

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
from scipy.sparse.linalg import spsolve
from scipy.integrate import quad
from scipy.interpolate import interp1d, PchipInterpolator
```

```
In [2]: beta_Gstar = 8 # kT
D0 = 0.01 # rescaled D/D0 so it won't be used

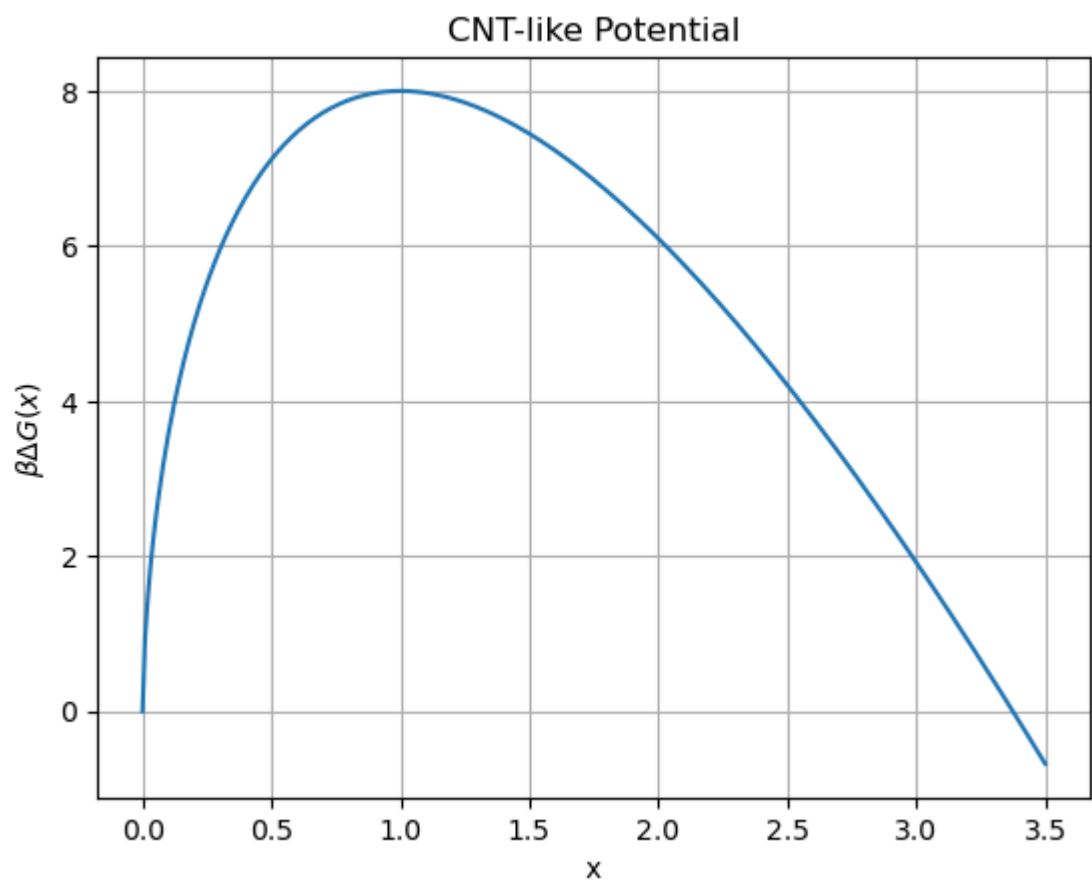
def beta_Gcnt(x):
    return 2*beta_Gstar*(-x+3.0/2*x**(2/3))

def Dcnt(x):
    # return D0*x**(2/3)
    return D0*x**0

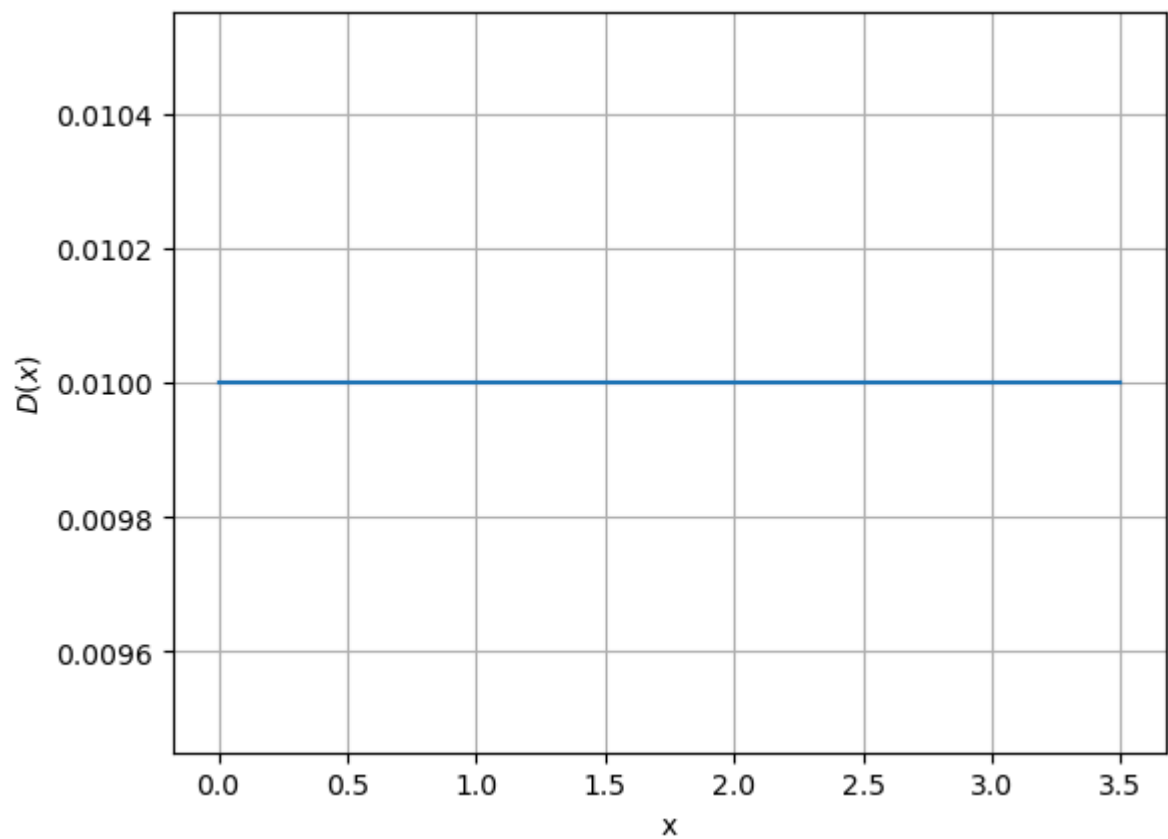
x_arr = np.linspace(0, 3.5, 351)
```

```
In [3]: plt.plot(x_arr, beta_Gcnt(x_arr))
plt.grid()
plt.xlabel('x')
plt.ylabel("$ \\beta \\Delta G(x)$")
plt.title('CNT-like Potential')
plt.show()

plt.plot(x_arr, Dcnt(x_arr))
plt.grid()
plt.xlabel('x')
plt.ylabel("$ D(x)$")
```



Out[3]: Text(0, 0.5, '\$ D(x)\$')



Numerical solve ODE with injecting boundary condition to find steady state solution

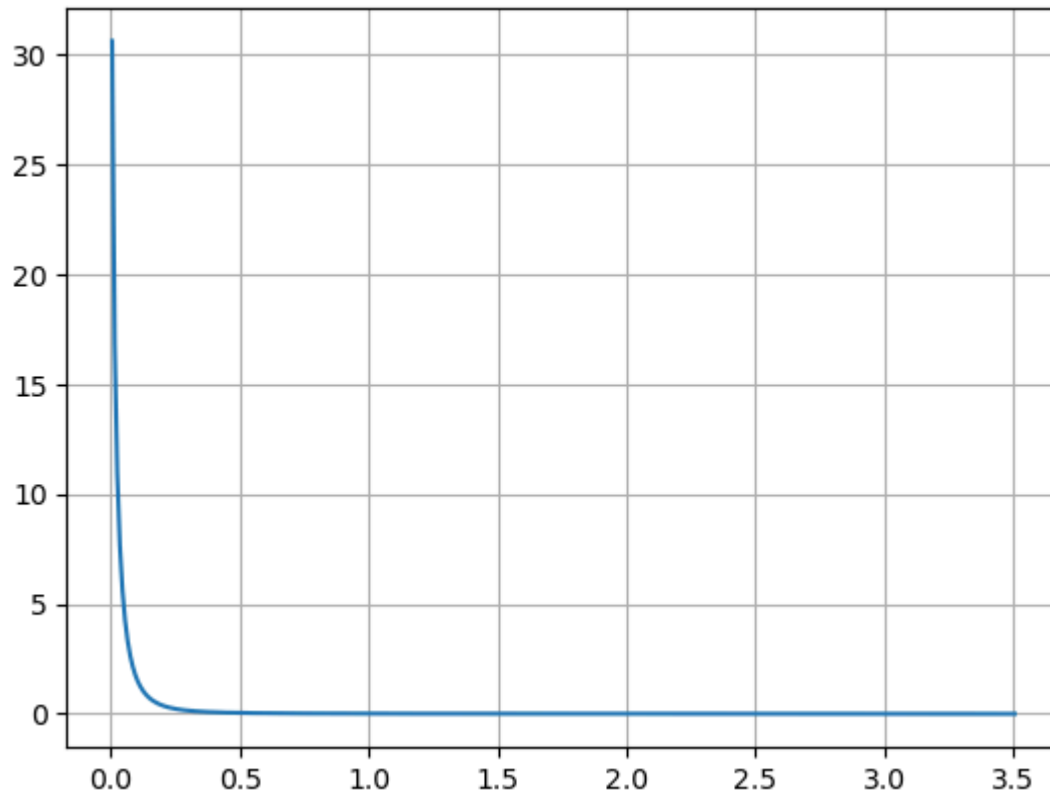
```
In [4]: def kappa(x):  
        return Dcnt(x)*np.exp(-beta_Gcnt(x))
```

```
N = x_arr.size  
h = x_arr[1]-x_arr[0]  
  
x_minus_half = x_arr[:]  
x_plus_half = x_arr+h  
  
b_arr = x_arr+h/2.0  
u_arr = np.zeros(b_arr.size)
```

```
In [5]: A = np.zeros((N-1, N-1))  
  
np.fill_diagonal(A, -(kappa(x_minus_half)+kappa(x_plus_half)))  
np.fill_diagonal(A[1:, ], kappa(x_minus_half[1:-1])) # subdiagonal  
np.fill_diagonal(A[:, 1:], kappa(x_plus_half[:-2])) # superdiagonal  
A[0, 1] += kappa(x_minus_half[0])  
  
f_vect = np.zeros(N-1)  
f_vect[0] = 1  
  
u_arr[0:-1] = spsolve(A, f_vect)  
Pst_arr = u_arr*np.exp(-beta_Gcnt(b_arr))  
Pst_arr /= (np.sum(Pst_arr)*h)  
  
inject_rate = Dcnt(b_arr[-1])*np.exp(-beta_Gcnt(b_arr[-1])+beta_Gcnt(b_arr[-  
print(inject_rate)  
  
plt.plot(b_arr, Pst_arr)  
plt.grid()
```

9.08394516091092e-05

/tmp/ipykernel_784189/3470158452.py:11: SparseEfficiencyWarning: spsolve requires A be CSC or CSR matrix format
u_arr[0:-1] = spsolve(A, f_vect)



Numerically Nest integrate for Steady-State Flux and Probability distribution function

```
In [6]: a = 0 # location of reflecting boundary
b = 3.5 # location of absorbing boundary

# Define the inner function to integrate as a function of y
def inner_integrand(y):
    return 1.0/Dcnt(y)*np.exp(beta_Gcnt(y))

# Define the inner integral as a function of x
def inner_integral(x):
    y_lower = x
    y_upper = b
    result, error = quad(inner_integrand, y_lower, y_upper)
    return result

# Define the outer integral
x_lower = a
x_upper = b

# Define the outer function to integrate (also as a function of x)
def outer_integrand(x):
    return np.exp(-beta_Gcnt(x))*inner_integral(x)

# Perform the outer integration
invert_st_flux, error = quad(outer_integrand, x_lower, x_upper)
st_flux = 1.0/invert_st_flux
print(st_flux)
```

0.00017239049166835254

```
In [7]: def st_P_func(x):
        def integrand(y):
            return 1.0/Dcnt(y)*np.exp(beta_Gcnt(y))
        # Perform the integration
        y_lower = x
        y_upper = b
        result, error = quad(integrand, y_lower, y_upper)
        result *= st_flux*np.exp(-beta_Gcnt(x))

        return result

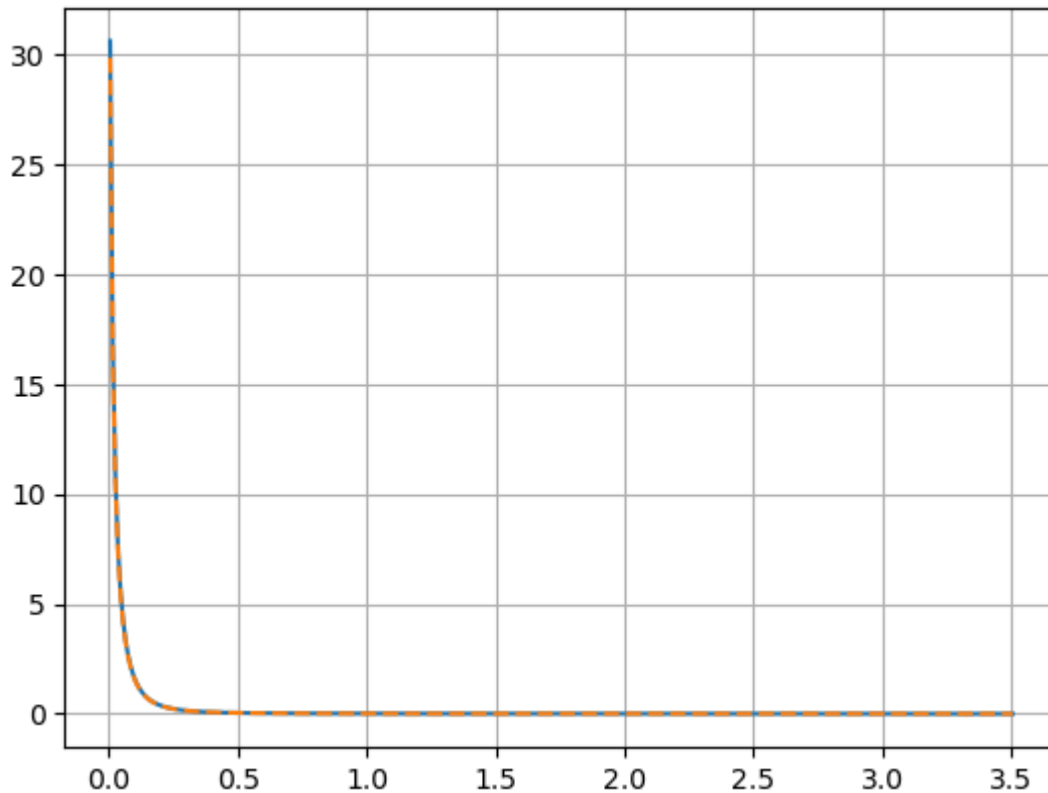
st_P_arr = np.zeros(x_arr.size)
for i in np.arange(x_arr.size):
    st_P_arr[i] = st_P_func(b_arr[i])

plt.plot(b_arr, Pst_arr)
plt.plot(b_arr, st_P_arr, '--')

plt.grid()

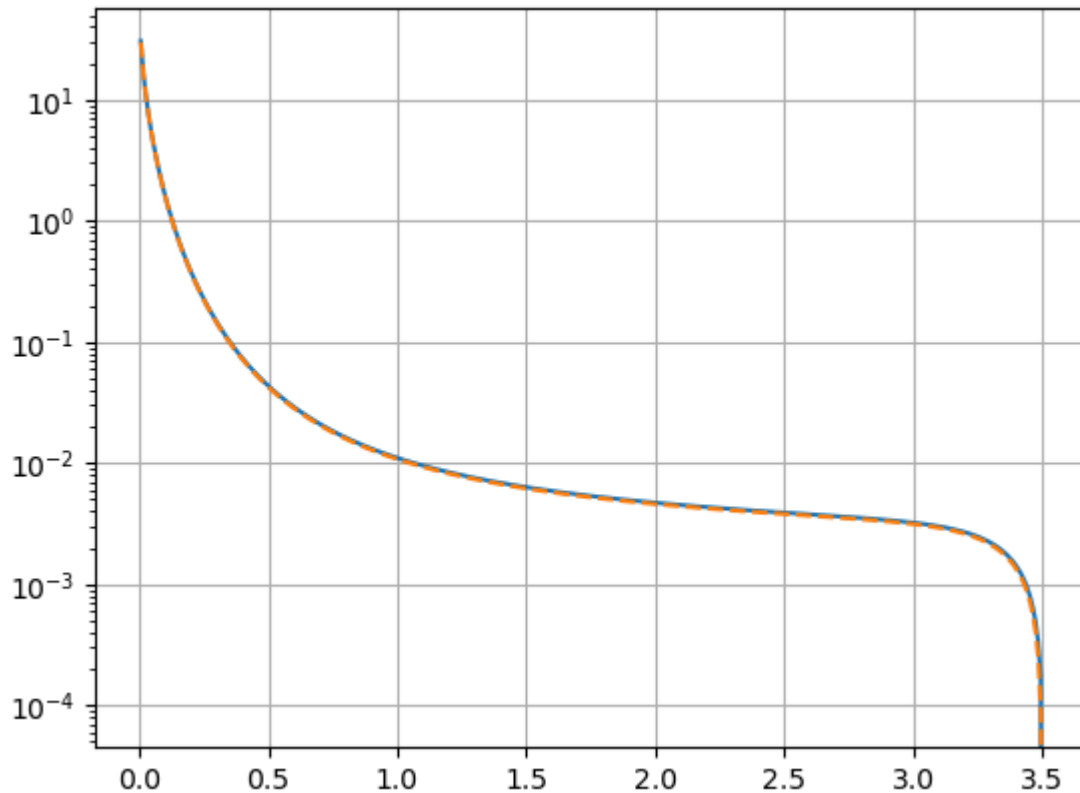
print(Pst_arr[:5], st_P_arr[:5])
```

```
[30.59977131 16.82759771 10.92183939  7.65030948  5.61999833] [29.83955161 1
6.40953295 10.65049676  7.46024445  5.48037421]
```



```
In [8]: plt.semilogy(b_arr, Pst_arr)
        plt.semilogy(b_arr, st_P_arr, '--')

        plt.grid()
```



Numerically Nest integrate for MFPT

```
In [9]: # a = 0.0 # location of reflecting boundary
x0 = a # Regura's method, overlap the starting point and reflecting boundary
# b = 3.5 # location of absorbing boundary

# Define the inner function to integrate as a function of z
def inner_integrand(z):
    return np.exp(-beta_Gcnt(z))

# Define the inner integral as a function of y
def inner_integral(y):
    z_lower = a
    z_upper = y
    result, error = quad(inner_integrand, z_lower, z_upper)
    return result

# Define the outer integral
y_lower = x0
y_upper = b

# Define the outer function to integrate (also as a function of y)
def outer_integrand(y):
    return np.exp(beta_Gcnt(y))*inner_integral(y)/Dcnt(y)

# Perform the outer integration (from x0 to b)
result, error = quad(outer_integrand, y_lower, y_upper)
```

```

In [10]: mfpt_arr = np.zeros(b_arr.size)
         for i in np.arange(b_arr.size):
             mfpt_arr[i], _ = quad(outer_integrand, y_lower, b_arr[i])

         idx_barrier = np.where((b_arr > 1.0) & (b_arr < 1.0 + h))
         t_star = mfpt_arr[idx_barrier][0]
         print(f"{2*t_star} = 2*t(x*)")
         print(f"{mfpt_arr[-1]} = t(b)")
         print(f"{invert_st_flux} = 1/J")
         print(f"{1/inject_rate/2} = 1/inject_rate")

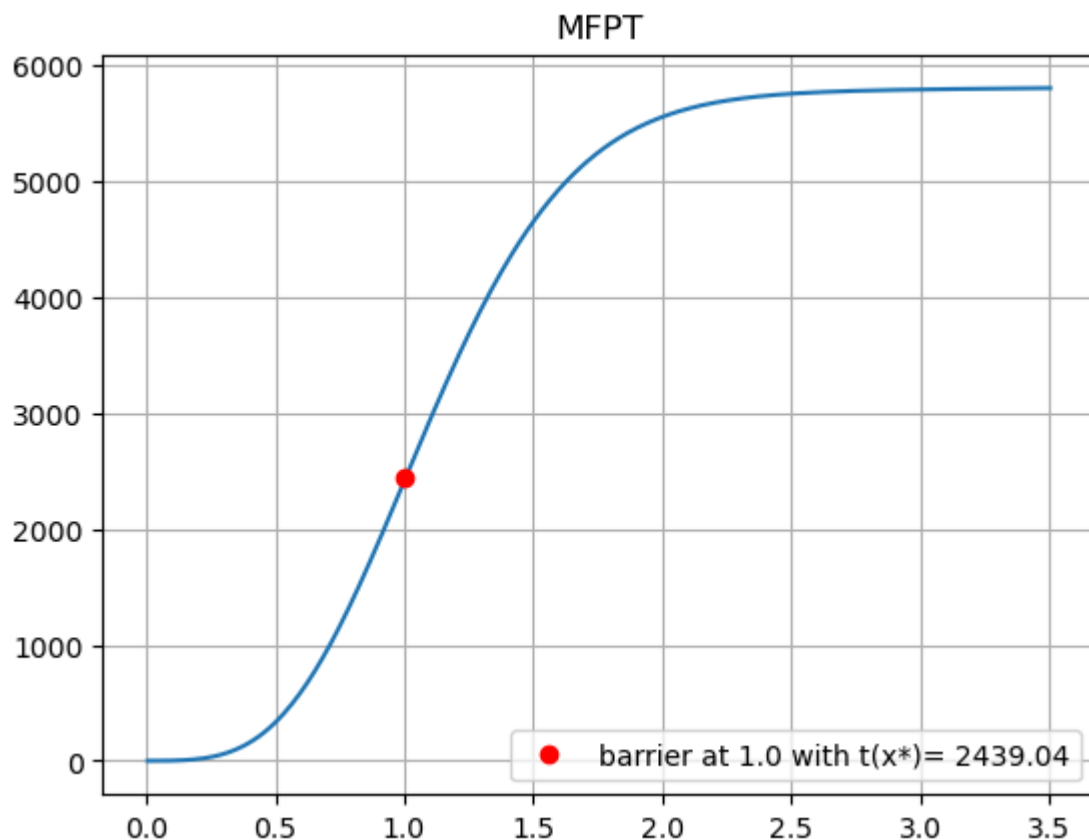
         plt.plot(b_arr, mfpt_arr)
         plt.plot(1.0, t_star, 'ro', label=f"barrier at 1.0 with t(x*)={t_star: .2f}")
         plt.title('MFPT')
         plt.legend()
         plt.grid()

```

```

4878.082469370472 = 2*t(x*)
5800.883826714521 = t(b)
5800.783966228342 = 1/J
5504.216407553268 = 1/inject_rate

```



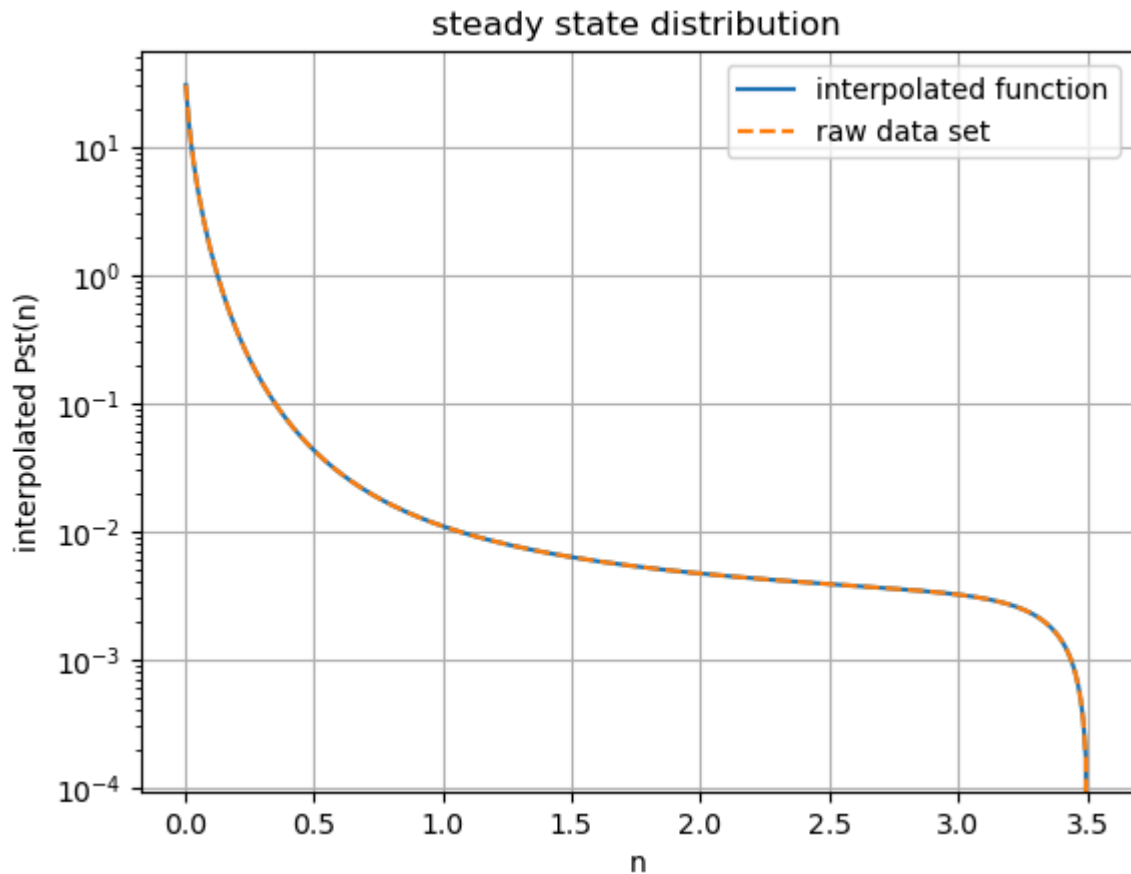
Reconstruct Free Energy from Numerical Solution of P_{st_arr} and Numerical Integration of $mfpt$

```

In [11]: interp_Pst_func = interp1d(b_arr, Pst_arr, kind='cubic', fill_value="extrapc
         # interp_Pst_func = PchipInterpolator(b_arr, Pst_arr)

```

```
plt.semilogy(b_arr, interp_Pst_func(b_arr), label="interpolated function")
plt.semilogy(b_arr, Pst_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()
```

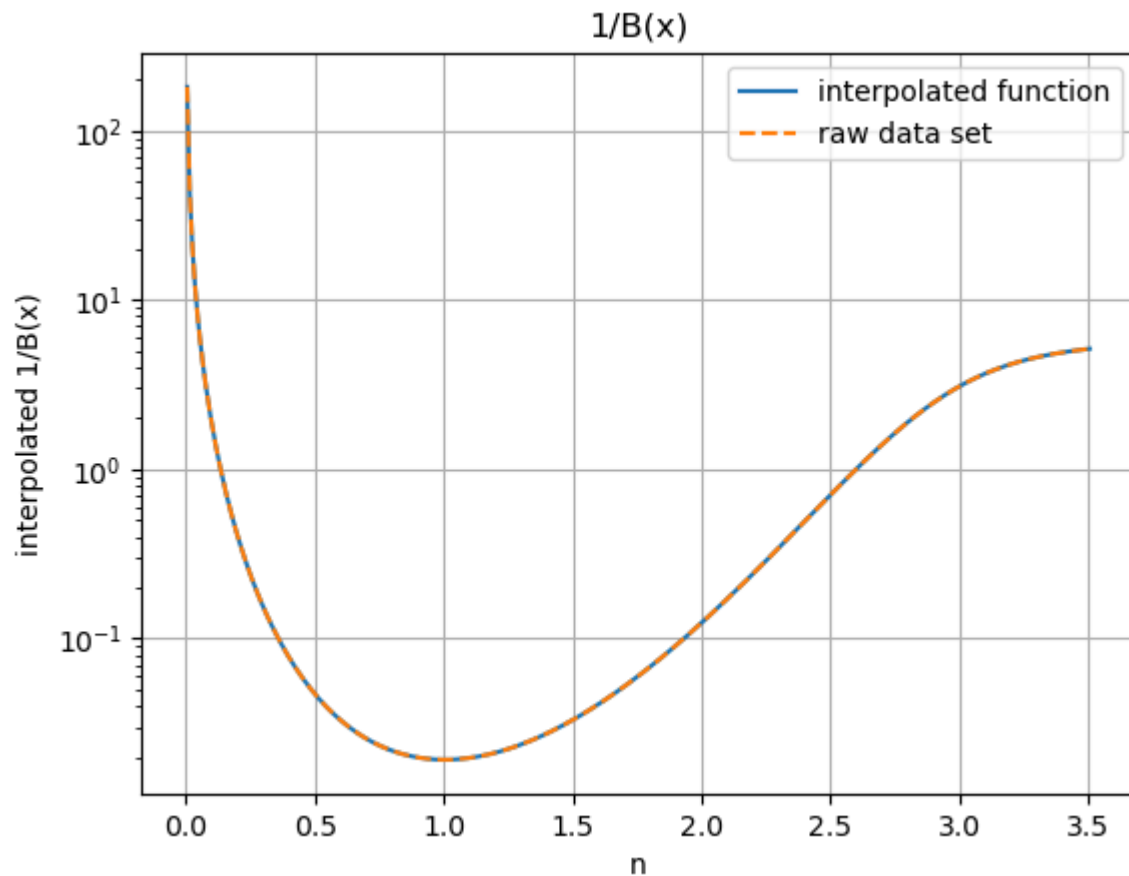


```
In [12]: # Pst(b) = 0, and also avoid D(x)=0
integral_Pst_arr = np.zeros(b_arr.size-1)
Bx_arr = np.zeros(b_arr.size-1)

for i in range(b_arr.size-1):
    integral_Pst_arr[i], _ = quad(interp_Pst_func, b_arr[i], b_arr[-1])
    Bx_arr[i] = -1.0/Pst_arr[i]*(integral_Pst_arr[i]-(mfpt_arr[-1]-mfpt_arr[

interp_invertBx_func = interp1d(b_arr[:-1], 1.0/Bx_arr, kind='cubic', fill_v

plt.semilogy(b_arr, interp_invertBx_func(b_arr), label="interpolated function")
plt.semilogy(b_arr[:-1], 1.0/Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```

```
In [13]: integral_invertBx_arr = np.zeros(b_arr.size-1)
beta_G_arr = np.zeros(b_arr.size-1)

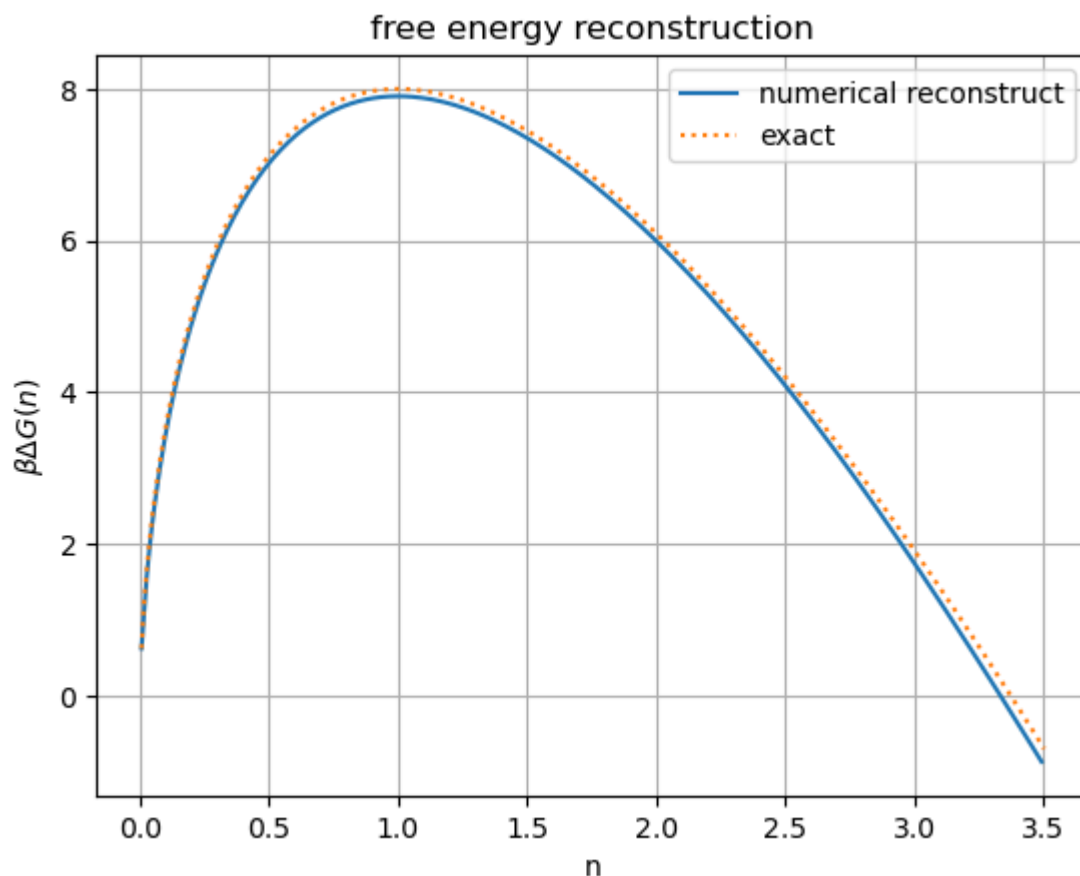
for i in range(b_arr.size-1):
    # Here x0 is b_arr[0]
    integral_invertBx_arr[i], _ = quad(interp_invertBx_func, b_arr[0], b_arr[i])
    beta_G_arr[i] = beta_Gcnt(b_arr[0])+np.log(Bx_arr[i]/Bx_arr[0])-integral_invertBx_arr[i]

print(_)

plt.plot(b_arr[:-1], beta_G_arr, label="numerical reconstruct")
plt.plot(b_arr, beta_Gcnt(b_arr), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \beta \Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

6.688236758529483e-08



```
In [14]: print(beta_G_arr[0], beta_Gcnt(b_arr[0]))
         beta_G_arr[:20]
```

```
0.6217642571710881 0.6217642571710881
```

```
Out[14]: array([0.62176426, 1.10776875, 1.56163295, 1.91170654, 2.22170962,
                2.4959099 , 2.74493635, 2.97328069, 3.1847236 , 3.38183371,
                3.56660717, 3.74058785, 3.90501315, 4.06089089, 4.20905636,
                4.35021196, 4.48495503, 4.61379922, 4.73719019, 4.85551783])
```

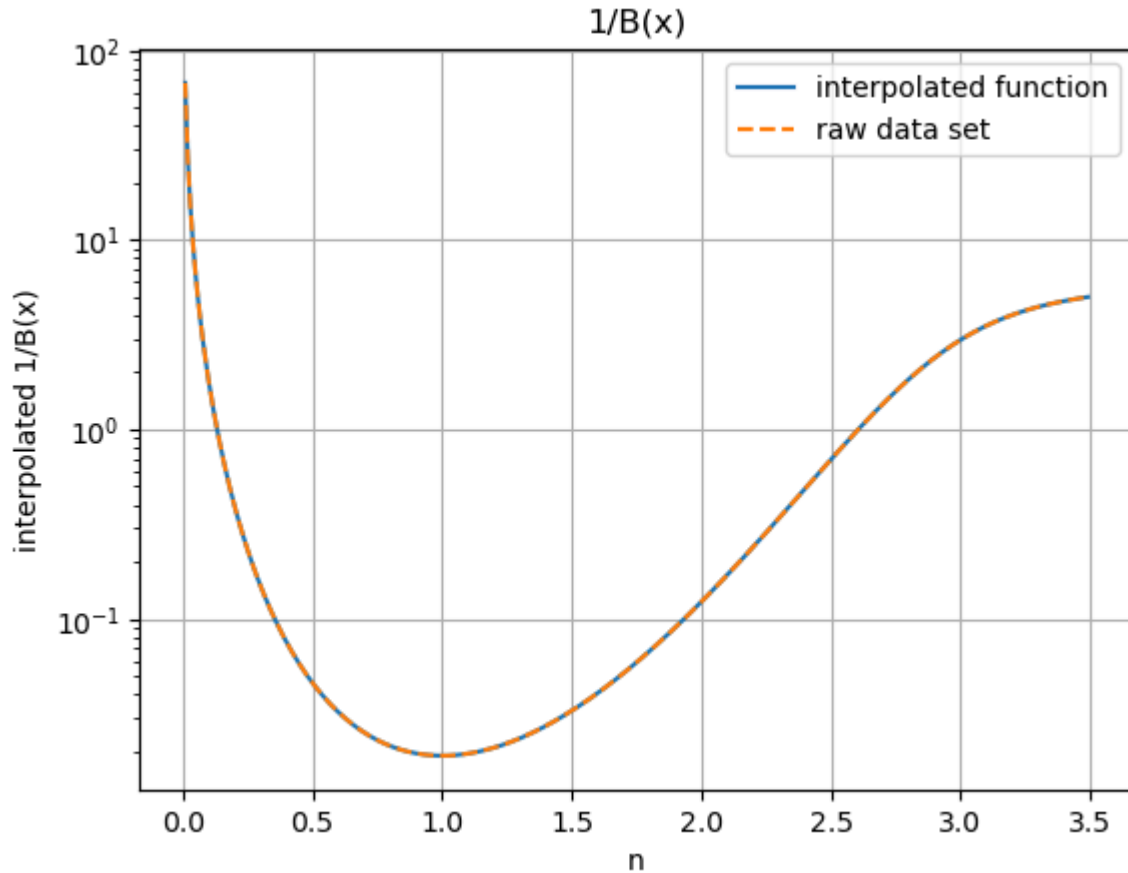
Reconstruct Free Energy from Numerical Integration of mfpt and Pst (st_P_func) - assume to be exact version

```
In [15]: # Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflect
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(st_P_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/st_P_func(x_arr[1+i])*(integral_Pst_arr[i]-st_flux*(mfpt))

interp_invertBx_func = interp1d(x_arr[1:-1], 1.0/Bx_arr, kind='cubic') # file

plt.semilogy(x_arr[1:-1], interp_invertBx_func(x_arr[1:-1]), label="interpolated")
plt.semilogy(x_arr[1:-1], 1.0/Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
```

```
plt.legend()
plt.grid()
```



```
In [16]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

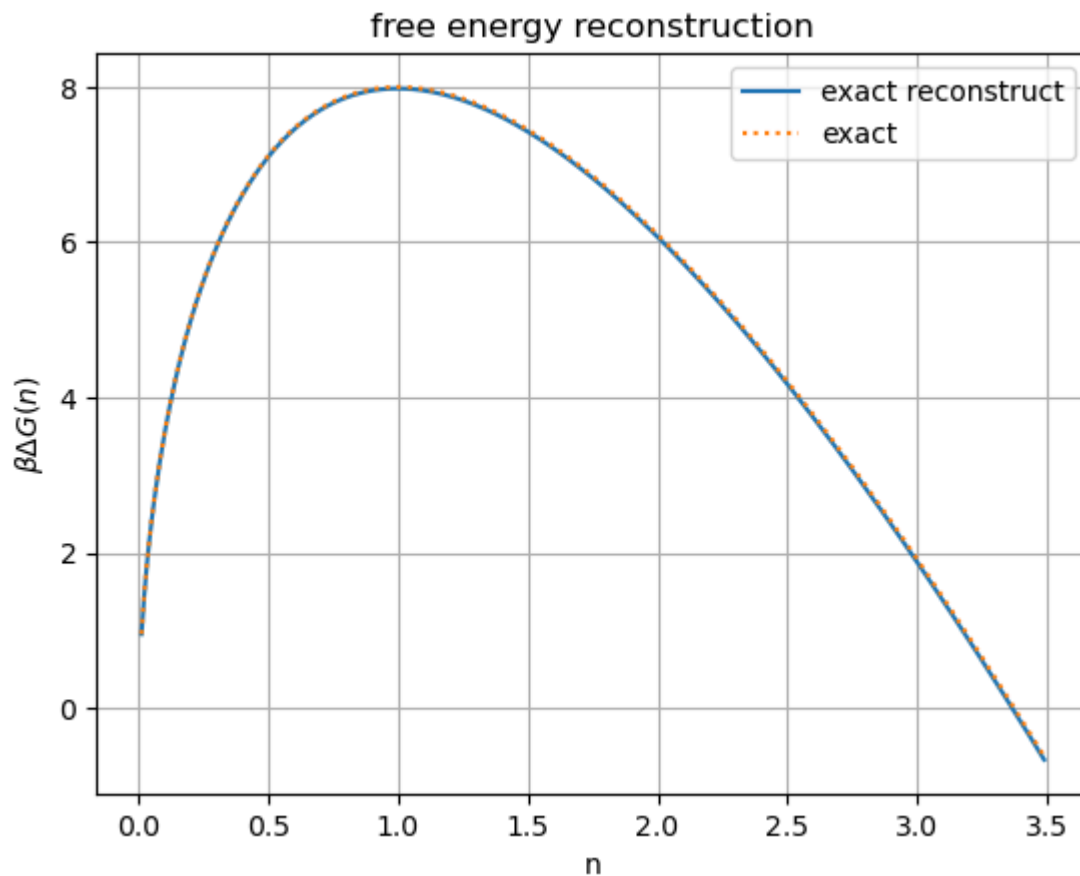
for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[1], x_arr
    beta_Grec2_arr[i] = beta_Gcnt(x_arr[1])+np.log(Bx_arr[i]/Bx_arr[0])-inte

print(_)

plt.plot(x_arr[1:-1], beta_Grec2_arr, label="exact reconstruct")
plt.plot(x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \beta \Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

4.893772083685819e-08



```
In [17]: print(beta_Grec2_arr[0], beta_Gcnt(x_arr[1]))
         beta_Grec2_arr[:20]
```

```
0.9539813200670669 0.9539813200670669
```

```
Out[17]: array([0.95398132, 1.43343661, 1.82586571, 2.15481149, 2.44531398,
                2.70622648, 2.94435174, 3.16386604, 3.36785    , 3.55856498,
                3.7377588 , 3.90681024, 4.06683332, 4.21874385, 4.36330646,
                4.50116787, 4.63288126, 4.7589245 , 4.87971397, 4.99561529])
```

```
In [ ]:
```

Verify Hill Relation: plot the $1/\text{flux}$, $\tau(b)$, and $2\tau(x^*)$ v.s different location of absorbing boundary

```
In [18]: def exact_flux(a, b):
         # Define the inner function to integrate as a function of y
         def inner_integrand(y):
             return 1.0/Dcnt(y)*np.exp(beta_Gcnt(y))

         # Define the inner integral as a function of x
         def inner_integral(x):
             y_lower = x
             y_upper = b
             result, error = quad(inner_integrand, y_lower, y_upper)
             return result
```

```

# Define the outer integral
x_lower = a
x_upper = b

# Define the outer function to integrate (also as a function of x)
def outer_integrand(x):
    return np.exp(-beta_Gcnt(x))*inner_integral(x)

# Perform the outer integration
invert_Jst, error = quad(outer_integrand, x_lower, x_upper)
return 1/invert_Jst

```

```

In [19]: # for valid value, exclude the reflecting boundary
Jst_arr = np.zeros(N-1)

for i in np.arange(N-1):
    Jst_arr[i] = exact_flux(x_arr[0], x_arr[1+i])

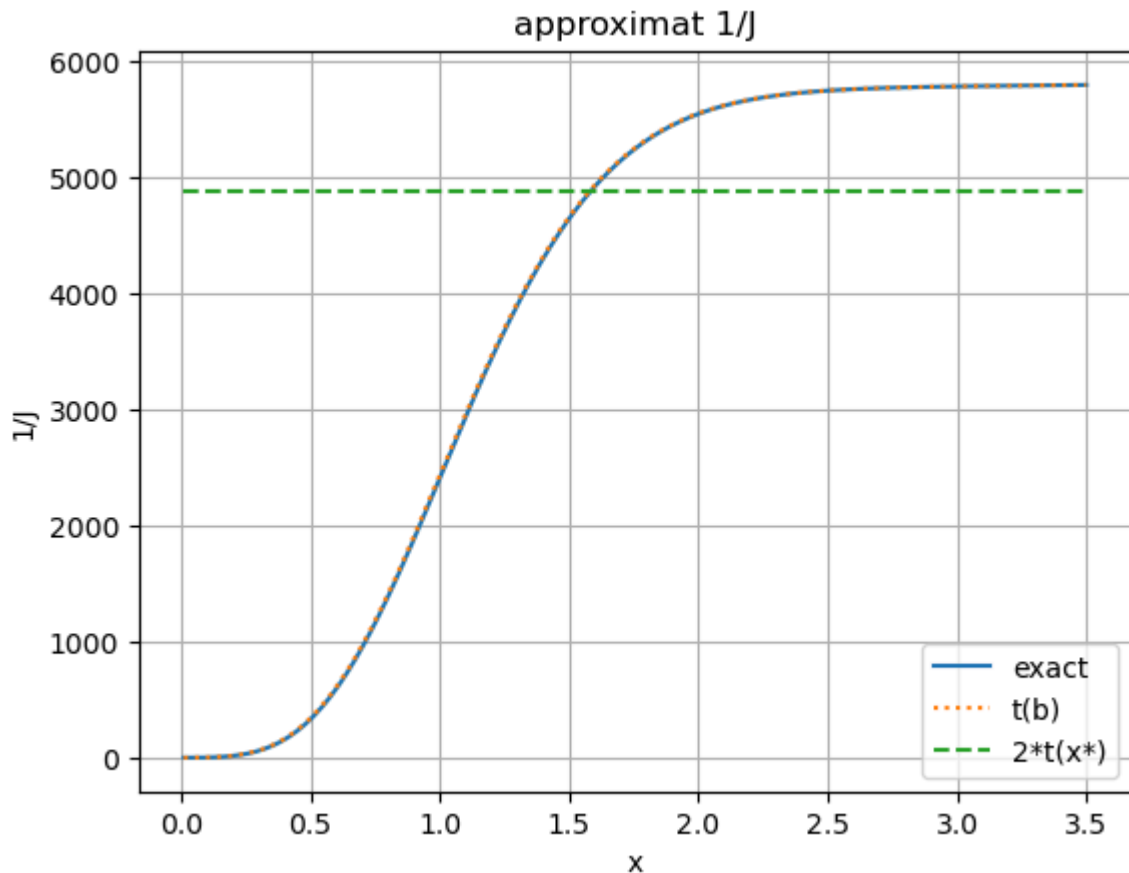
```

```

In [20]: plt.plot(x_arr[1:], 1/Jst_arr, label="exact")
plt.plot(x_arr[1:], mfpt_arr[1:], ':', label="t(b)")
plt.plot(x_arr[1:], 2*t_star*np.ones(x_arr[1:].size), '--', label="2*t(x*)")

# Plot formatting
plt.xlabel('x')
plt.ylabel('1/J')
plt.title('approximat 1/J')
plt.legend()
plt.grid()

```



In []:

Transfer Matrix with Recycling Boundary Condition

```
In [21]: from transfer_matrix_reptile import TransferMatrix_ReInAb

ria_trans = TransferMatrix_ReInAb(hx=h, x_arr=x_arr, beta_U=beta_Gcnt, crite
```

```
In [22]: # plt.plot(x_arr[:-1], ria_trans.steady_state, label="RIA")
# # plt.plot(x_arr[:-1], 1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.ei
# plt.plot(x_arr, st_P_arr, '--', label="exact")
# plt.plot(b_arr, Pst_arr, ':', label="numerical")

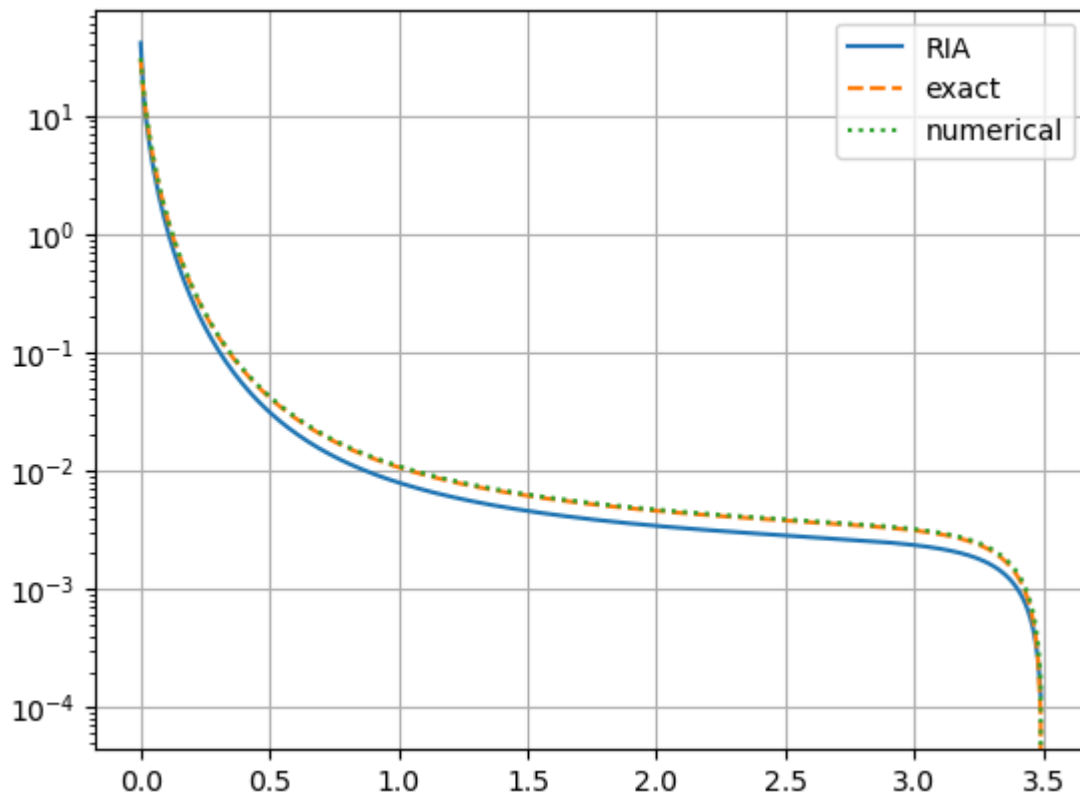
plt.semilogy(x_arr[:-1], ria_trans.steady_state, label="RIA")
# plt.semilogy(x_arr[:-1], 1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.
plt.semilogy(x_arr, st_P_arr, '--', label="exact")
plt.semilogy(x_arr, Pst_arr, ':', label="numerical")

plt.legend()
plt.grid()

print(ria_trans.relax_timescale)
```

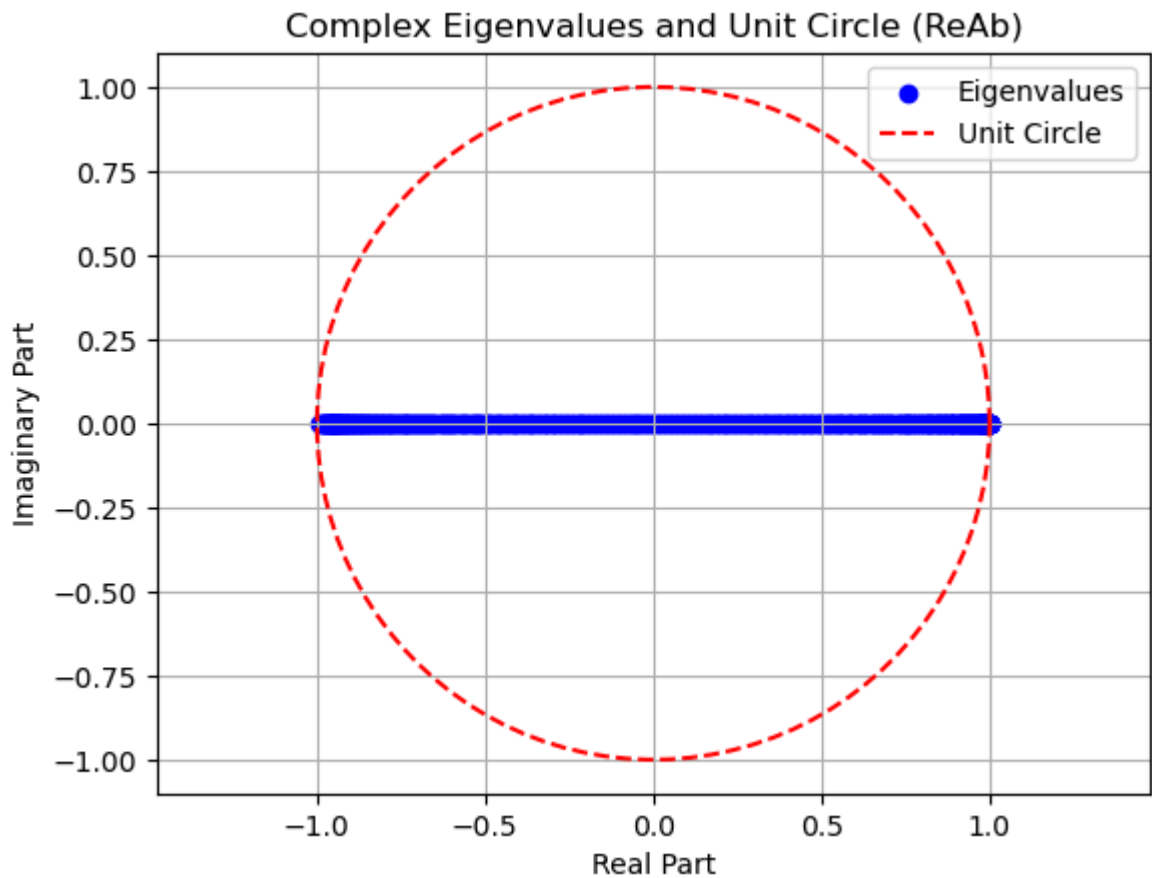
(4352.656550130287-0j)

```
/home/yjiang23/anaconda3/lib/python3.11/site-packages/matplotlib/cbook.py:16
99: ComplexWarning: Casting complex values to real discards the imaginary pa
rt
    return math.isfinite(val)
/home/yjiang23/anaconda3/lib/python3.11/site-packages/matplotlib/cbook.py:13
45: ComplexWarning: Casting complex values to real discards the imaginary pa
rt
    return np.asarray(x, float)
```



```
In [23]: ria_trans.plot_eigenvalues()
         print(ria_trans.eig6_w)
```

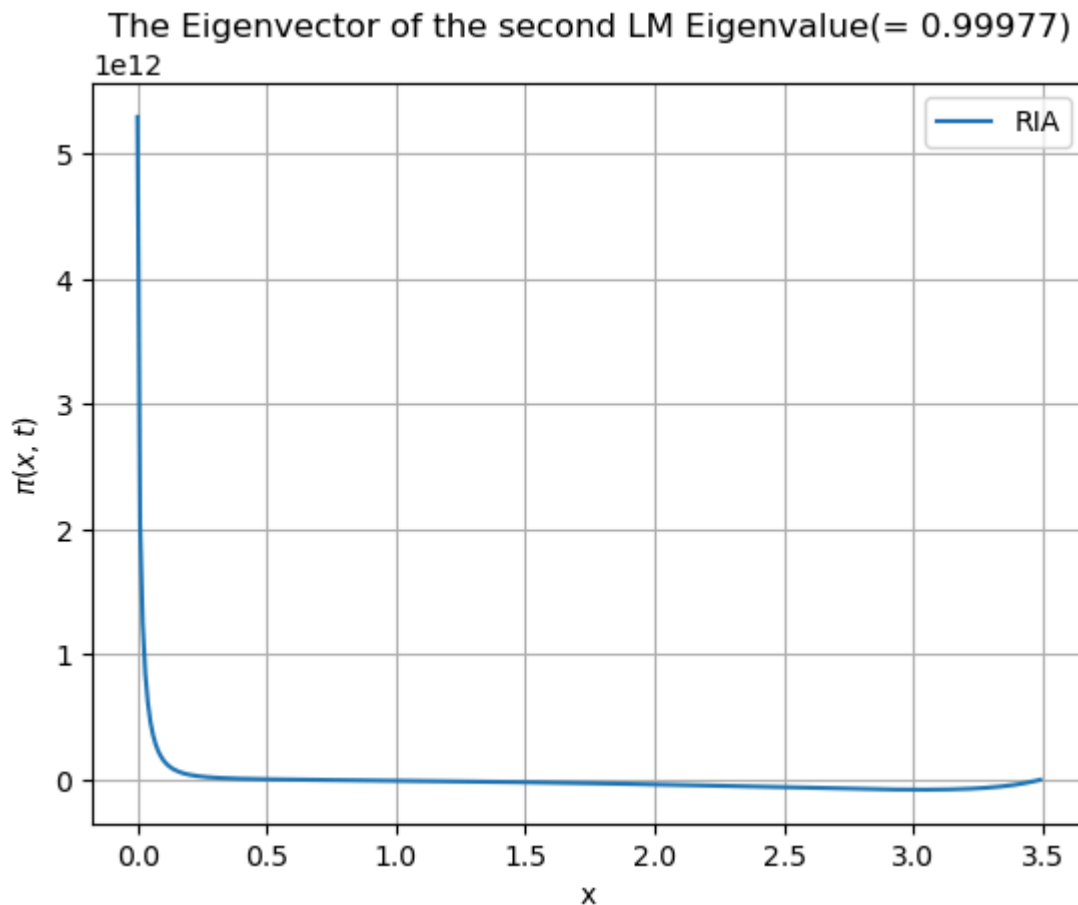
```
/home/yjiang23/Desktop/research/MFPT/MFPT_reconst_experiment/transfer_matrix_reptile.py:547: RuntimeWarning: k >= N - 1 for N * N square matrix. Attempting to use scipy.linalg.eig instead.
  eigenvalues, eigenvectors_mat = eigs(self.trans_mat, k=num_eigenvalues)
```



```
[1.          +0.j  0.99977028+0.j  0.99961714+0.j  0.99928545+0.j
 0.99911414+0.j  0.99848607+0.j]
```

```
In [24]: plt.plot(x_arr[:-1], 1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.eig6_v
# Plot formatting
plt.xlabel('x')
plt.ylabel('$ \pi(x,t) $')
plt.title(f'The Eigenvector of the second LM Eigenvalue(= {ria_trans.eig6_w[
plt.legend()
plt.grid(True)
print(1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.eig6_v[:, 1][:10])
```

```
[5.29151637e+12+0.j  2.04130994e+12+0.j  1.24718448e+12+0.j
 8.46879403e+11+0.j  6.10008138e+11+0.j  4.57150092e+11+0.j
 3.52744184e+11+0.j  2.78445060e+11+0.j  2.23877712e+11+0.j
 1.82777073e+11+0.j]
```

In []:

Extract Steady State Distribution and MFPT from Simulation

```
In [25]: from mfpt_Pst_RW_simulate import simulate_ReAb, simulate_ReAb_accelerate

num_particles = 600
init_position_arr = np.zeros(num_particles, dtype=float)
simu_x_arr = np.linspace(a, b, 351)
hx = simu_x_arr[1]-simu_x_arr[0]
ht = hx**2/(2*D0)
n_arr = np.arange(a, b+0.01, 0.01)
n_arr = np.round(n_arr, decimals=5)
hx == 0.01
```

Out[25]: True

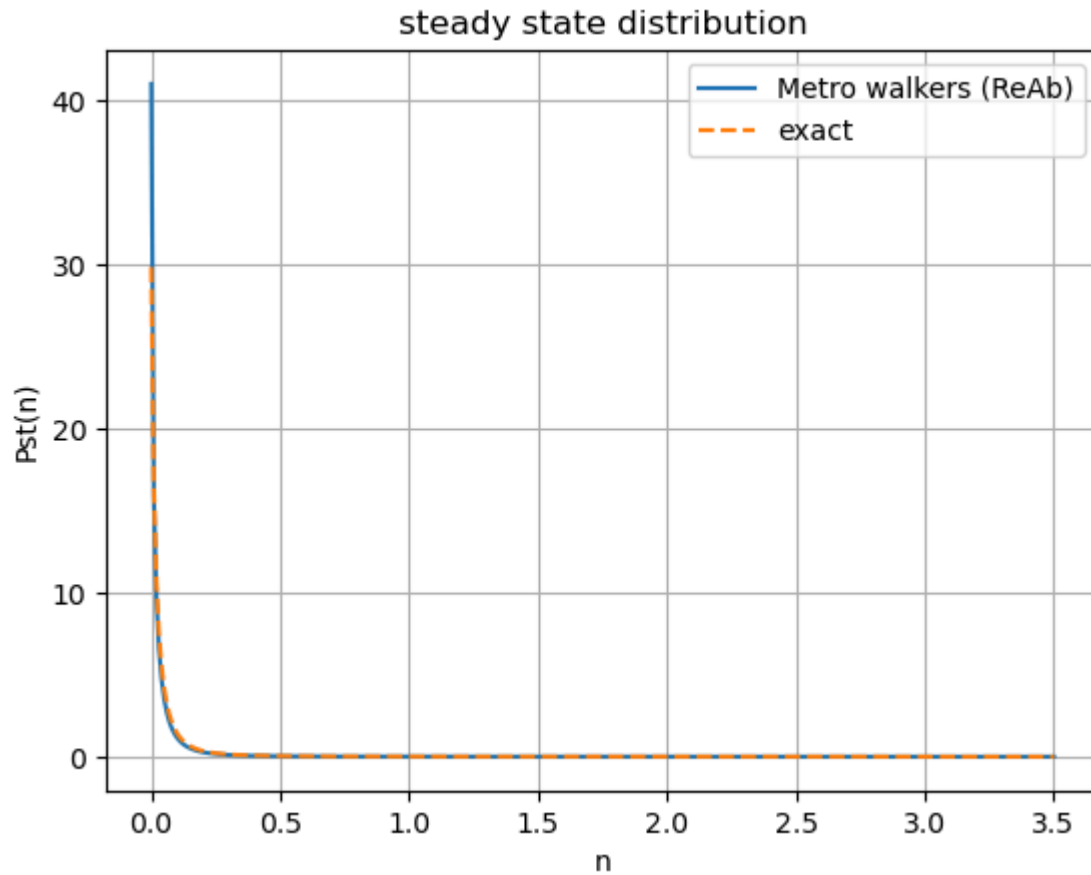
```
In [26]: count_n, ti_n = simulate_ReAb_accelerate(init_position_arr=init_position_arr)
```

```
In [27]: Pst_n = count_n/(hx*np.sum(count_n))
plt.plot(n_arr, Pst_n, label="Metro walkers (ReAb)")
plt.plot(x_arr, st_P_arr, '--', label="exact")
# plt.plot(x_arr[:-1], ria_trans.steady_state, label="RIA")
# plt.plot(x_arr[:-1], 1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.eig6_v[:, 1], label="exact")
```

```

# Plot formatting
plt.xlabel('n')
plt.ylabel('Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()

```

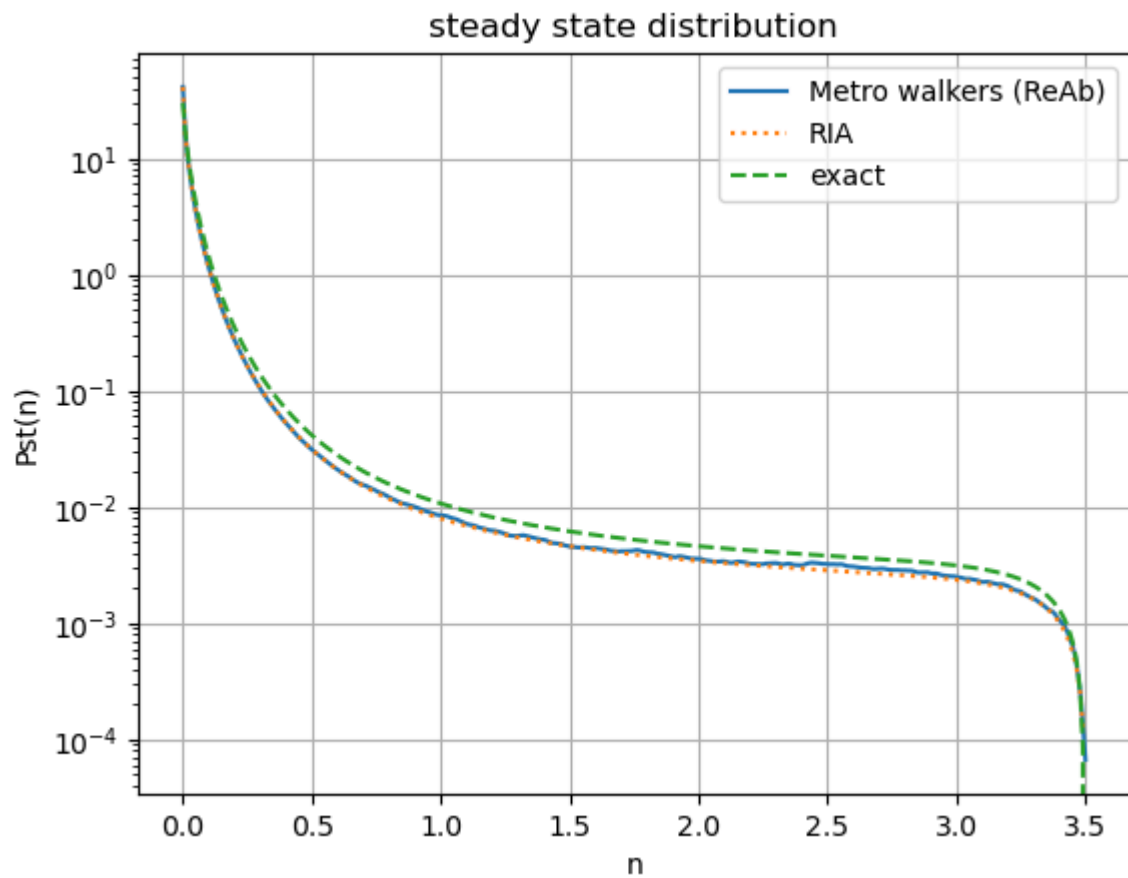


```

In [28]: plt.semilogy(n_arr, Pst_n, label="Metro walkers (ReAb)")
plt.semilogy(x_arr[:-1], ria_trans.steady_state, ':', label="RIA")
# plt.semilogy(x_arr[:-1], 1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*ria_trans.
plt.semilogy(x_arr, st_P_arr, '--', label="exact")

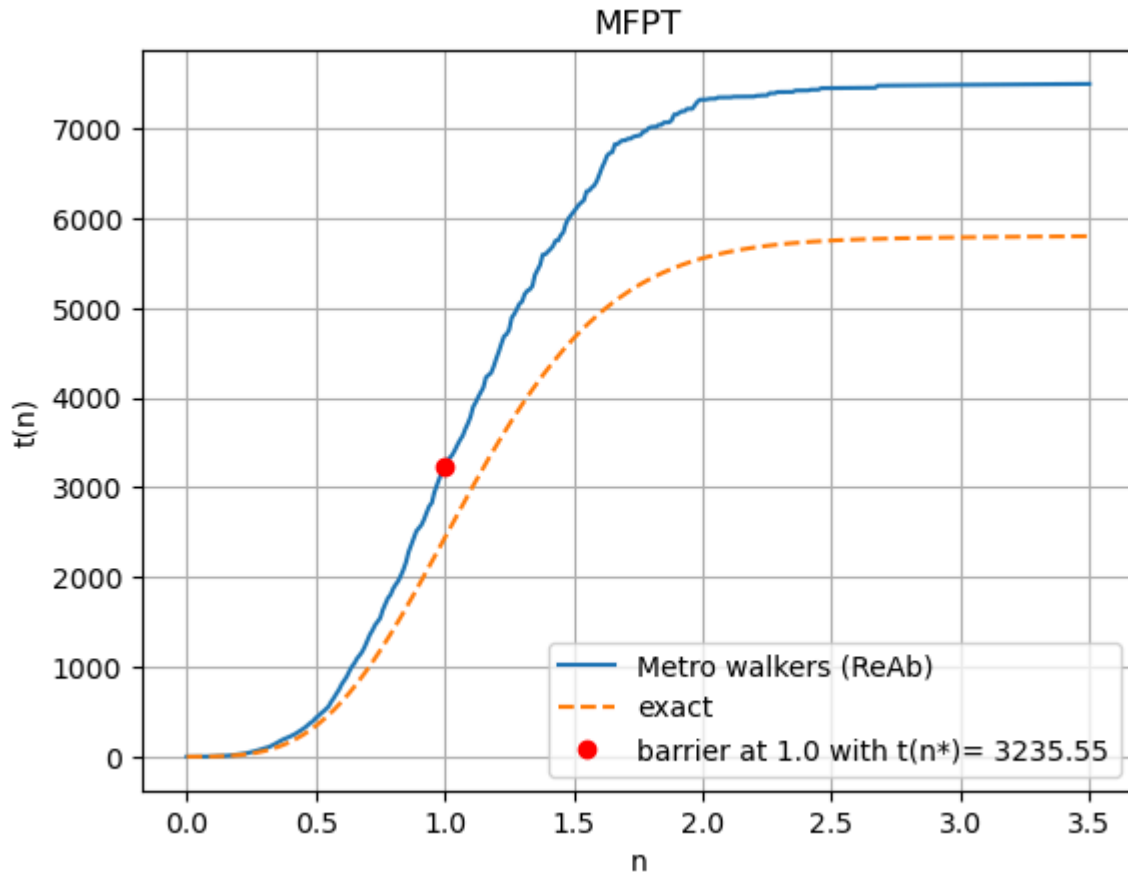
# Plot formatting
plt.xlabel('n')
plt.ylabel('Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()

```



```
In [29]: mfpt_simu_arr = np.mean(ti_n, axis=0)
idx_barrier = np.where(n_arr == 1.0)[0][0]
t_star = mfpt_simu_arr[idx_barrier]

plt.plot(n_arr, mfpt_simu_arr, label="Metro walkers (ReAb)")
plt.plot(x_arr, mfpt_arr, '--', label="exact")
plt.plot(1.0, t_star, 'ro', label=f'barrier at 1.0 with t(n*)={t_star: .2f}')
# Plot formatting
plt.xlabel('n')
plt.ylabel('t(n)')
plt.title('MFPT')
plt.legend()
plt.grid()
```



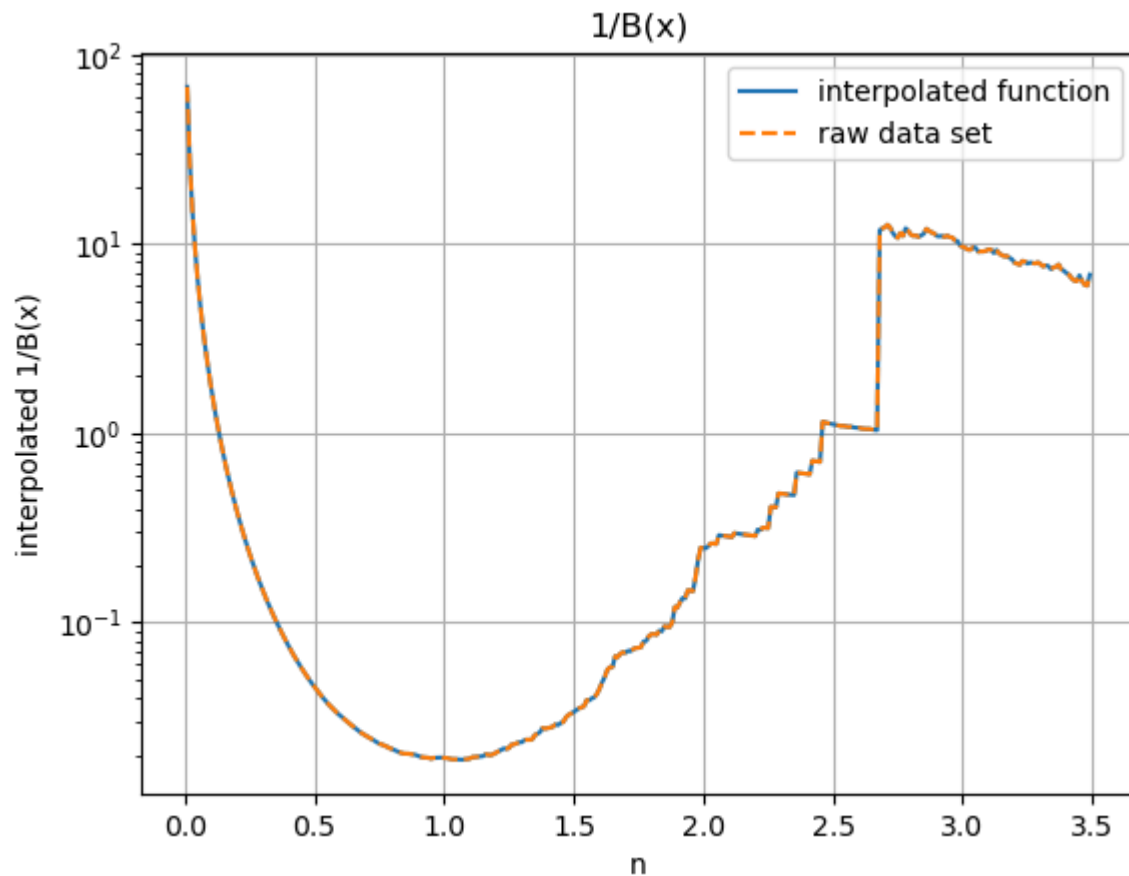
Reconstruct Free Energy Using mfpt (mfpt_simu_arr) and Pst (Pst_n) extracted from Simulation

(1) Exact Steady State Distribution with simulated MFPT

```
In [30]: # Except for the absorbing boundary  $P_{st}(b) = 0$ ,  $D(x)=0$ , also avoid at reflection
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(st_P_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/st_P_func(x_arr[1+i])*(integral_Pst_arr[i]-(mfpt_simu_arr[i]-mfpt_simu_arr[-1]))

interp_invertBx_func = interp1d(x_arr[1:-1], 1.0/Bx_arr, kind='cubic') # file

plt.semilogy(x_arr[1:-1], interp_invertBx_func(x_arr[1:-1]), label="interpolated 1/B(x)")
plt.semilogy(x_arr[1:-1], 1.0/Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```



```
In [31]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[1], x_arr
    beta_Grec2_arr[i] = beta_Gcnt(x_arr[1])+np.log(Bx_arr[i]/Bx_arr[0])-inte

print(_)

plt.plot(x_arr[1:-1], beta_Grec2_arr, label="simulation reconstruct")
plt.plot(x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \\beta \\Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

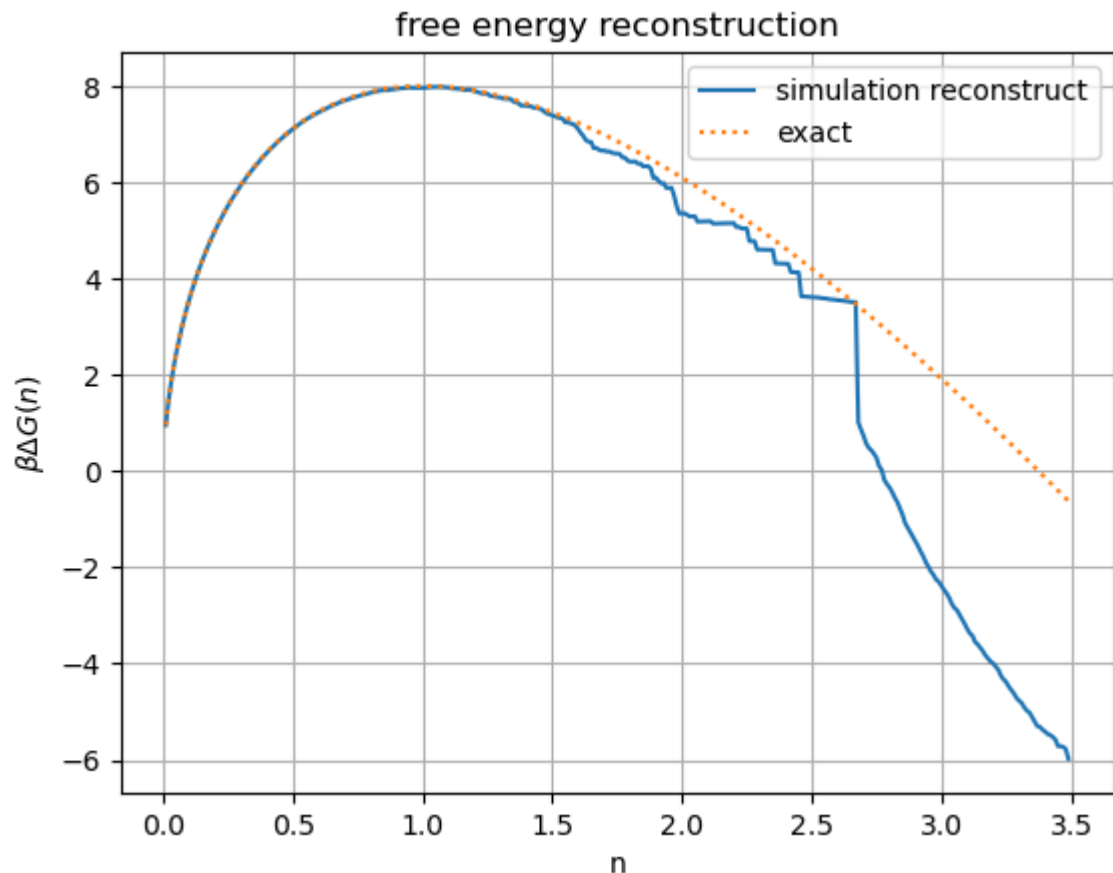
```
/tmp/ipykernel_784189/2563123347.py:6: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.
```

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.

```
integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[i], x_arr[i+1])
```

```
0.012095718480184713
```



(2) Transfer Matrix Steady State Distribution with exact MFPT and then with simulated MFPT

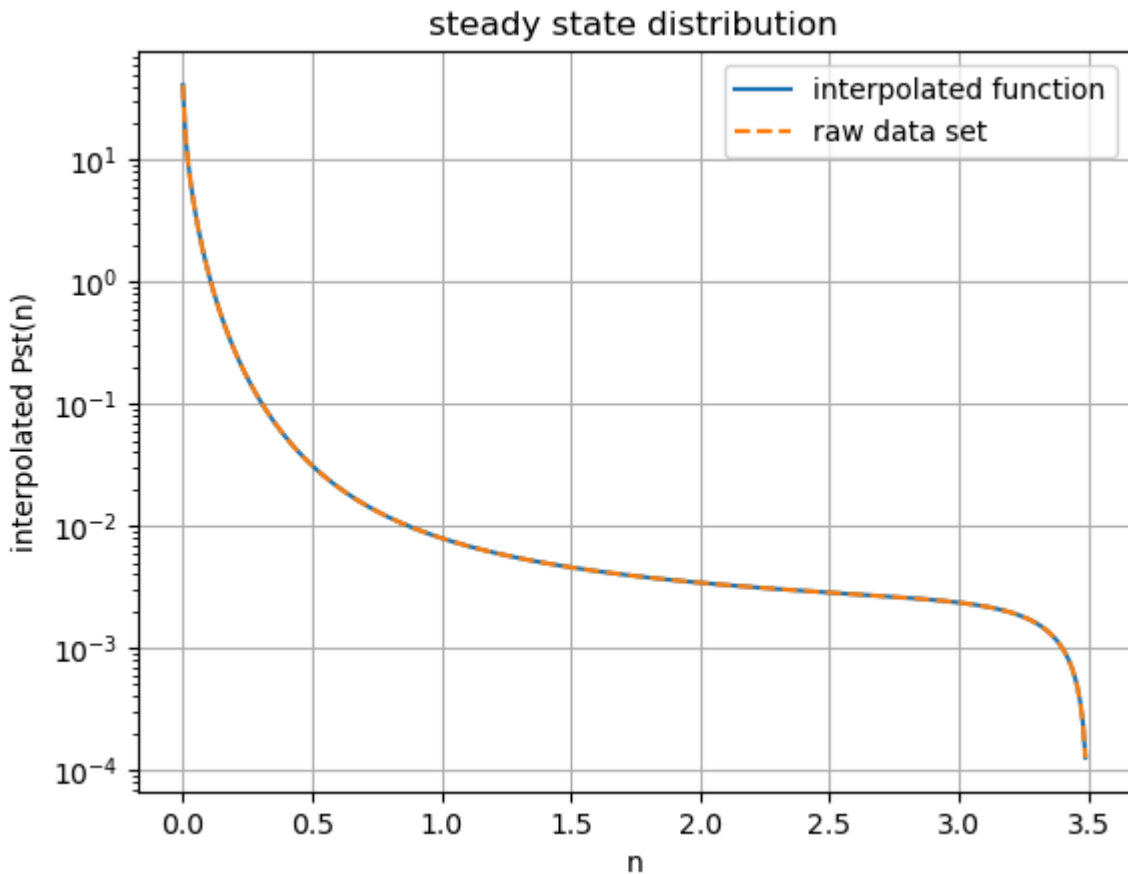
```
In [32]: interp_Pst_func = interp1d(x_arr[:-1], np.array(ria_trans.steady_state, dtype=float))
# interp_Pst_func = interp1d(x_arr[:-1], np.array(1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*r

plt.semilogy(x_arr[:-1], interp_Pst_func(x_arr[:-1])), label="interpolated function")
plt.semilogy(x_arr[:-1], ria_trans.steady_state, '--', label="raw data set")
# plt.semilogy(x_arr[:-1], np.array(1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*r

# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()
```

```
/tmp/ipykernel_784189/2788019905.py:1: ComplexWarning: Casting complex values
to real discards the imaginary part
```

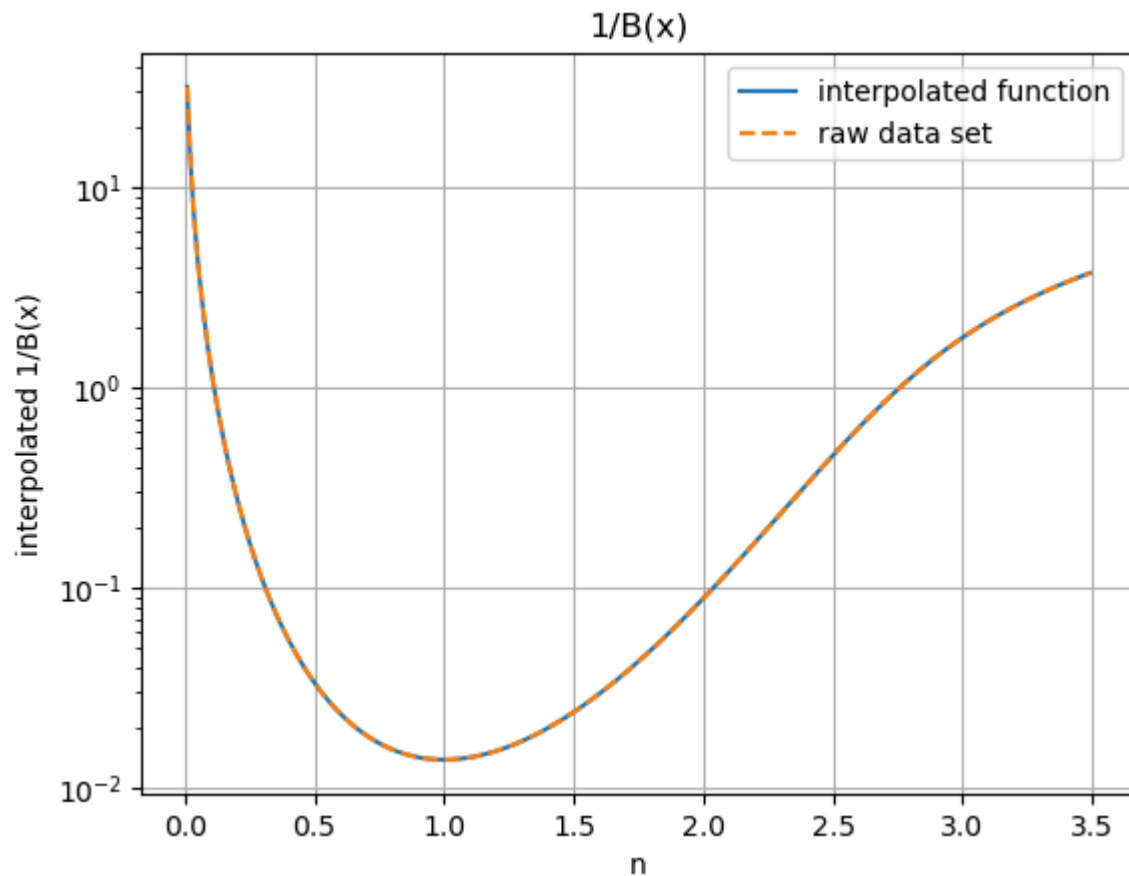
```
interp_Pst_func = interp1d(x_arr[:-1], np.array(ria_trans.steady_state, dtype=float), kind='cubic', fill_value="extrapolate")
```



```
In [33]: # Except for the absorbing boundary  $Pst(b) = 0$ ,  $D(x)=0$ , also avoid at reflect
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(interp_Pst_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/interp_Pst_func(x_arr[1+i])*(integral_Pst_arr[i]-(mfpt_
    #  $Bx\_arr[i] = -1.0/interp\_Pst\_func(x\_arr[1+i])*(integral\_Pst\_arr[i]-st\_t$ 

interp_invertBx_func = interp1d(x_arr[1:-1], 1.0/Bx_arr, kind='cubic') # fil

plt.semilogy(x_arr[1:-1], interp_invertBx_func(x_arr[1:-1]), label="interpol
plt.semilogy(x_arr[1:-1], 1.0/Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```



```
In [34]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

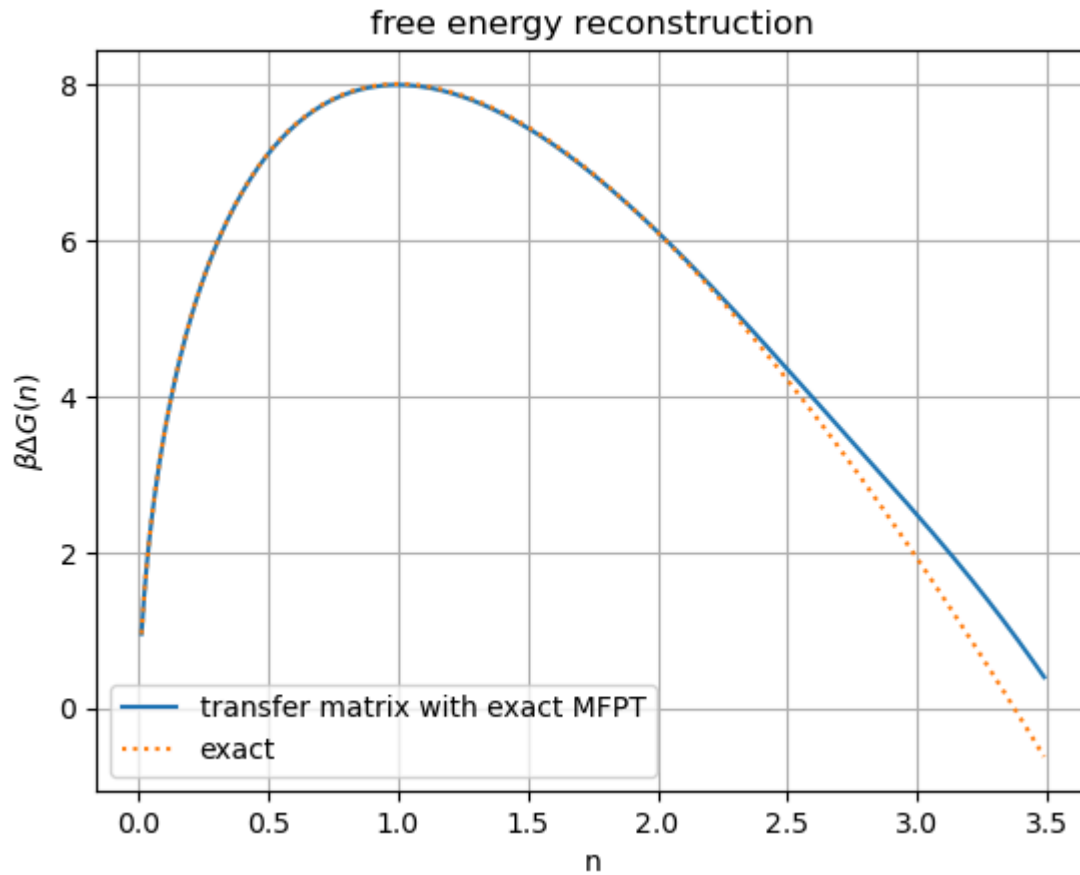
for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[1], x_arr
    beta_Grec2_arr[i] = beta_Gcnt(x_arr[1])+np.log(Bx_arr[i]/Bx_arr[0])-inte

print(_)

plt.plot(x_arr[1:-1], beta_Grec2_arr, label="transfer matrix with exact MFPT")
plt.plot(x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \\beta \\Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

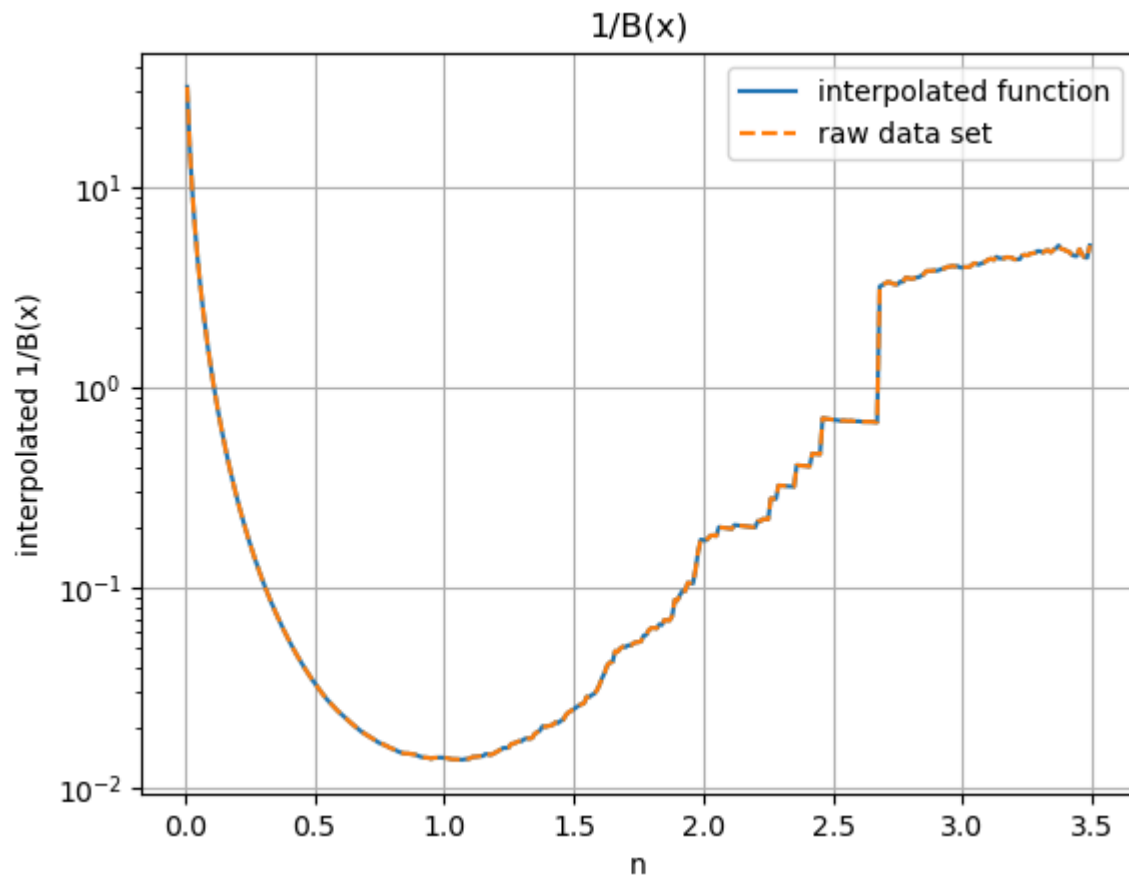
3.583373171061787e-08



```
In [35]: # Except for the absorbing boundary  $P_{st}(b) = 0$ ,  $D(x)=0$ , also avoid at reflection
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(interp_Pst_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/interp_Pst_func(x_arr[1+i])*(integral_Pst_arr[i]-(mfpt_

interp_invertBx_func = interp1d(x_arr[1:-1], 1.0/Bx_arr, kind='cubic') # file

plt.semilogy(x_arr[1:-1], interp_invertBx_func(x_arr[1:-1]), label="interpolated 1/B(x)")
plt.semilogy(x_arr[1:-1], 1.0/Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```



```
In [36]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[1], x_arr
    beta_Grec2_arr[i] = beta_Gcnt(x_arr[1])+np.log(Bx_arr[i]/Bx_arr[0])-inte

print(_)

plt.plot(x_arr[1:-1], beta_Grec2_arr, label="transfer matrix with simulated
plt.plot(x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \\beta \\Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

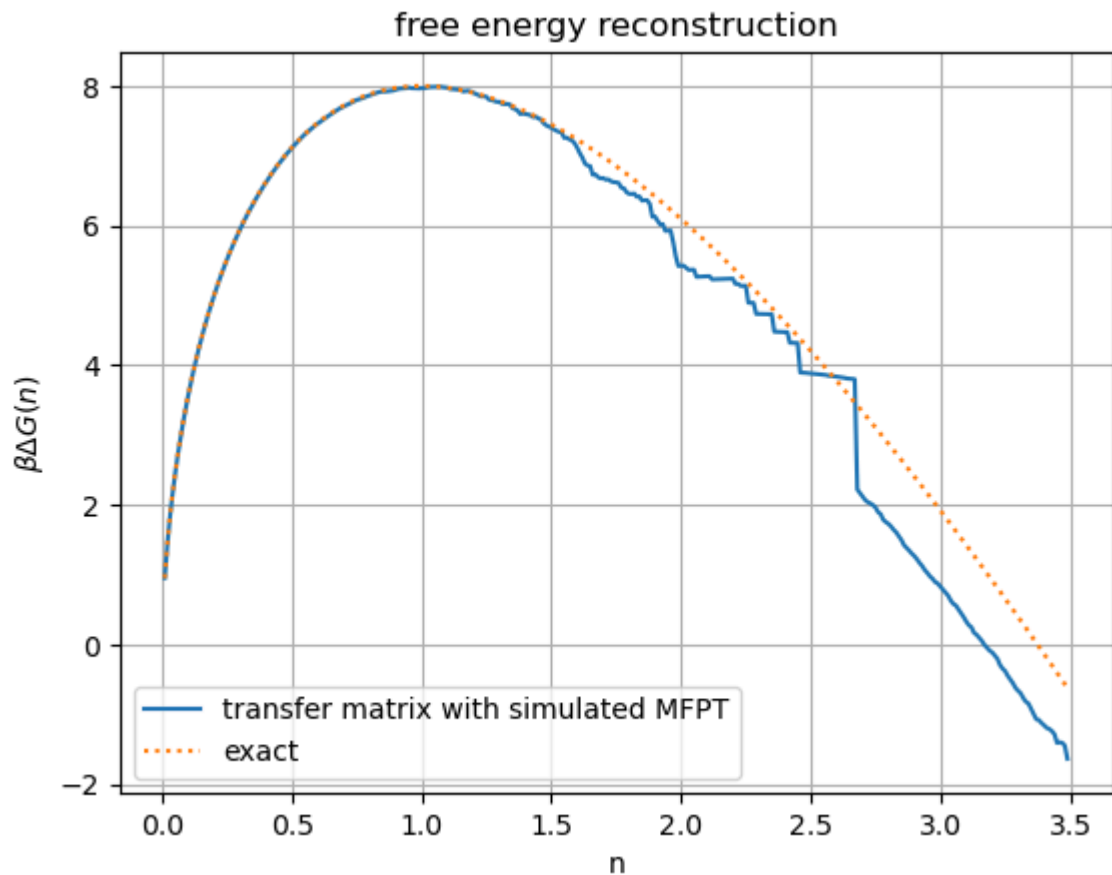
0.0047117370194555445

```
/tmp/ipykernel_784189/2741261074.py:6: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.
```

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.

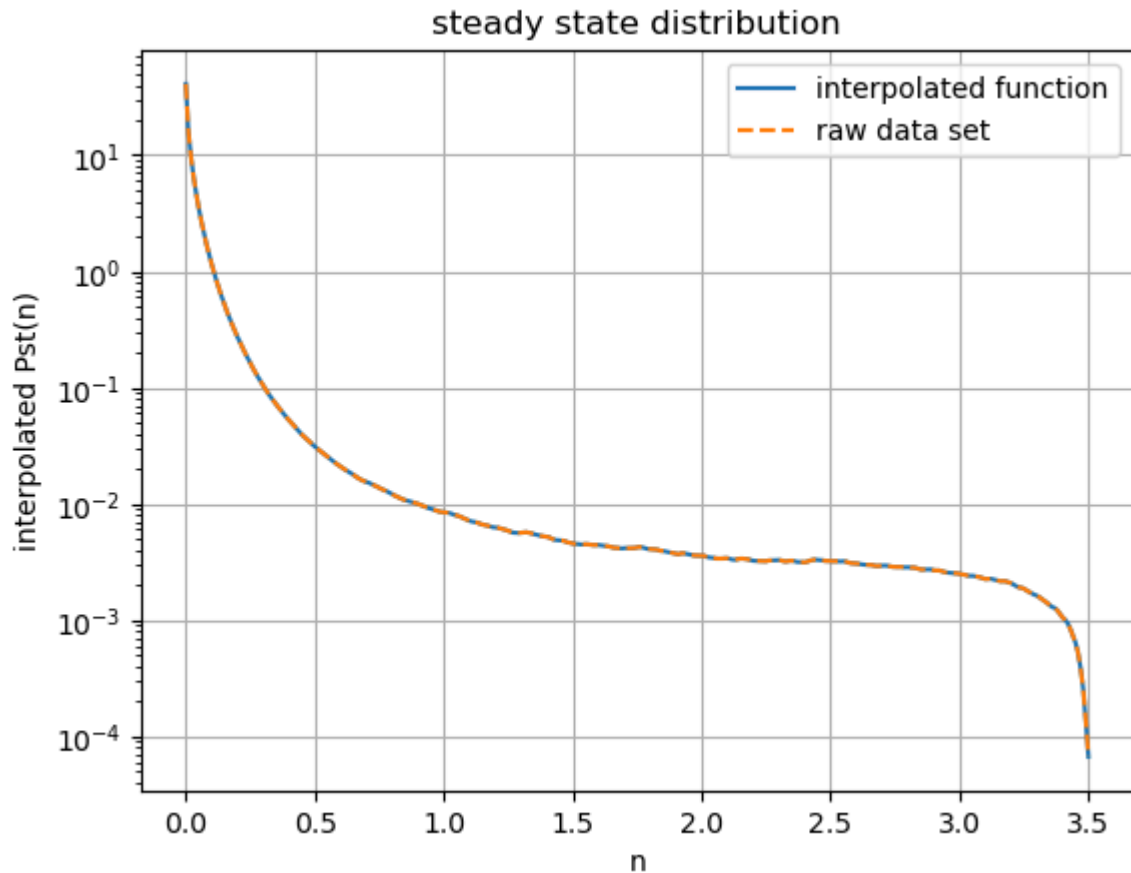
```
integral_invertBx_arr[i], _ = quad(interp_invertBx_func, x_arr[1], x_arr[1+i])
```



(3) Simulated Steady State Distribution with exact MFPT and then with simulated MFPT

```
In [37]: interp_simu_Pst_func = interp1d(simu_x_arr, Pst_n, kind='cubic', fill_value=
# interp_Pst_func = PchipInterpolator(b_arr, Pst_arr)

plt.semilogy(simu_x_arr, interp_simu_Pst_func(simu_x_arr), label="interpolat
plt.semilogy(simu_x_arr, Pst_n, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()
```



```
In [38]: # Except for the absorbing boundary  $Pst(b) = 0$ ,  $D(x)=0$ , also avoid at reflection
simu_Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(interp_simu_Pst_func, simu_x_arr[1+i], simu_x_arr[-1])
    simu_Bx_arr[i] = -1.0/Pst_n[1+i]*(integral_Pst_arr[i]-(mfpt_arr[-1]-mfpt_arr[i]))

interp_simu_invertBx_func = interp1d(x_arr[1:-1], 1.0/simu_Bx_arr, kind='cubic')

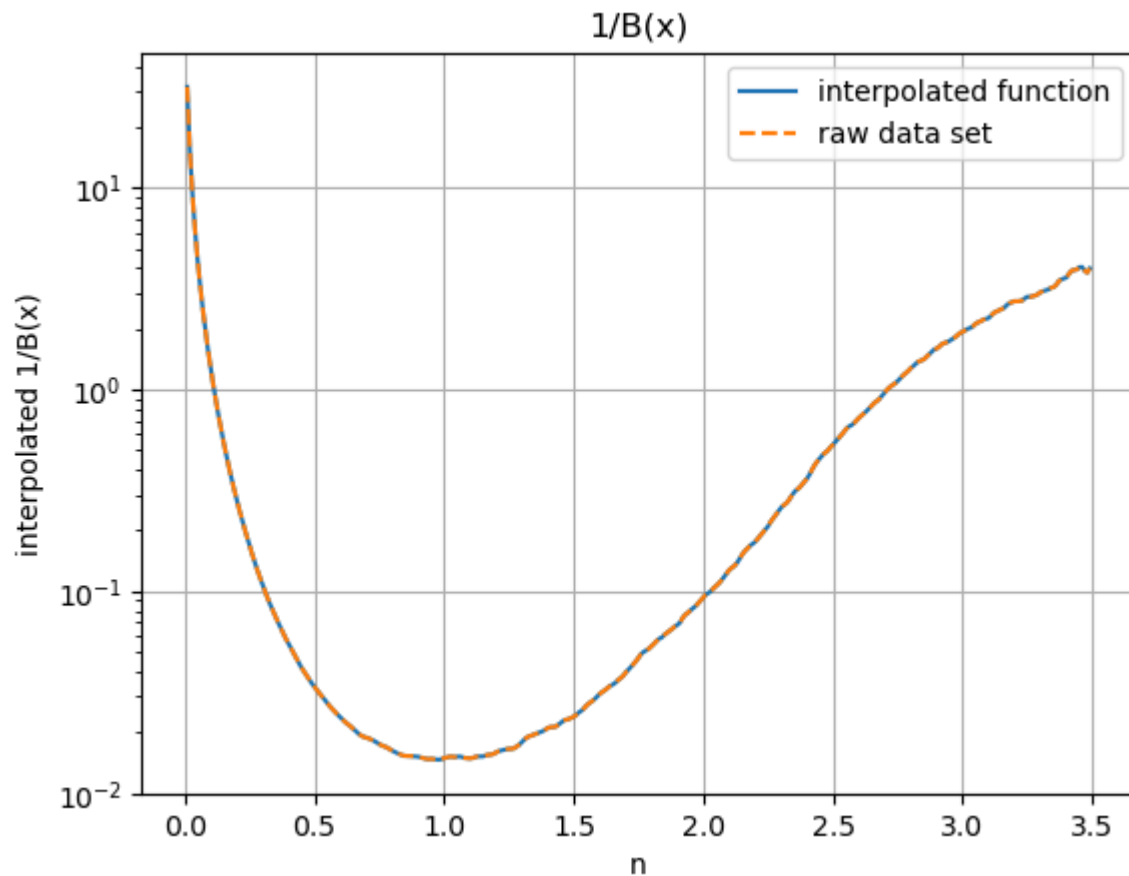
plt.semilogy(simu_x_arr[1:-1], interp_simu_invertBx_func(x_arr[1:-1]), label='interpolated 1/B(x)')
plt.semilogy(simu_x_arr[1:-1], 1.0/simu_Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```

/tmp/ipykernel_784189/3951444635.py:5: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.

```
integral_Pst_arr[i], _ = quad(interp_simu_Pst_func, simu_x_arr[1+i], simu_x_arr[-1])
```



```
In [39]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_simu_invertBx_func, simu_x_arr
    beta_Grec2_arr[i] = beta_Gcnt(simu_x_arr[1])+np.log(simu_Bx_arr[i]/simu_

print(_)

plt.plot(simu_x_arr[1:-1], beta_Grec2_arr, label="simulated Pst reconstruct")
plt.plot(simu_x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \\beta \\Delta G(n) $')
plt.title('free energy reconstruction')
plt.legend()
plt.grid()
```

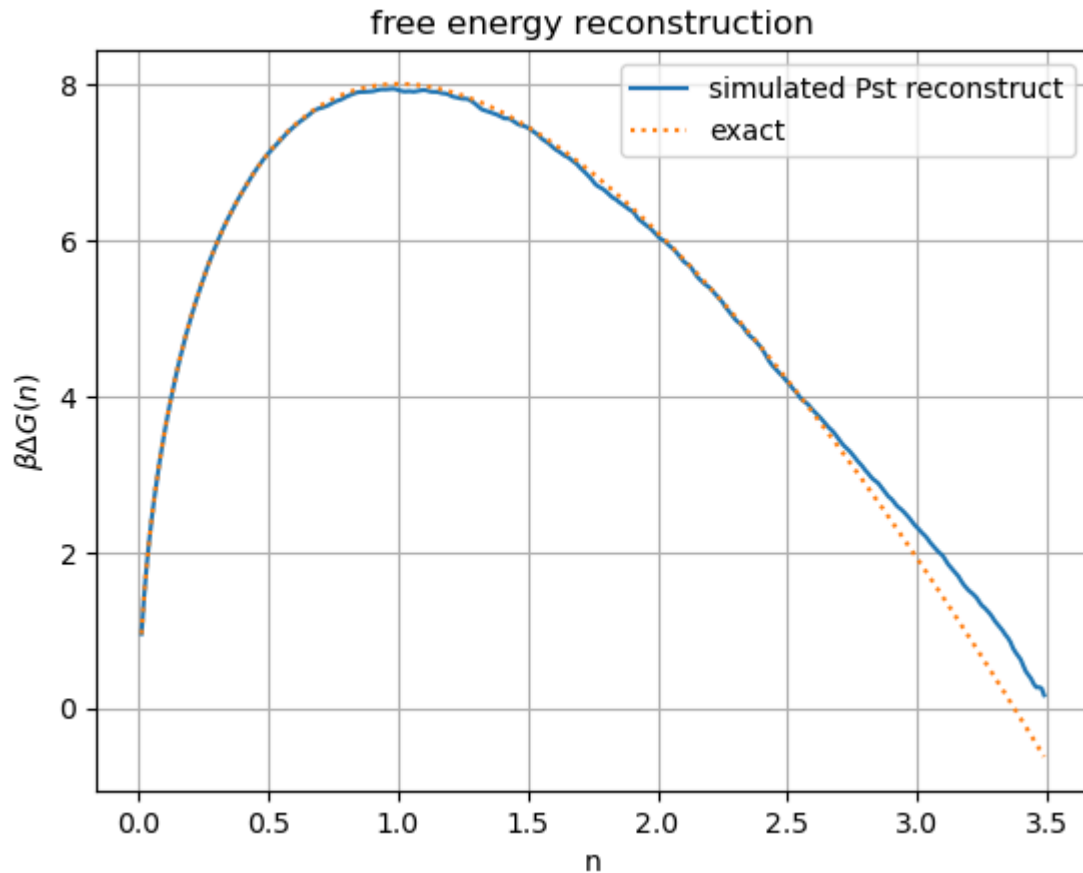
/tmp/ipykernel_784189/4156853672.py:6: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.

```
integral_invertBx_arr[i], _ = quad(interp_simu_invertBx_func, simu_x_arr[1], simu_x_arr[1+i])
```

0.0003577887668912735



```
In [40]: # Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflection
simu_Bx_arr = np.zeros(N+2)
integral_Pst_arr = np.zeros(N+2)
for i in range(N+2):
    integral_Pst_arr[i], _ = quad(interp_simu_Pst_func, simu_x_arr[1+i], simu_x_arr[1+i])
    simu_Bx_arr[i] = -1.0/Pst_n[1+i]*(integral_Pst_arr[i]-(mfpt_simu_arr[1+i]-mfpt_simu_arr[1]))

interp_simu_invertBx_func = interp1d(simu_x_arr[1:-1], 1.0/simu_Bx_arr, kind='spline', fill_value=0)

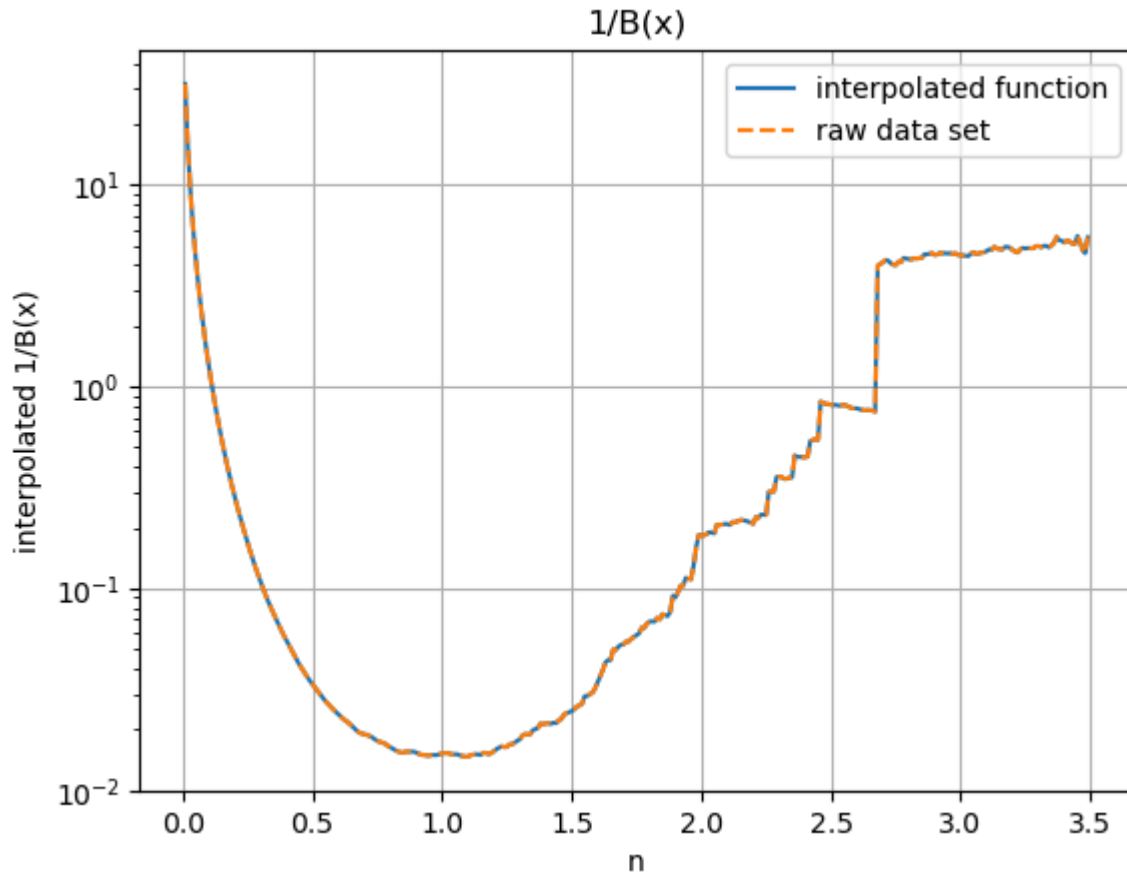
plt.semilogy(simu_x_arr[1:-1], interp_simu_invertBx_func(x_arr[1:-1]), label='interpolated 1/B(x)')
plt.semilogy(simu_x_arr[1:-1], 1.0/simu_Bx_arr, '--', label="raw data set")
# Plot formatting
plt.xlabel('n')
plt.ylabel('interpolated 1/B(x)')
plt.title('1/B(x)')
plt.legend()
plt.grid()
```

/tmp/ipykernel_784189/1053423012.py:5: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.

```
integral_Pst_arr[i], _ = quad(interp_simu_Pst_func, simu_x_arr[1+i], simu_x_arr[-1])
```



```
In [41]: integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

for i in range(N-2):
    # Here x0 is x_arr[1]
    integral_invertBx_arr[i], _ = quad(interp_simu_invertBx_func, simu_x_arr[1+i], simu_x_arr[-1])
    beta_Grec2_arr[i] = beta_Gcnt(simu_x_arr[1+i]) + np.log(simu_Bx_arr[i]/simu_Bx_arr[1])

print(_)

plt.plot(simu_x_arr[1:-1], beta_Grec2_arr, label="simulated Pst&MFPT reconst")
plt.plot(simu_x_arr[1:-1], beta_Gcnt(x_arr[1:-1]), ':', label="exact")

# Plot formatting
plt.xlabel('n')
plt.ylabel('$ \beta \Delta G(n) $')
plt.title('free energy reconstruction')
```

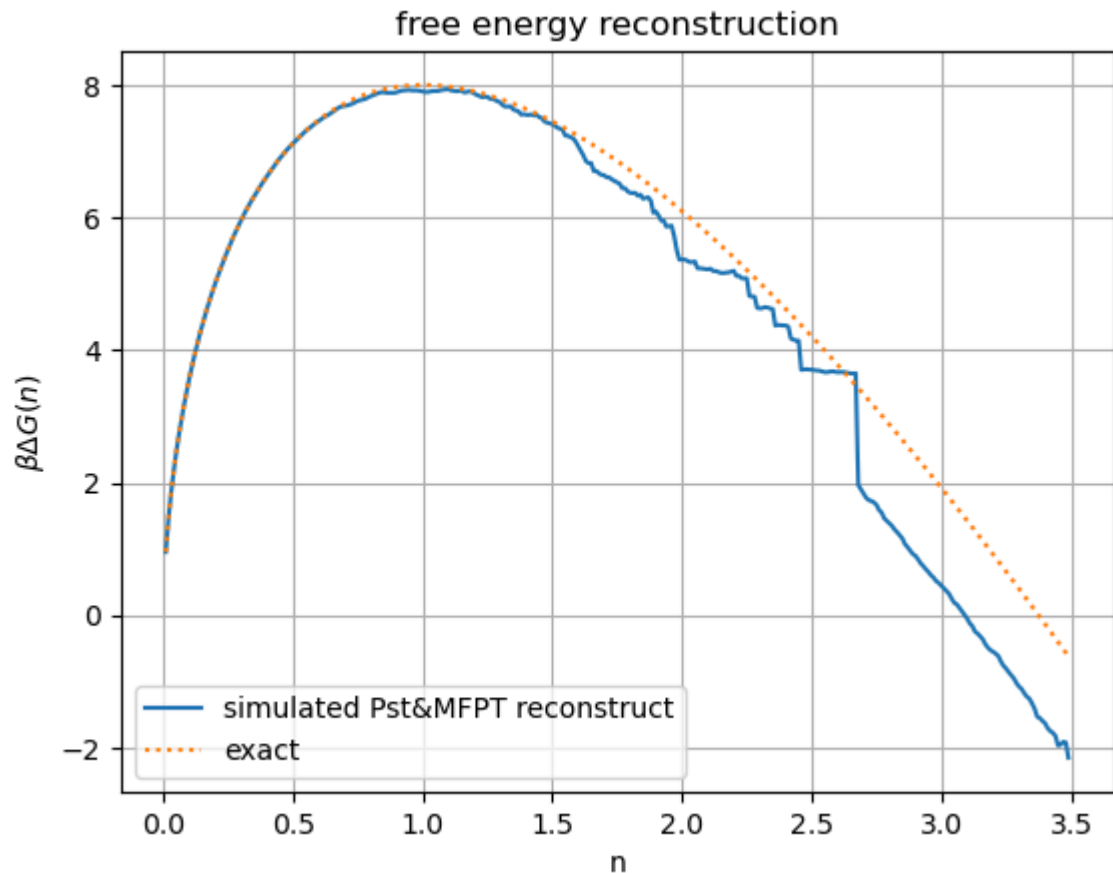
```
plt.legend()  
plt.grid()
```

/tmp/ipykernel_784189/1290495388.py:6: IntegrationWarning: The maximum number of subdivisions (50) has been achieved.

If increasing the limit yields no improvement it is advised to analyze the integrand in order to determine the difficulties. If the position of a

local difficulty can be determined (singularity, discontinuity) one will probably gain from splitting up the interval and calling the integrator on the subranges. Perhaps a special-purpose integrator should be used.
integral_invertBx_arr[i], _ = quad(interp_simu_invertBx_func, simu_x_arr[1], simu_x_arr[1+i])

0.00755549516305902



In []:

In []: