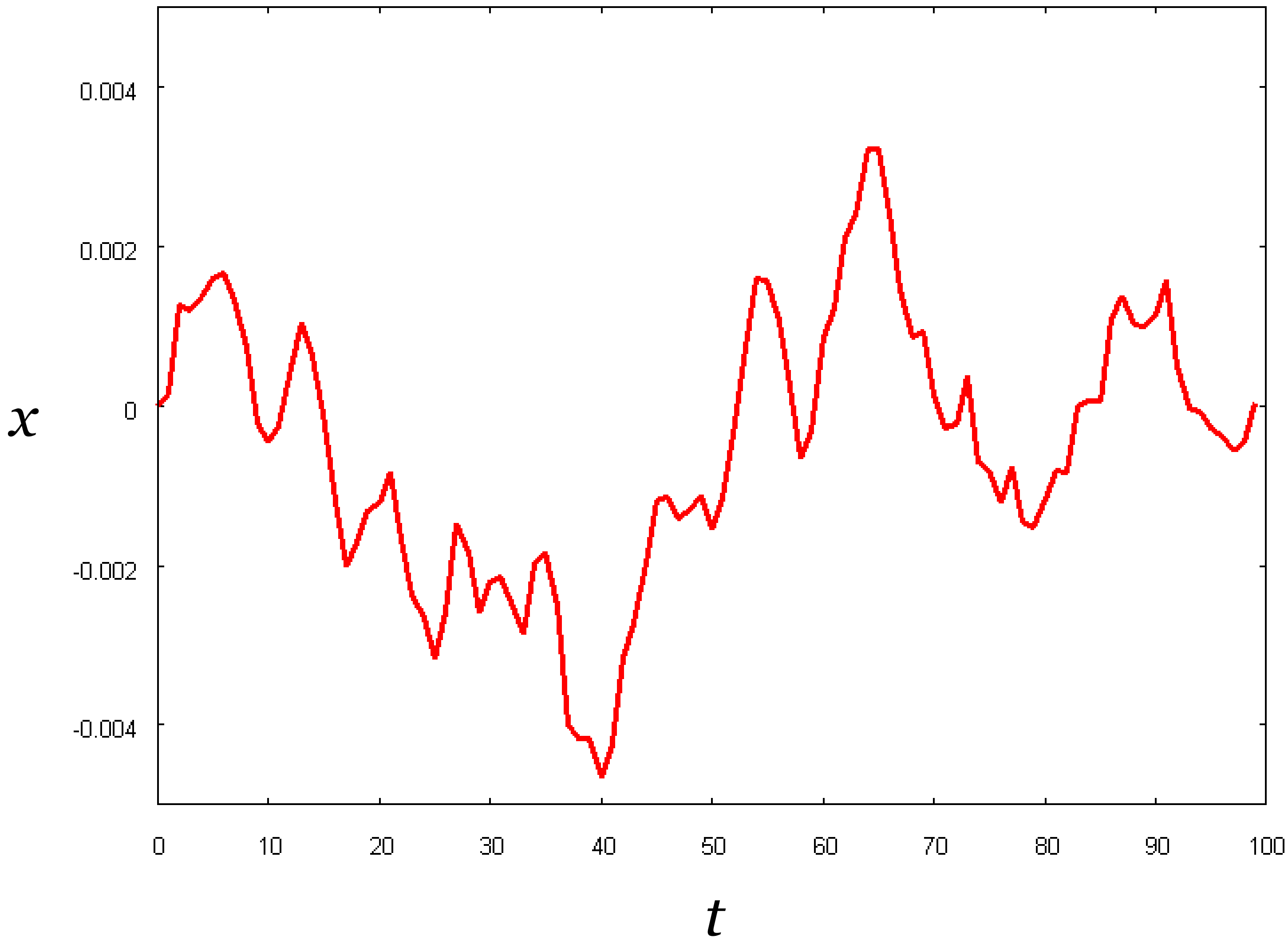
1次元で調和ポテンシャル中の場合

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\gamma\frac{\mathrm{d}x}{\mathrm{d}t} - ax + \xi(t)$$

$$\Phi(x) = \frac{a}{2}x^2$$

$$\left\langle \xi(t) \right\rangle = 0$$

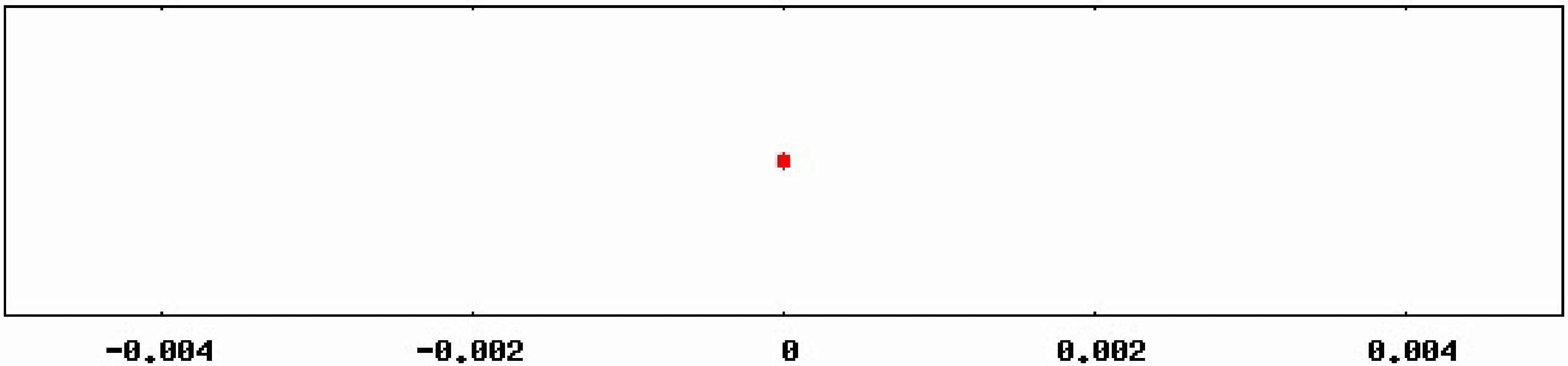
$$\left\langle \xi(t) \cdot \xi(s) \right\rangle = M\delta\left(t - s\right)$$



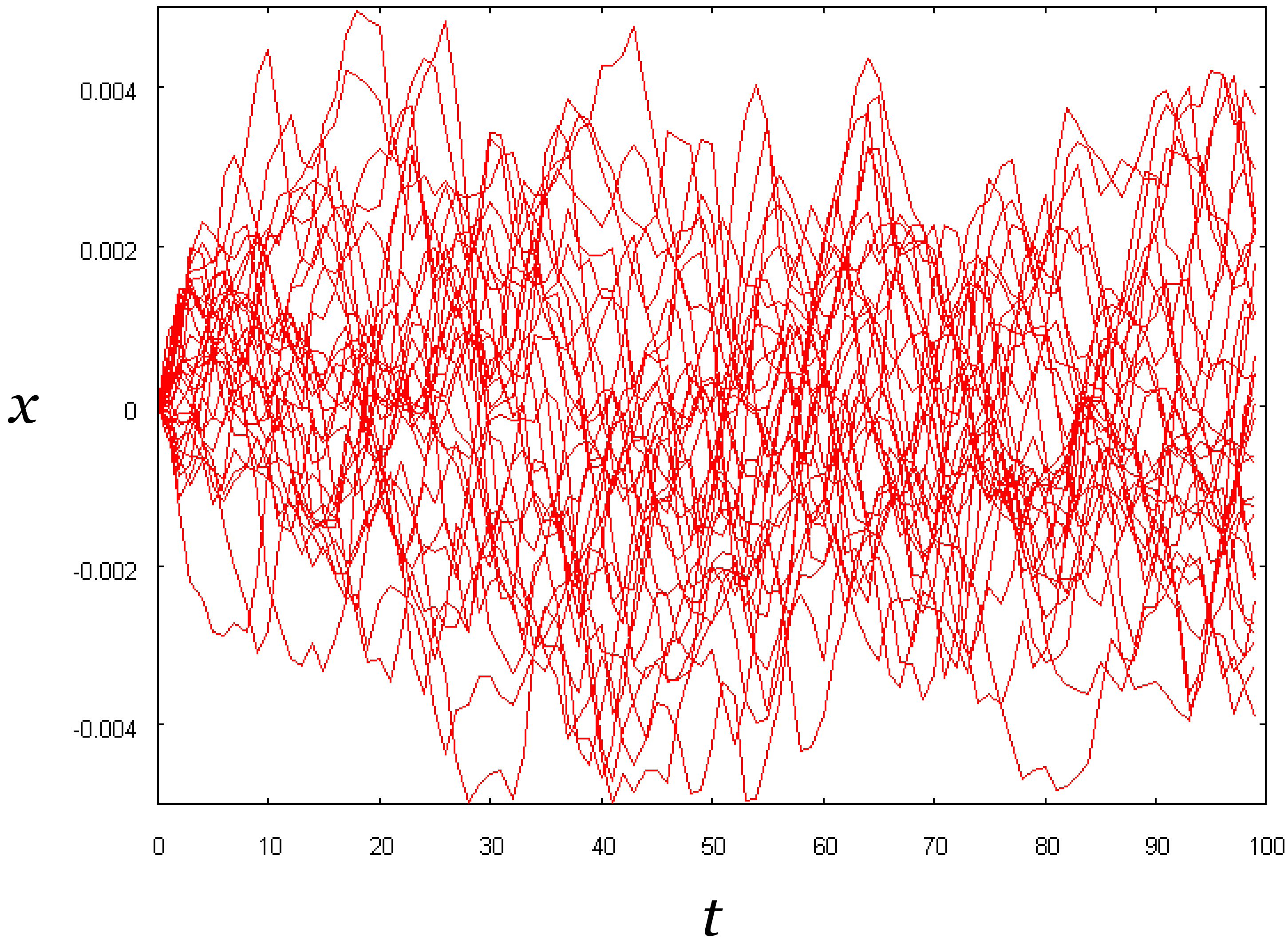
0.004
0.002
0
-0.002
-0.004
x
0
10
20
30
40
50
60
70
80
90
100
t

1次元で調和ポテンシャル中の場合

（多くの粒子を入れると･･･）

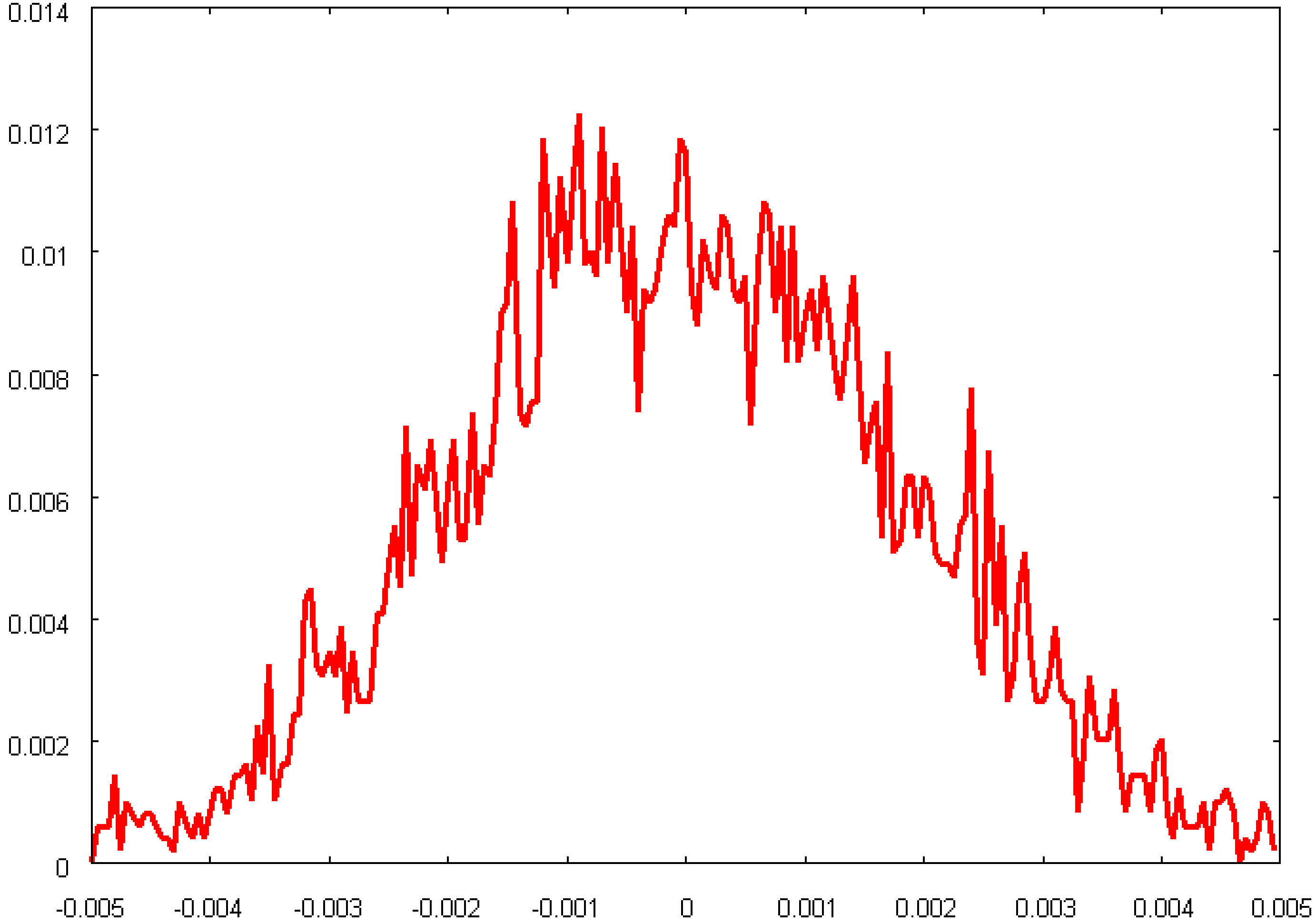


x



0.004
0.002
0
-0.002
-0.004
x
0
10
20
30
40
50
60
70
80
90
100
t

分布



$P(x)$

x

$U(x) = ax^2/2$

ポテンシャル力を受ける粒子のLangevin方程式

$$m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\gamma\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\mathrm{d}U}{\mathrm{d}x} + \xi(t)$$

慣性項に比べて粘性項が十分に大きい場合には:

$$0 = -\gamma\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\mathrm{d}U}{\mathrm{d}x} + \xi(t)$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{1}{\gamma}\frac{\mathrm{d}U}{\mathrm{d}x} + \frac{1}{\gamma}\xi(t)$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{1}{\gamma}\frac{\mathrm{d}U}{\mathrm{d}x} + \frac{1}{\gamma}\xi(t)$$

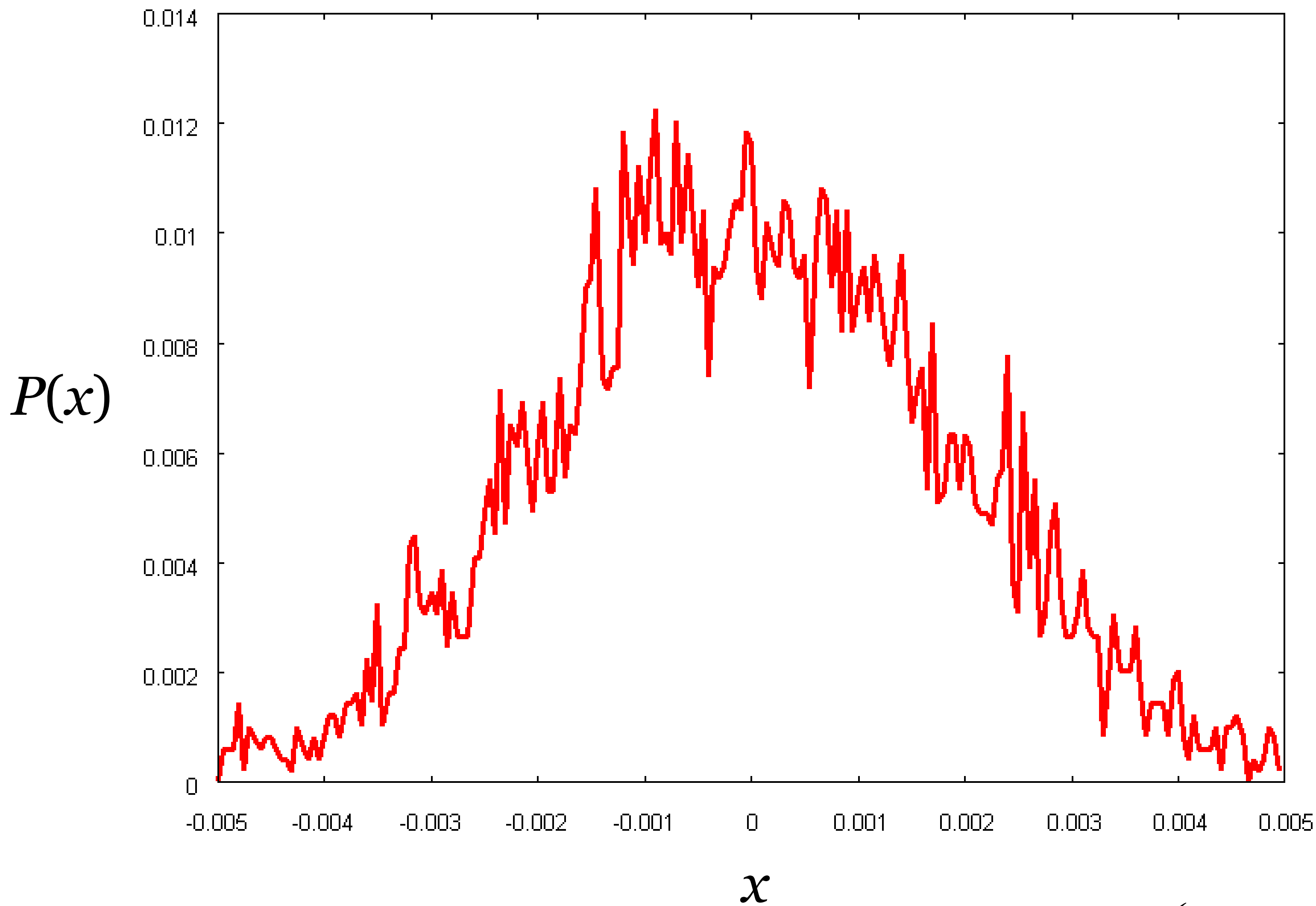
に対応するフォッカープランク方程式

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{\gamma}\frac{\mathrm{d}U}{\mathrm{d}x} + \frac{\partial}{\partial x}\frac{k_\mathrm{B}T}{\gamma}\right)P(x,t)$$

この定常解は、

$$P = P_0 \exp\left(-\frac{U(x)}{k_\mathrm{B}T}\right)$$

分 布

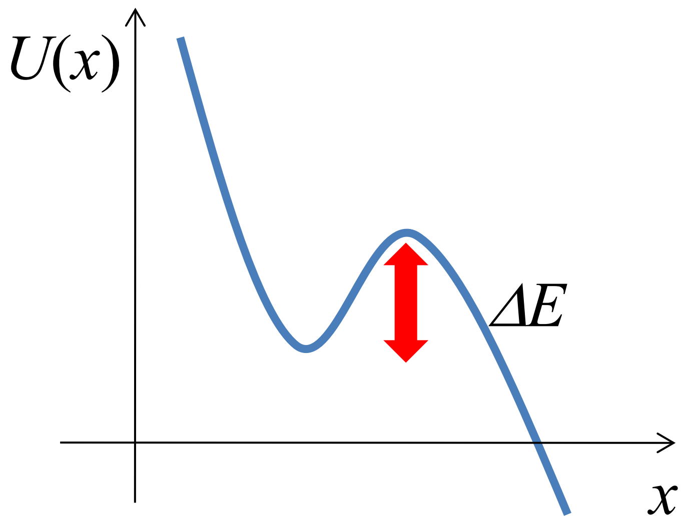


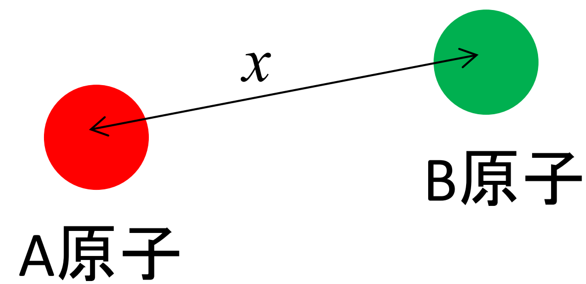
$$U(x) = ax^2/2$$

$$P = P_0 \exp\left(-\frac{U(x)}{k_B T}\right)$$

化学反応のモデル:KramersのEscape rate

化学反応の古典的描像





はじめ、結合していたA原子とB分子はどれくらいの割合で分離するか?

フォッカープランク方程式を用いるとその割合が計算できる

$$P \propto \exp\left(-\frac{\Delta E}{k_{\mathrm{B}}T}\right)$$