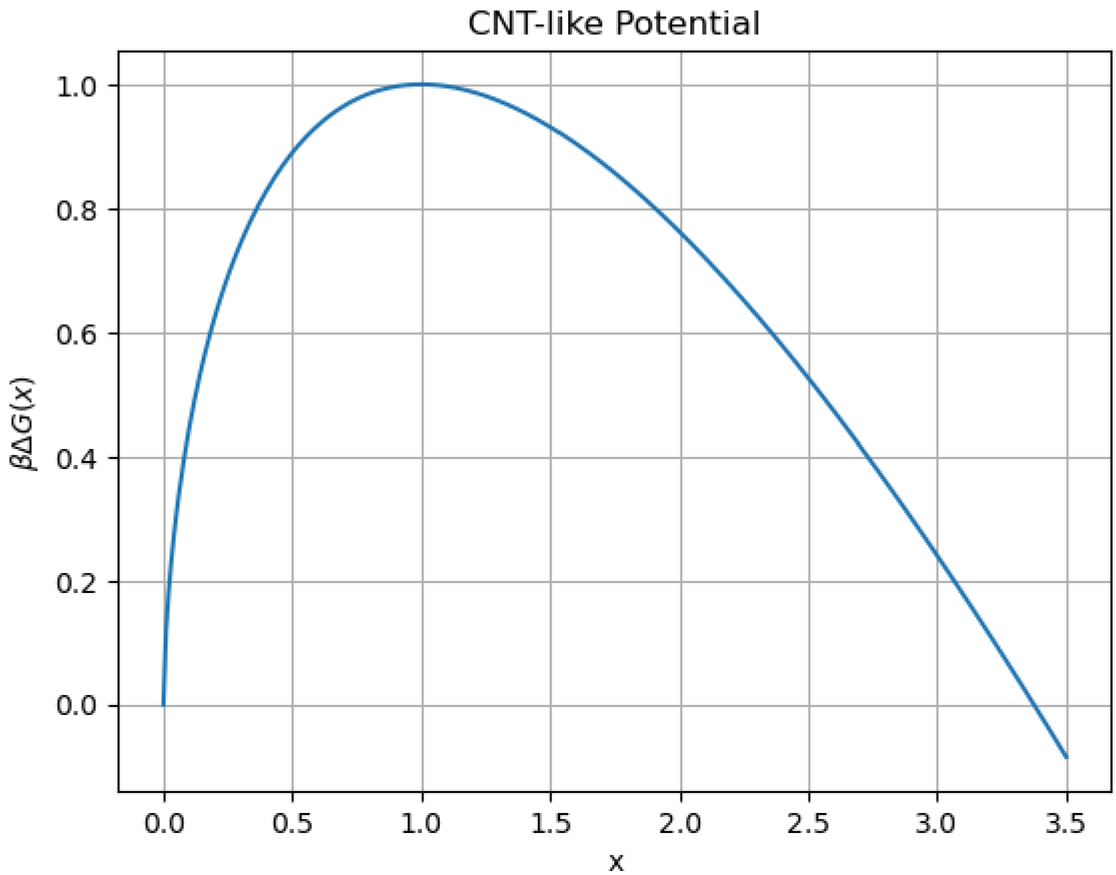
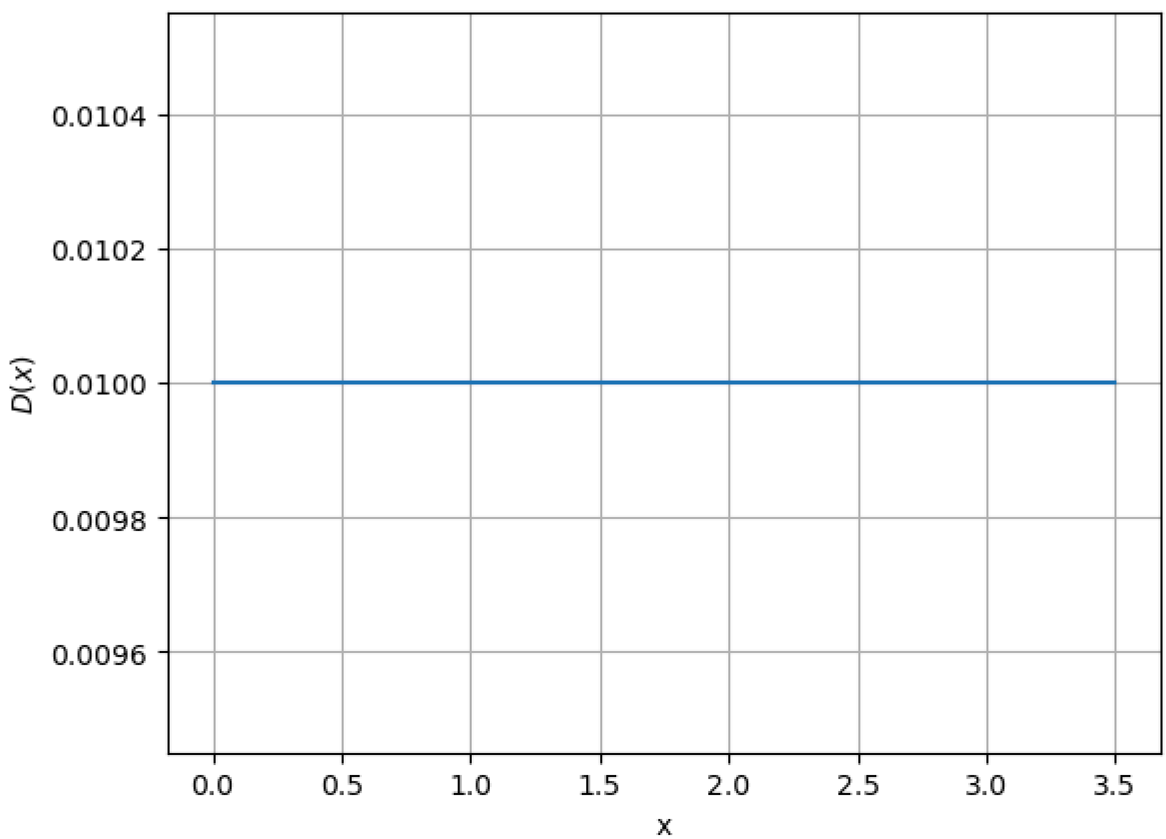
In [1]:
```python
import numpy as np
import matplotlib.pyplot as plt
from scipy.sparse.linalg import spsolve
from scipy.integrate import quad
from scipy.interpolate import interp1d, PchipInterpolator
```

In [2]:
```python
beta_Gstar = 1 # 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]:
```python
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)$')`



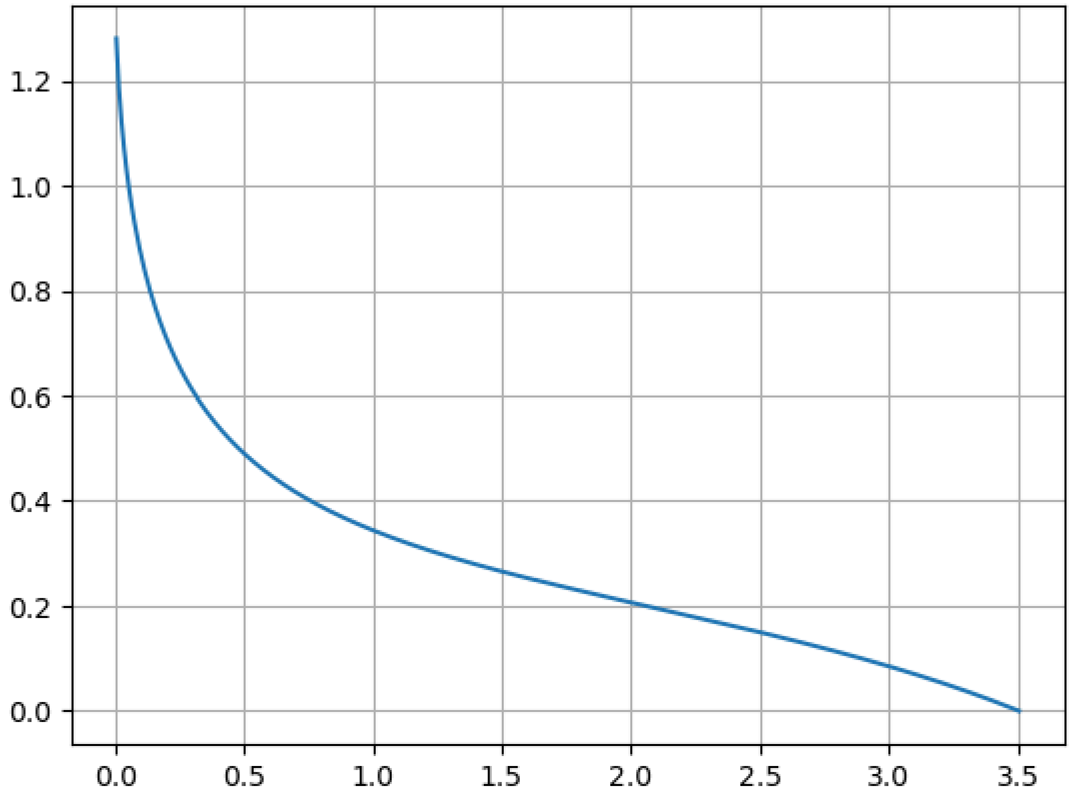
Numerical solve ODE with injecting boundary condition to find steady state solution

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()
```

```
0.0009888206574441799
```

```
/tmp/ipykernel_715167/3470158452.py:11: SparseEfficiencyWarning: spsolve req
uires A be CSC or CSR matrix format
  u_arr[0:-1] = spsolve(A, f_vect)
```



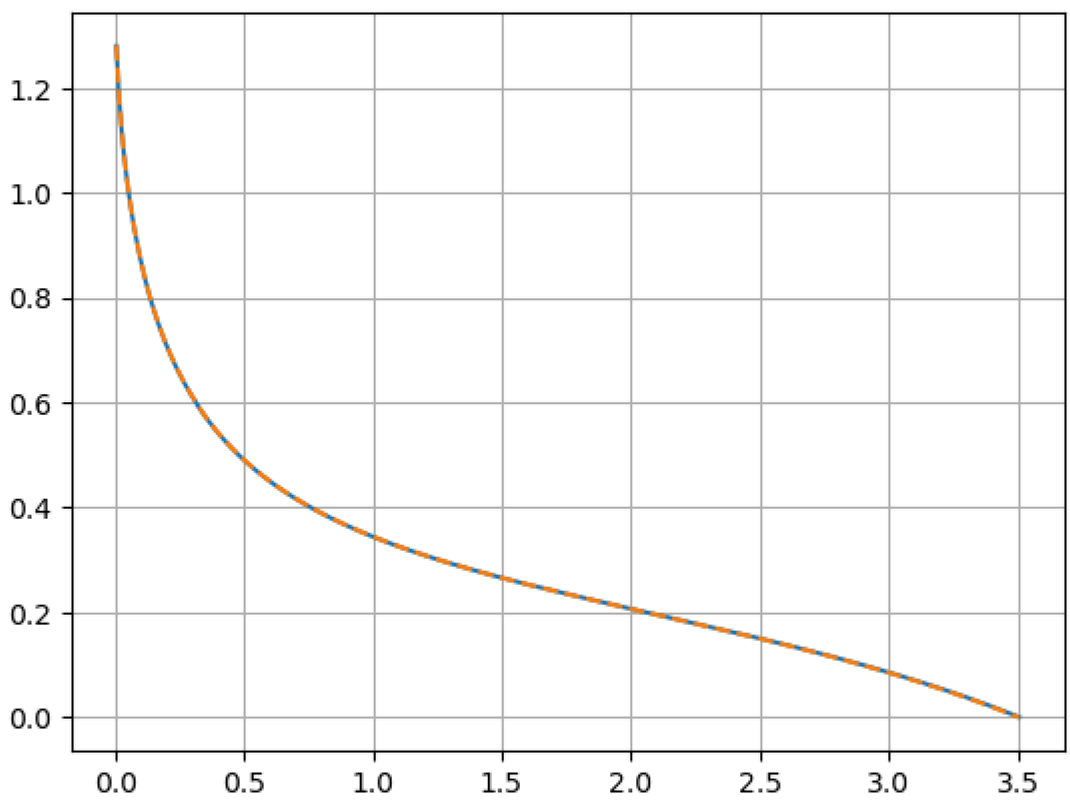
Numerically Nest integrate for Steady-State Flux and Probability distribution function

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)
```

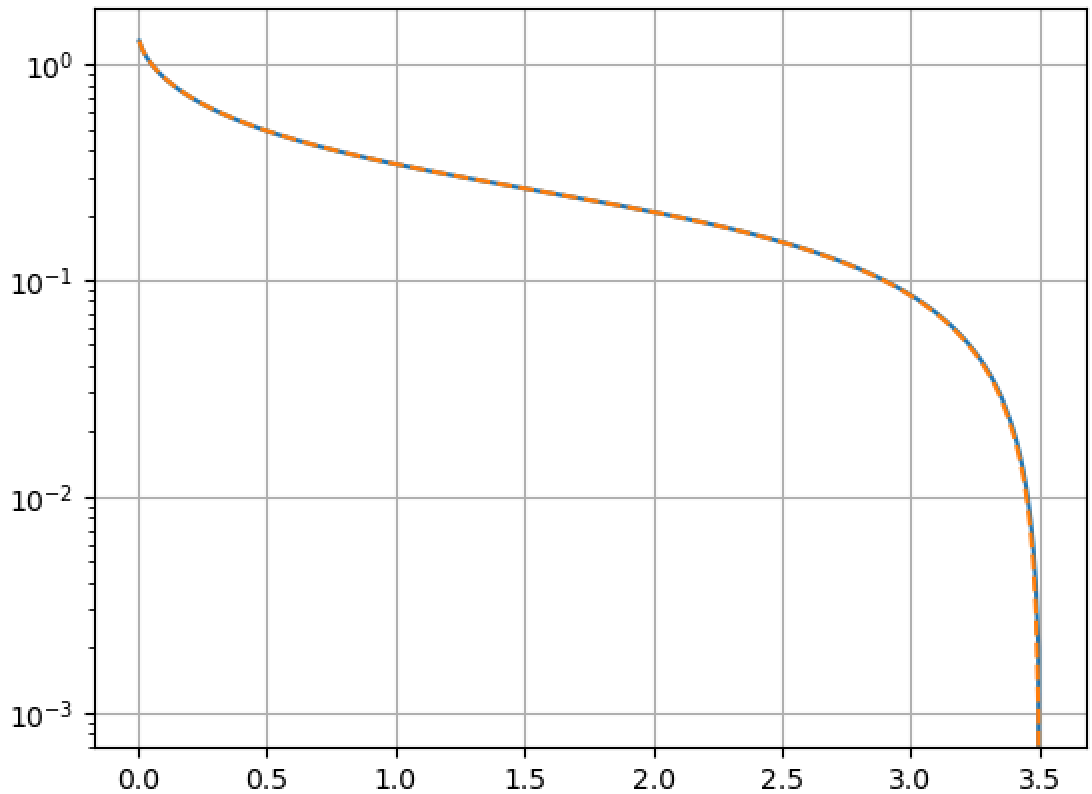
```
0.0019741547658293423
```

In [7]:
```python
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])
```

```
[1.2802321  1.18612277 1.12181534 1.07105989 1.02862339] [1.28150099 1.18729
925 1.12292753 1.07212091 1.02964137]
```



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

plt.grid()
```



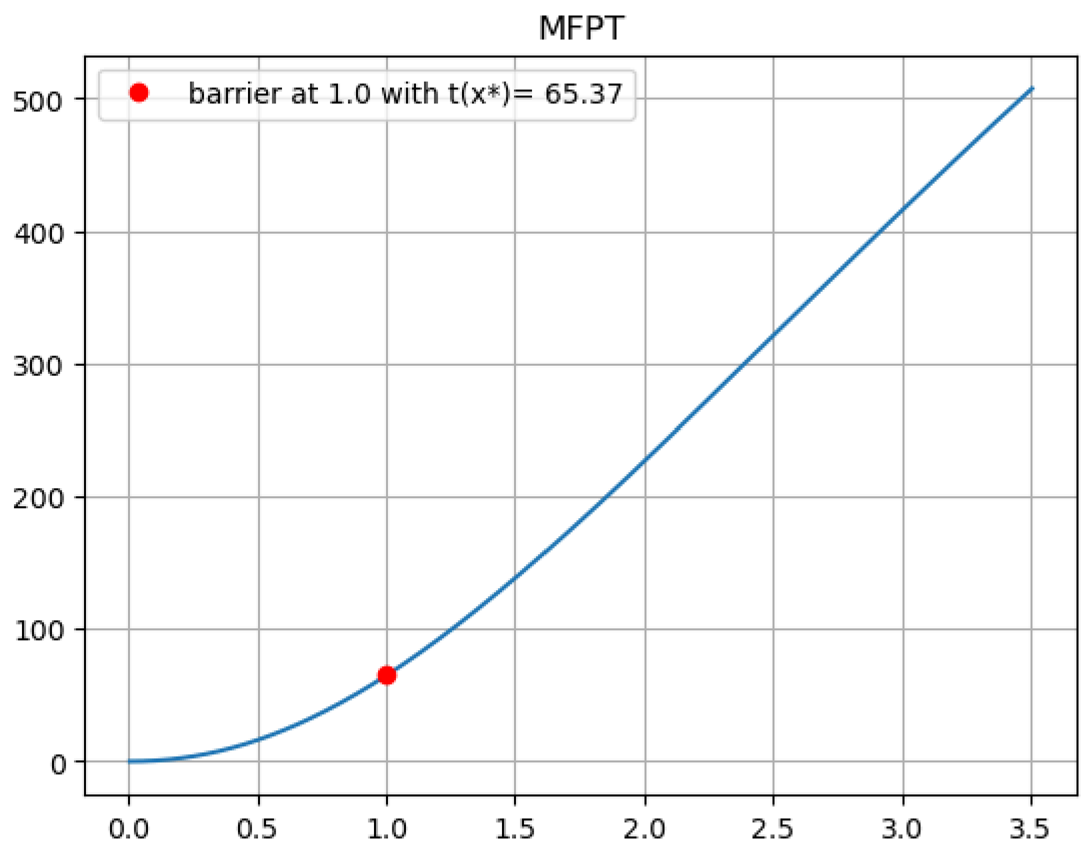
Numerically Nest integrate for MFPT

In [9]:

```
# a = 0.0  # location of reflecting boundary
x0 = a   # Regura's method, overlap the starting point and reflecting bounda
# 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()
```

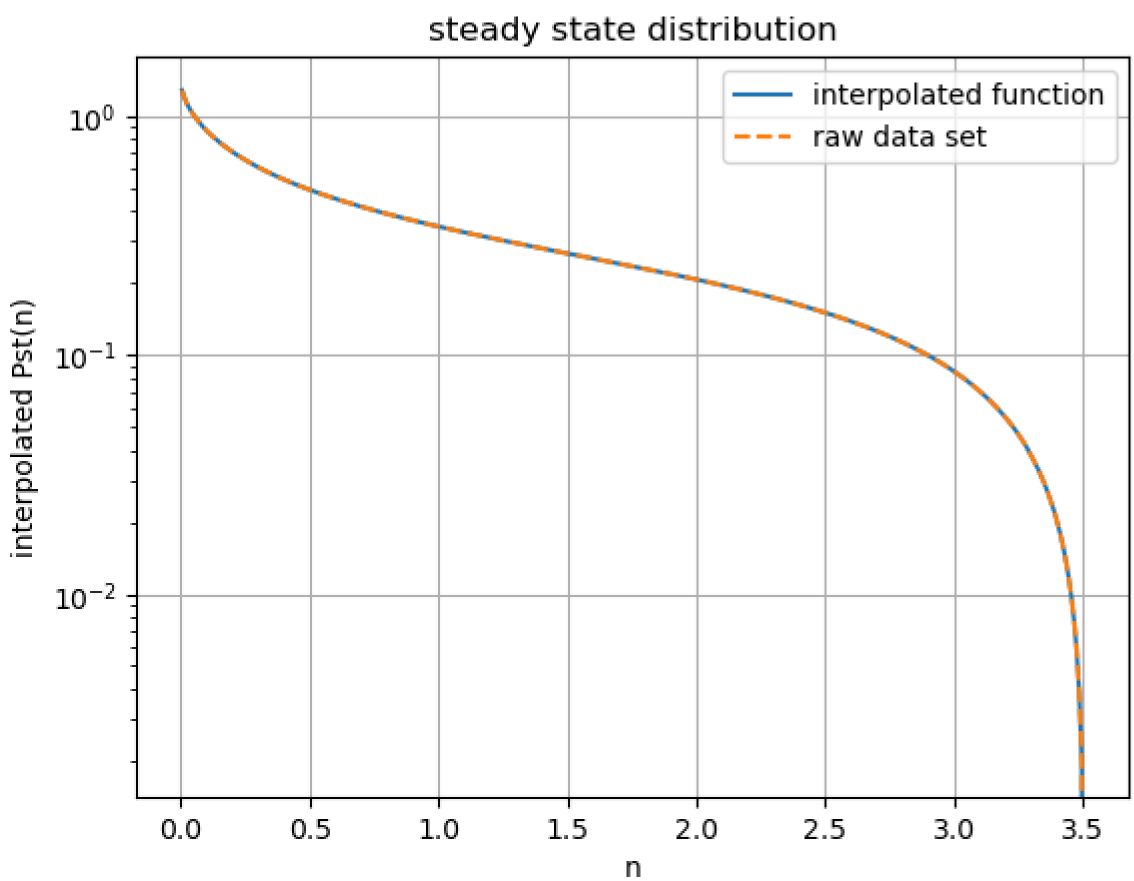
```
130.742547948485 = 2*t(x*)
507.432410682415 = t(b)
506.5458986848481 = 1/J
505.65286661016745 = 1/inject_rate
```



Reconstruct Free Energy from Numerical Solution of Pst_arr and Numerical Integration of mfpt

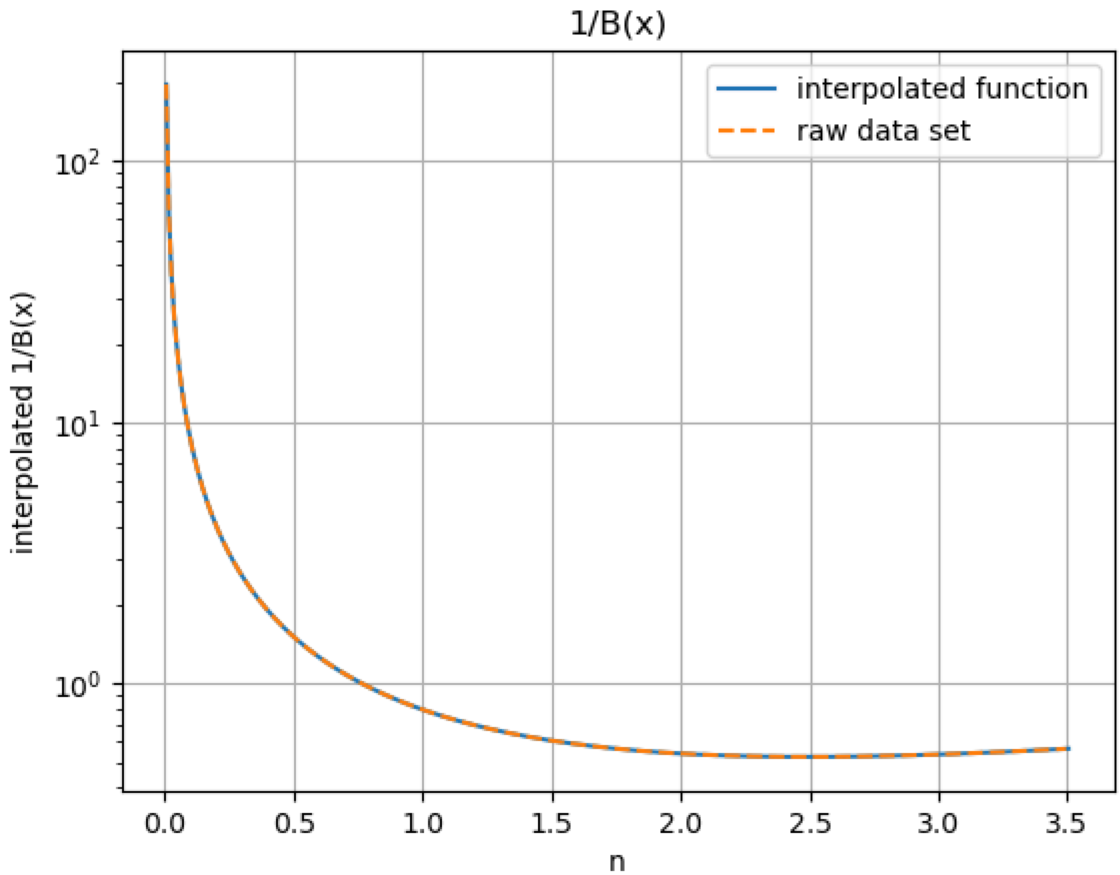
In [11]:
```
interp_Pst_func = interp1d(b_arr, Pst_arr, kind='cubic', fill_value="extrapo
# interp_Pst_func = PchipInterpolator(b_arr, Pst_arr)
```

```
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()
```



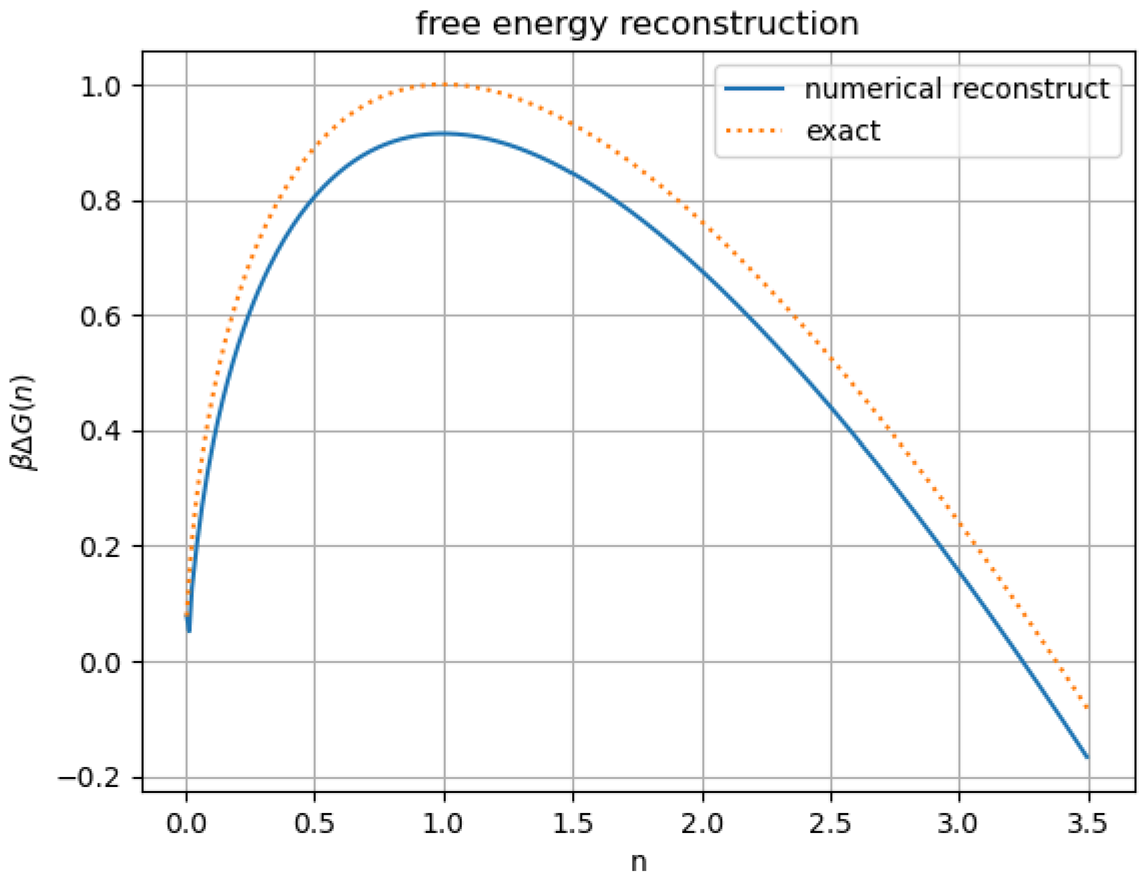
In [12]:

```
# 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 functio
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
    beta_G_arr[i] = beta_Gcnt(b_arr[0])+np.log(Bx_arr[i]/Bx_arr[0])-integral

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()
```

```
6.363314946367095e-08
```



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

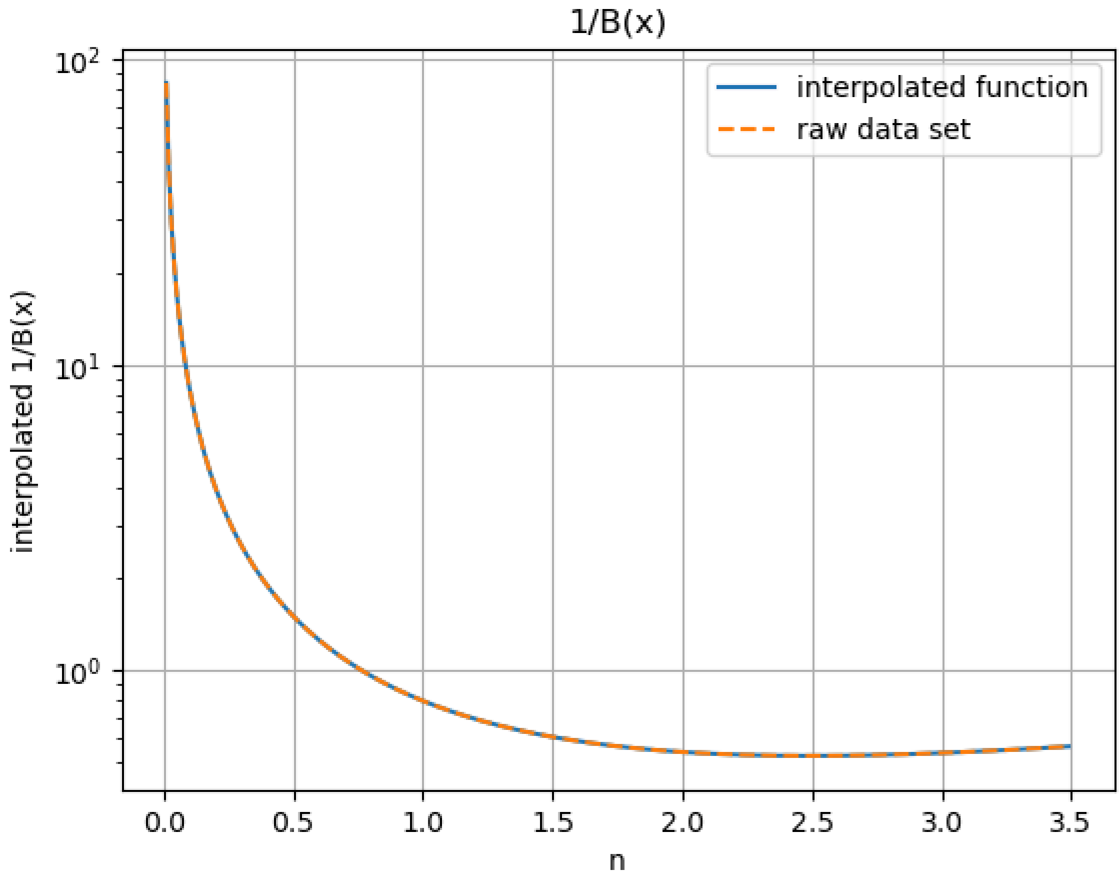
```
0.07772053214638601 0.07772053214638601
```

Out[14]:
```
array([0.07772053, 0.05149163, 0.12529789, 0.16449664, 0.20449   ,
       0.23843903, 0.269656  , 0.29817452, 0.32460986, 0.34924543,
       0.37234105, 0.394087  , 0.41463872, 0.43412204, 0.45264131,
       0.47028444, 0.48712604, 0.50323034, 0.51865302, 0.53344284])
```

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

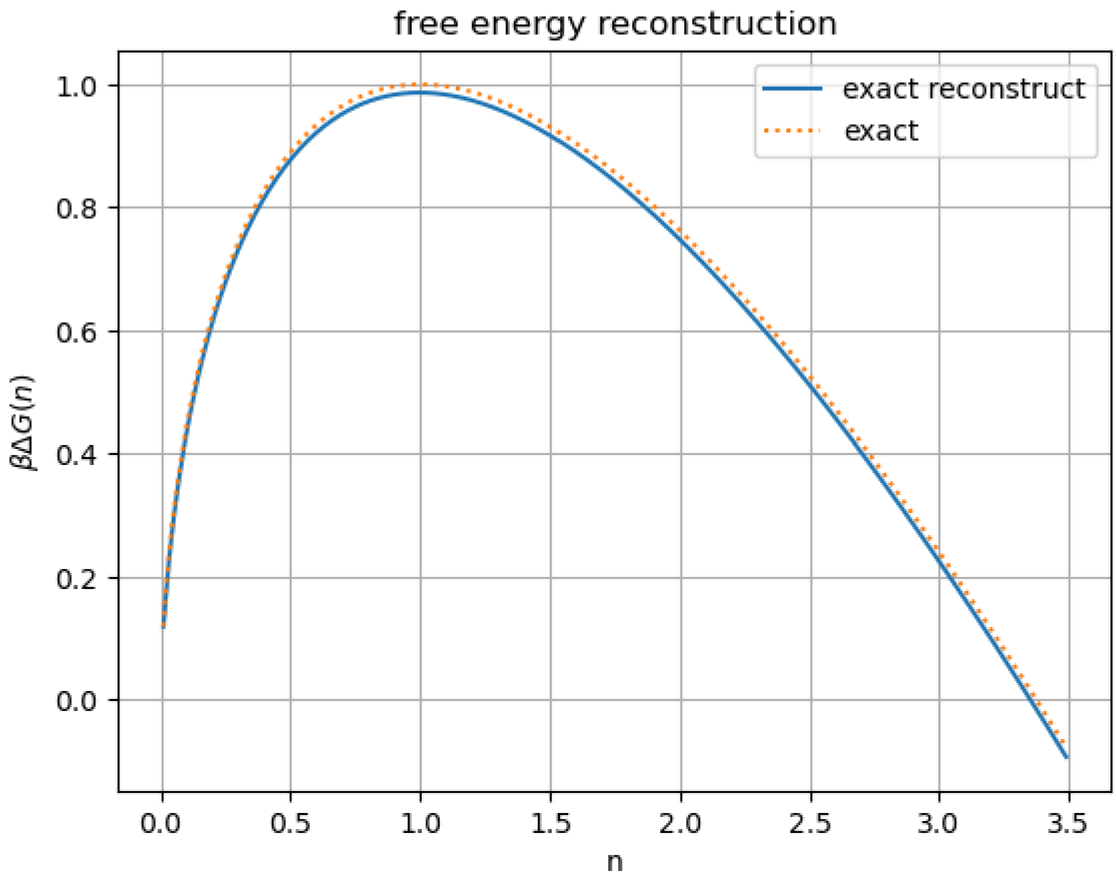
In [15]:
```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(st_P_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/st_P_func(x_arr[1+i])*(integral_Pst_arr[i]-st_flux*(mfp

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 [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()
```

```
5.7164179242266215e-08
```



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

```
0.11924766500838337 0.11924766500838337
```

Out[17]:
```
array([0.11924767, 0.1691753 , 0.22040473, 0.26070953, 0.29704432,
       0.32948162, 0.35914368, 0.38647549, 0.41187964, 0.43563178,
       0.45795054, 0.47900689, 0.49893944, 0.51786205, 0.53586979,
       0.55304312, 0.5694509 , 0.58515255, 0.6001999 , 0.61463847])
```

In [ ]:

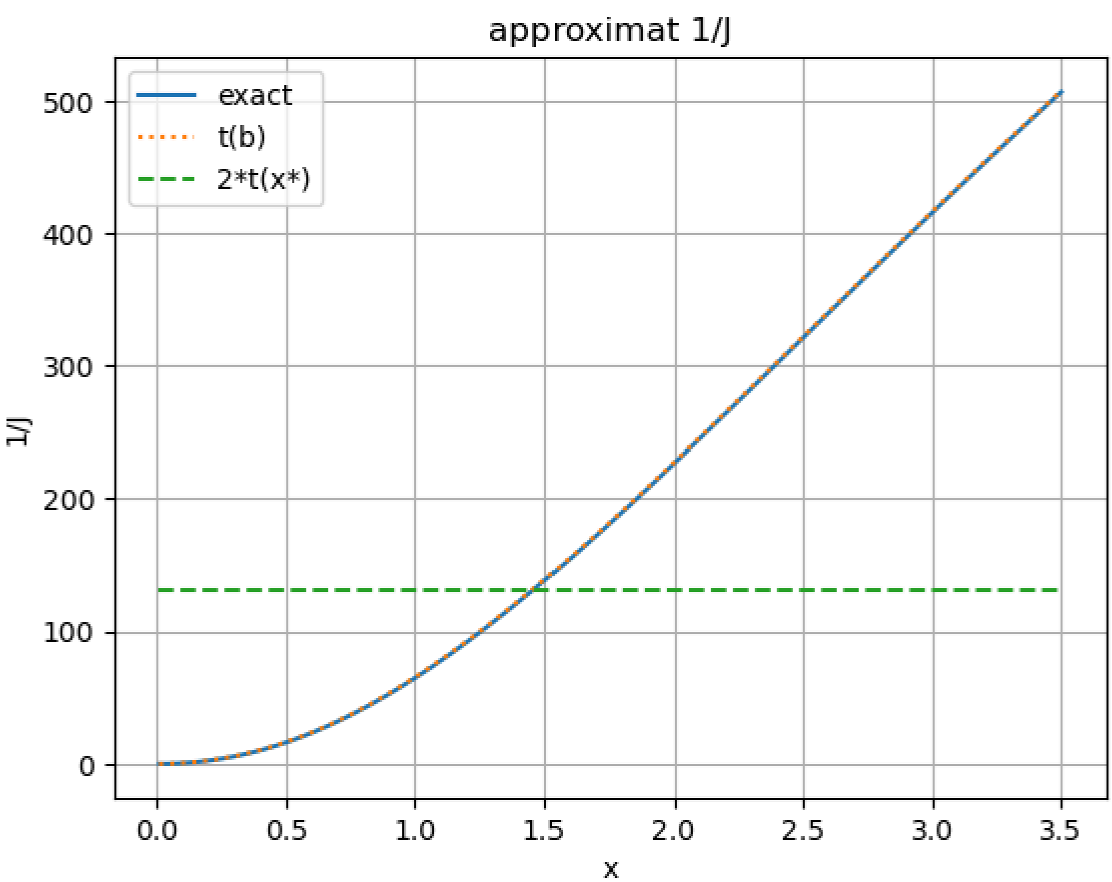
Verify Hill Relation: plot the $1/flux,\ \tau(b),\ and\ 2\tau(x*)$ v.s different location of absorbing boundary

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 refleting 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 [ ]:

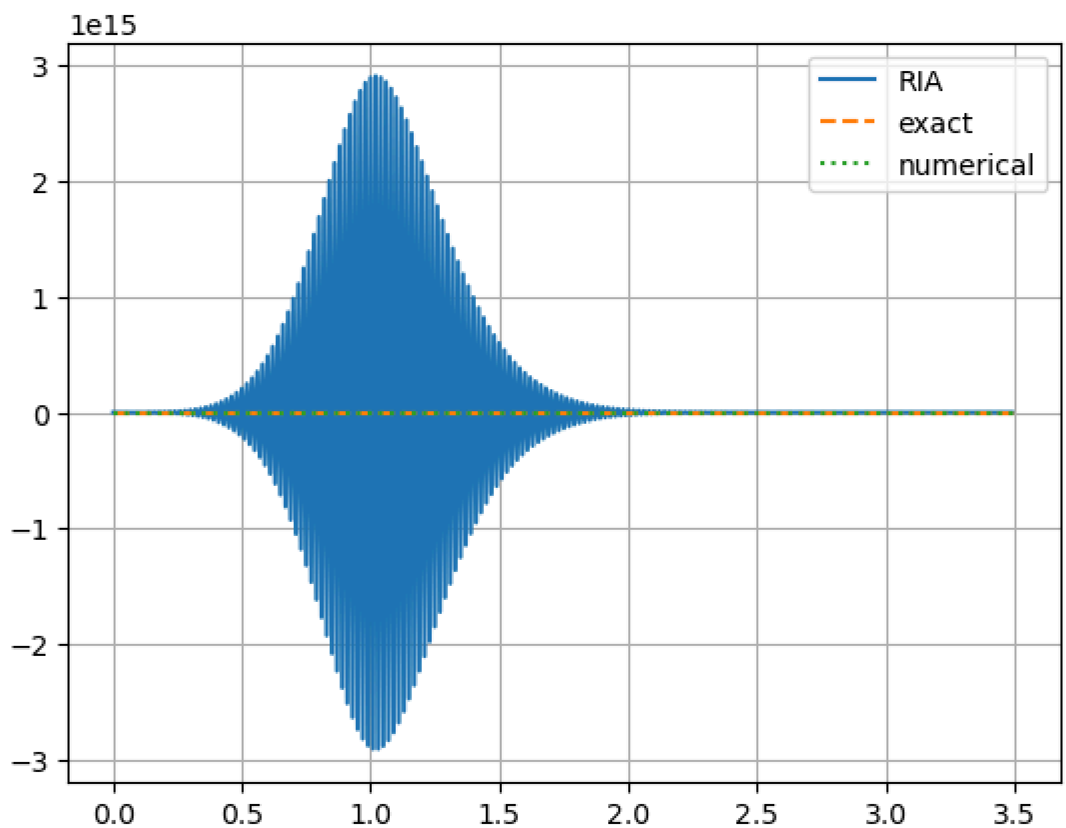
Transfer Matrix with Recycling Boundary Condition

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.eig6
plt.plot(x_arr, st_P_arr, '--', label="exact")
plt.plot(b_arr, Pst_arr, ':', label="numerical")

plt.legend()
plt.grid()

print(ria_trans.relax_timescale)
```

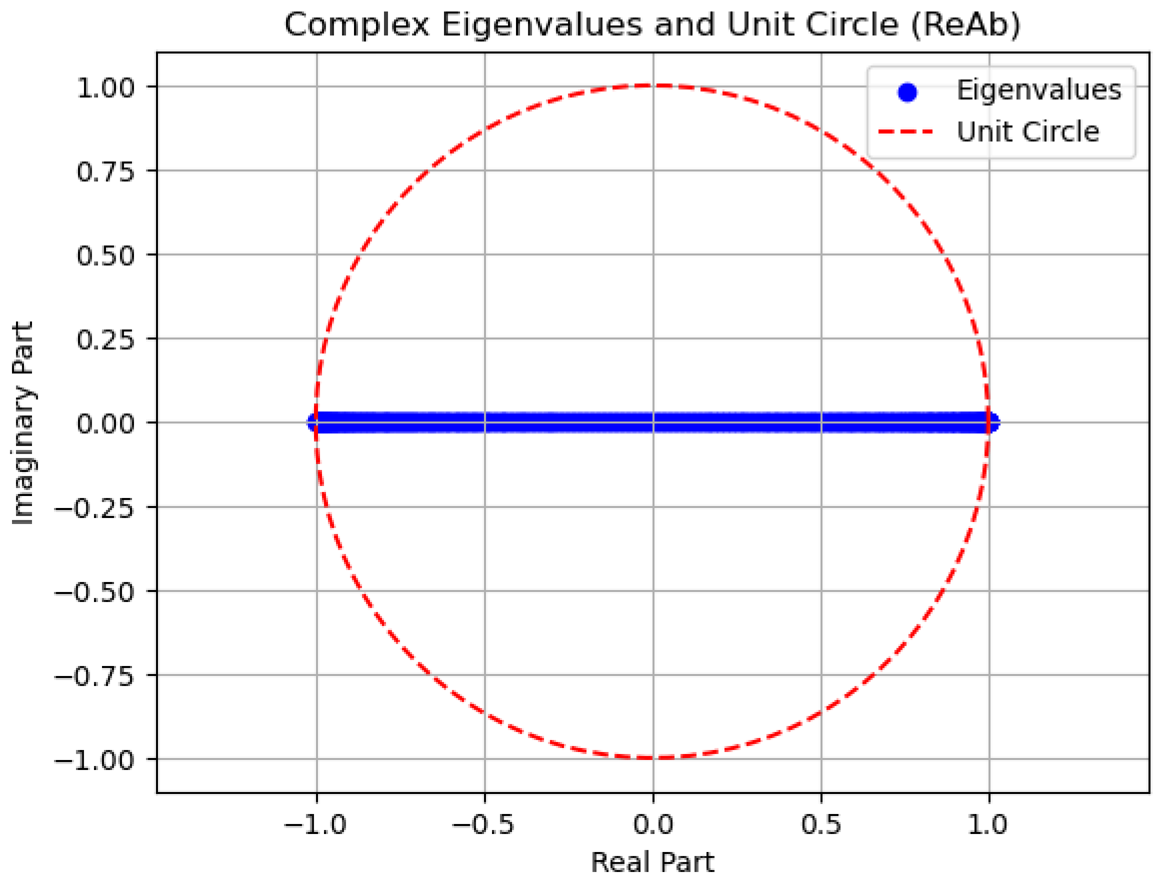
```
(-750599937895083.2+0j)
```

```
/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)
```

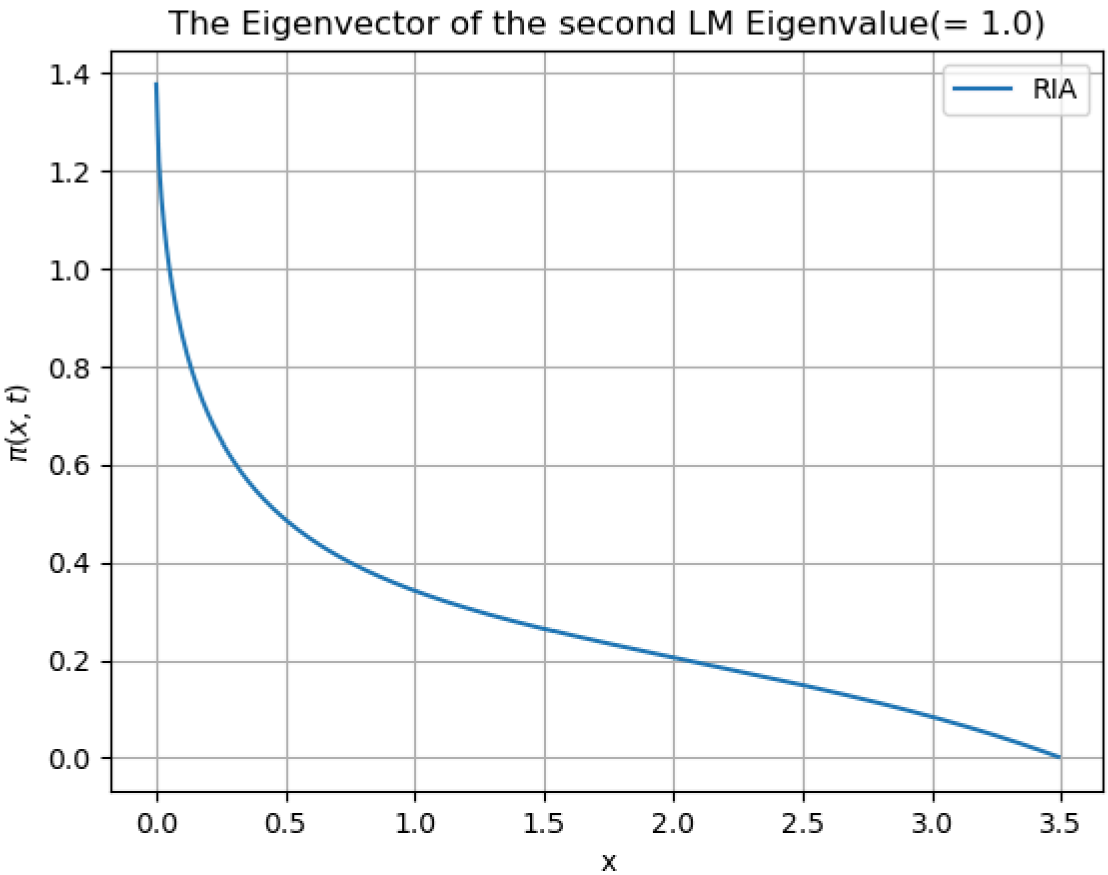
```
/home/yjiang23/Desktop/research/MFPT/MFPT_reconst_experiment/transfer_matrix
_reptile.py:547: RuntimeWarning: k >= N - 1 for N * N square matrix. Attempt
ing to use scipy.linalg.eig instead.
  eigenvalues, eigenvectors_mat = eigs(self.trans_mat, k=num_eigenvalues)
```




```
[-0.99868881+0.00000000e+00j  1.        +0.00000000e+00j
  0.99984489+3.77827968e-05j  0.99984489-3.77827968e-05j
  0.99936949+6.32850985e-05j  0.99936949-6.32850985e-05j]
```

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])
```

```
[1.37656144+0.j 1.21986363+0.j 1.14480918+0.j 1.08854073+0.j
 1.04261155+0.j 1.00350731+0.j 0.96934239+0.j 0.9389602 +0.j
 0.91158889+0.j 0.88668243+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

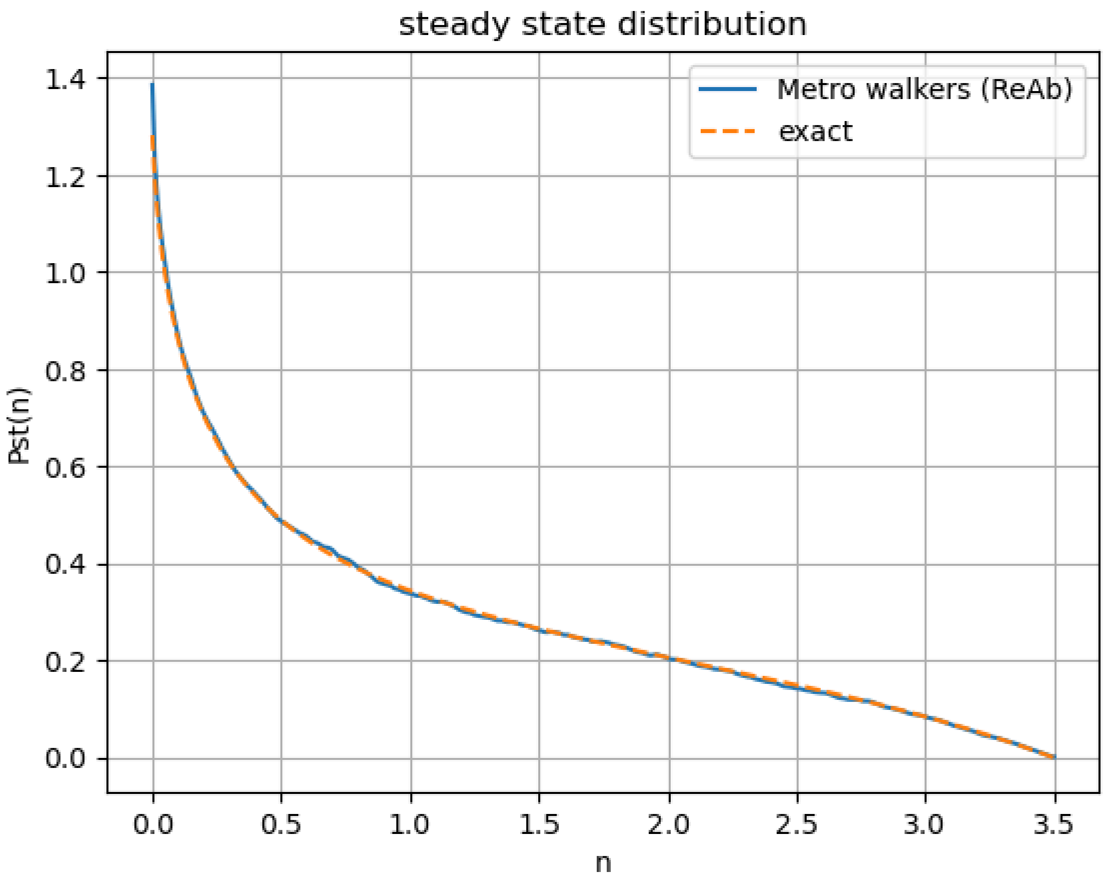
In [26]:

```
count_n, ti_n = simulate_ReAb_accelerate(init_position_arr=init_position_arr
```

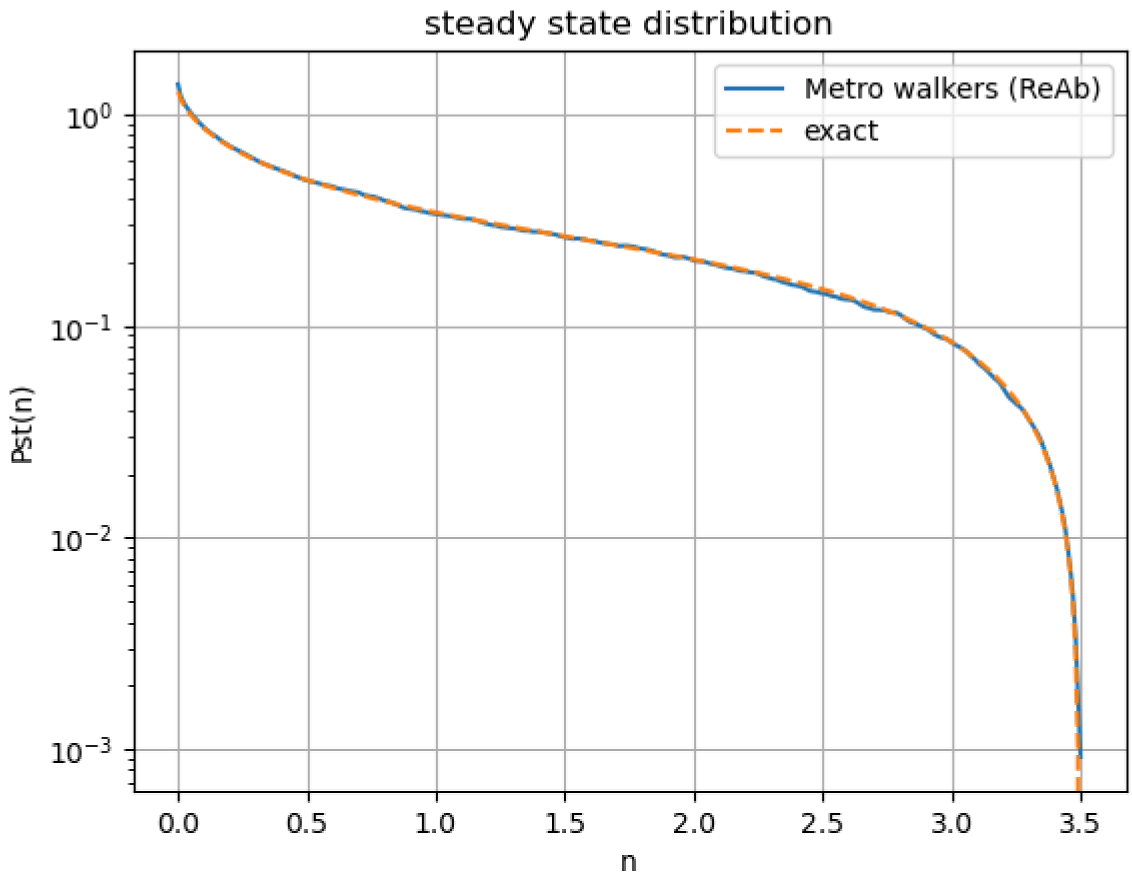
In [27]:

```
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
```

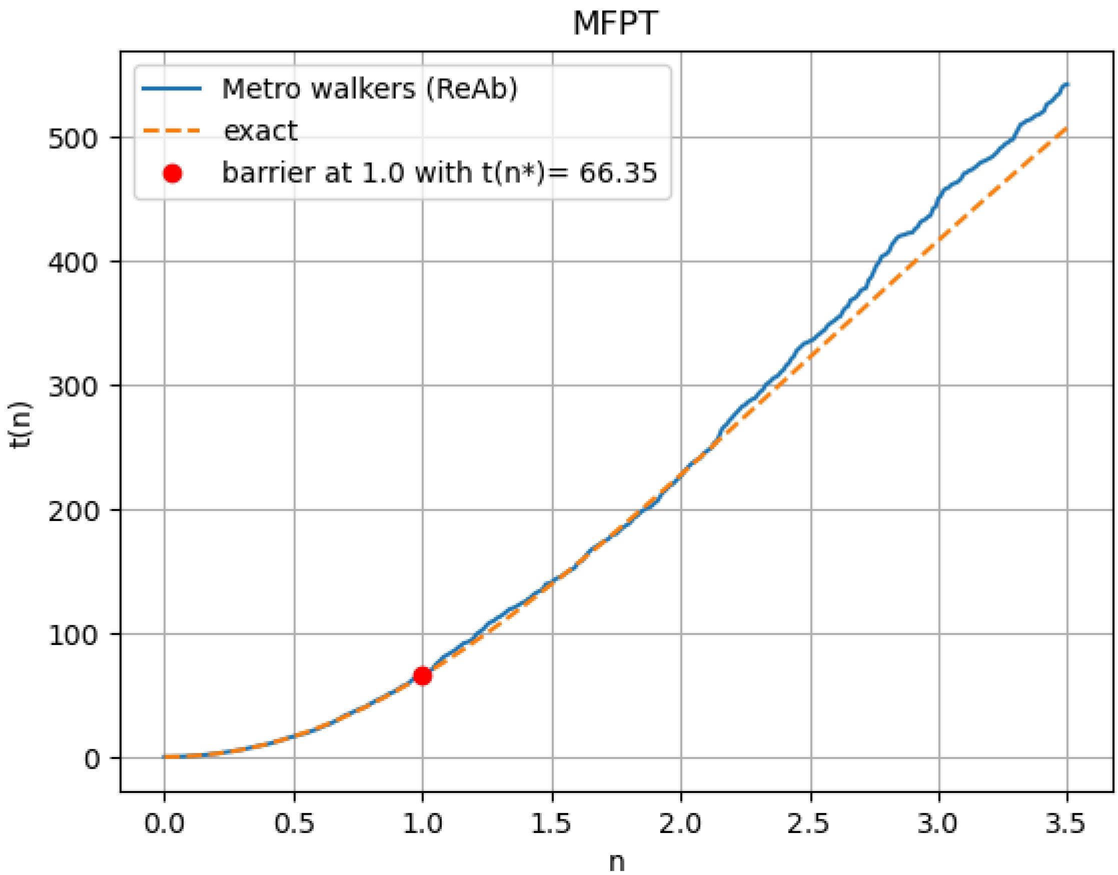
```python
# Plot formatting
plt.xlabel('n')
plt.ylabel('Pst(n)')
plt.title('steady state distribution')
plt.legend()
plt.grid()
```



In [28]:
```python
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()
```



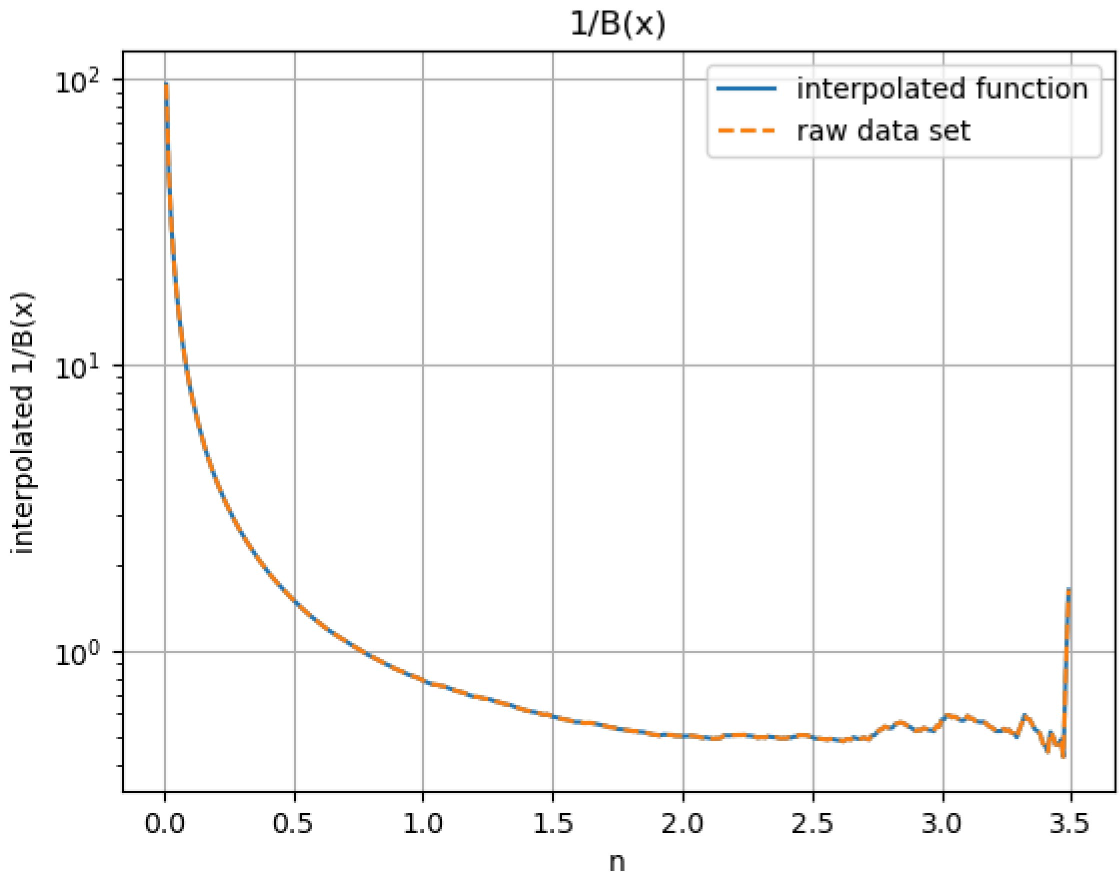
In [29]:
```
mfpt_simu_arr = np.mean(ti_n, axis=0)
idx_barrier = np.where(n_arr == 1.0)[0][0]
t_star = mfpt_simu_arr[idx_barrier]

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

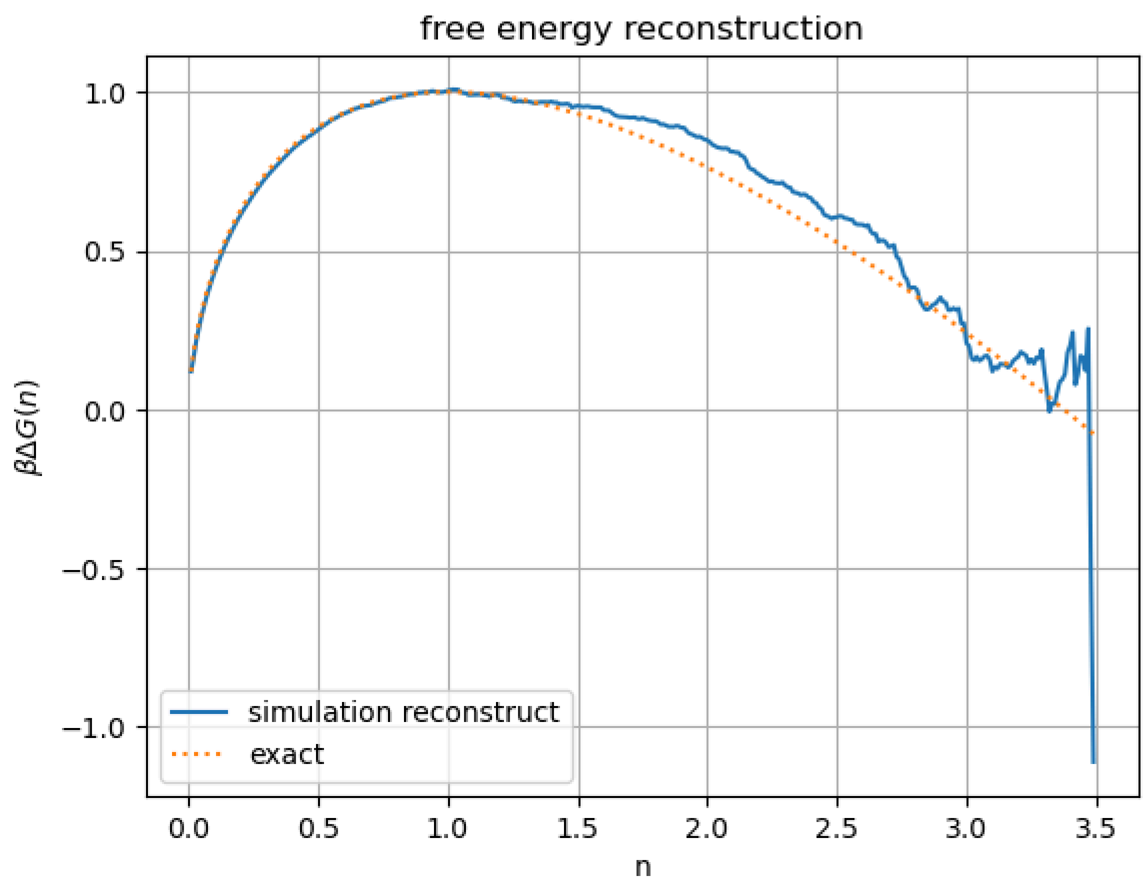
(1) Exact Steady State Distribution with simulated MFPT

In [30]:
```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
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_a

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 [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()
```

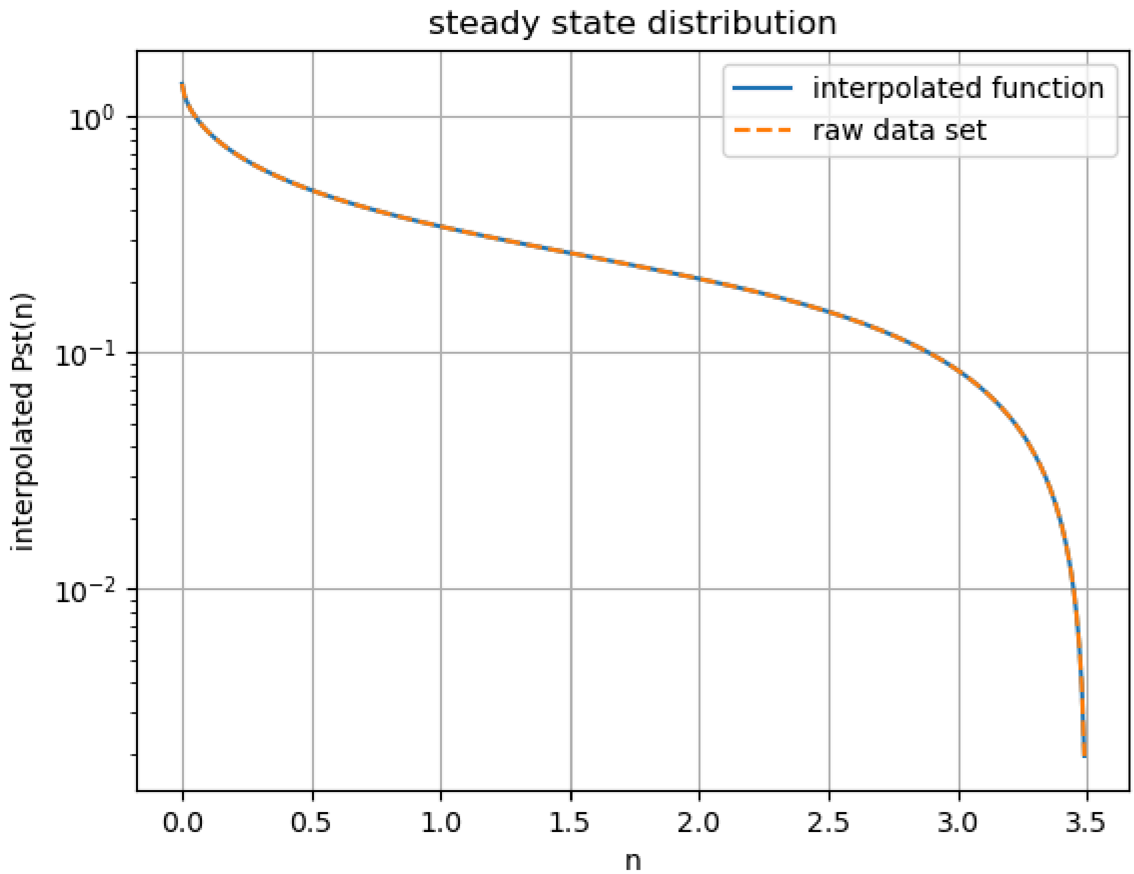
```
/tmp/ipykernel_715167/2563123347.py:6: IntegrationWarning: The maximum numbe
r of subdivisions (50) has been achieved.
  If increasing the limit yields no improvement it is advised to analyze
  the integrand in order to determine the difficulties.  If the position of
a
  local difficulty can be determined (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])
0.0028546762269776593
```



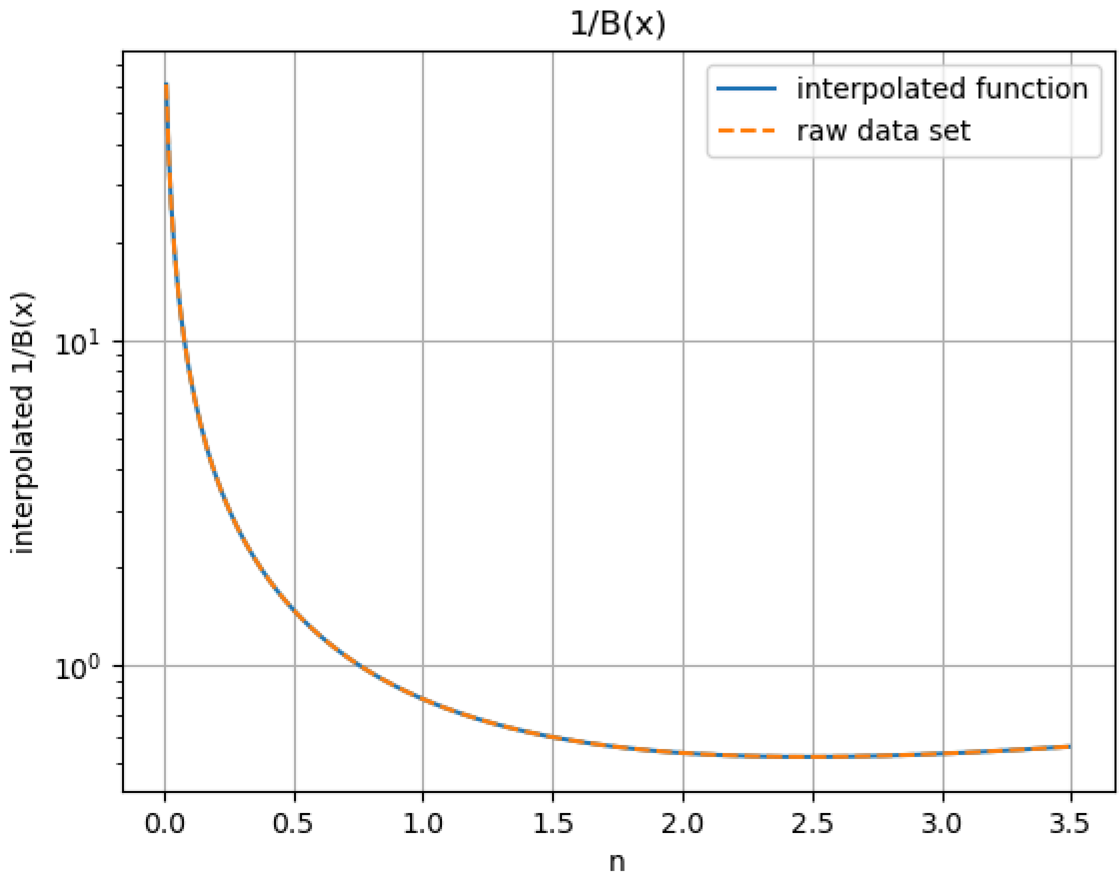
(2) Transfer Matrix Steady State Distribution with exact MFPT and then with simulated MFPT

In [32]:
```
interp_Pst_func = interp1d(x_arr[:-1], np.array(1.0/(h*np.sum(ria_trans.eig6
# interp_Pst_func = interp1d(x_arr[:-1], np.array(ria_trans.steady_state, dt

plt.semilogy(x_arr[:-1], interp_Pst_func(x_arr[:-1]), label="interpolated fu
# 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]))*ria

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

```
/tmp/ipykernel_715167/510819784.py:1: ComplexWarning: Casting complex values
to real discards the imaginary part
  interp_Pst_func = interp1d(x_arr[:-1], np.array(1.0/(h*np.sum(ria_trans.ei
g6_v[:, 1]))*ria_trans.eig6_v[:, 1], dtype=float), kind='cubic', fill_value
="extrapolate")
/tmp/ipykernel_715167/510819784.py:6: ComplexWarning: Casting complex values
to real discards the imaginary part
  plt.semilogy(x_arr[:-1], np.array(1.0/(h*np.sum(ria_trans.eig6_v[:, 1]))*r
ia_trans.eig6_v[:, 1], dtype=float), '--', label="raw data set")
```

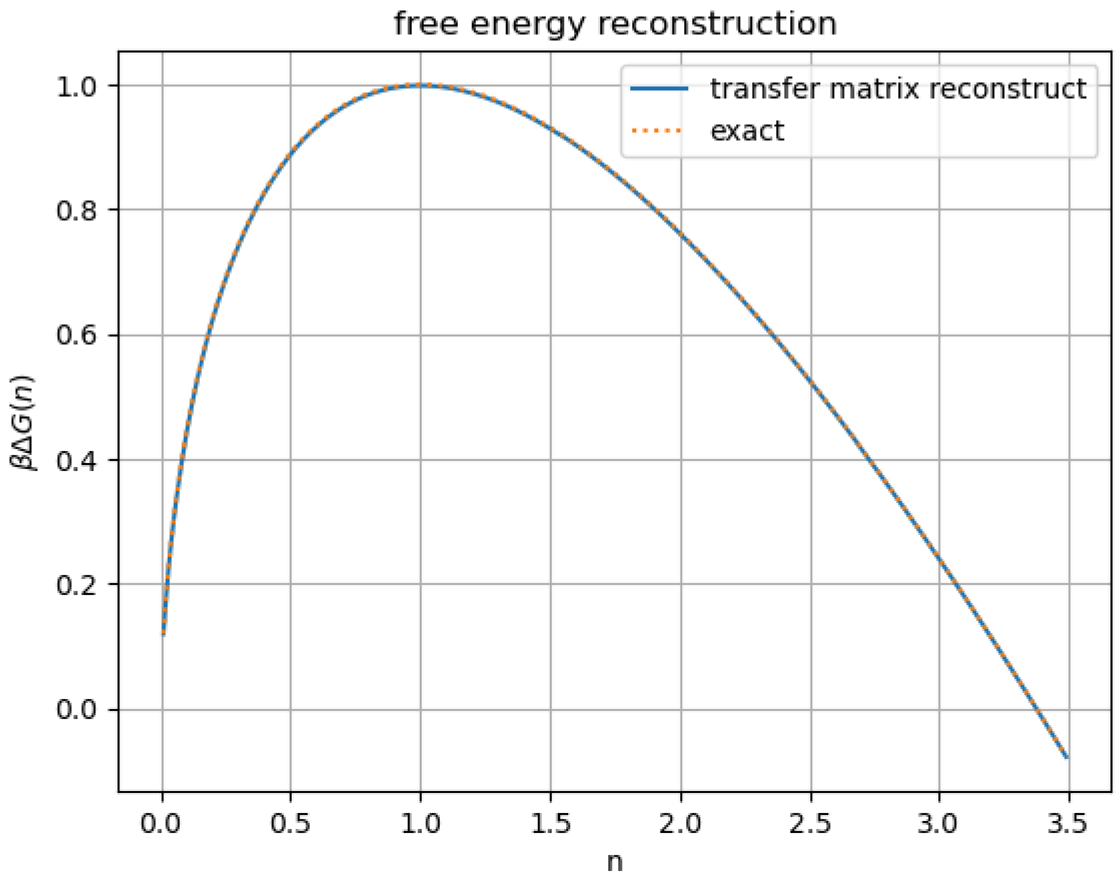


In [33]:
```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(interp_Pst_func, x_arr[1+i], x_arr[-1])
    Bx_arr[i] = -1.0/interp_Pst_func(x_arr[1+i])*(integral_Pst_arr[i]-(mfpt_

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



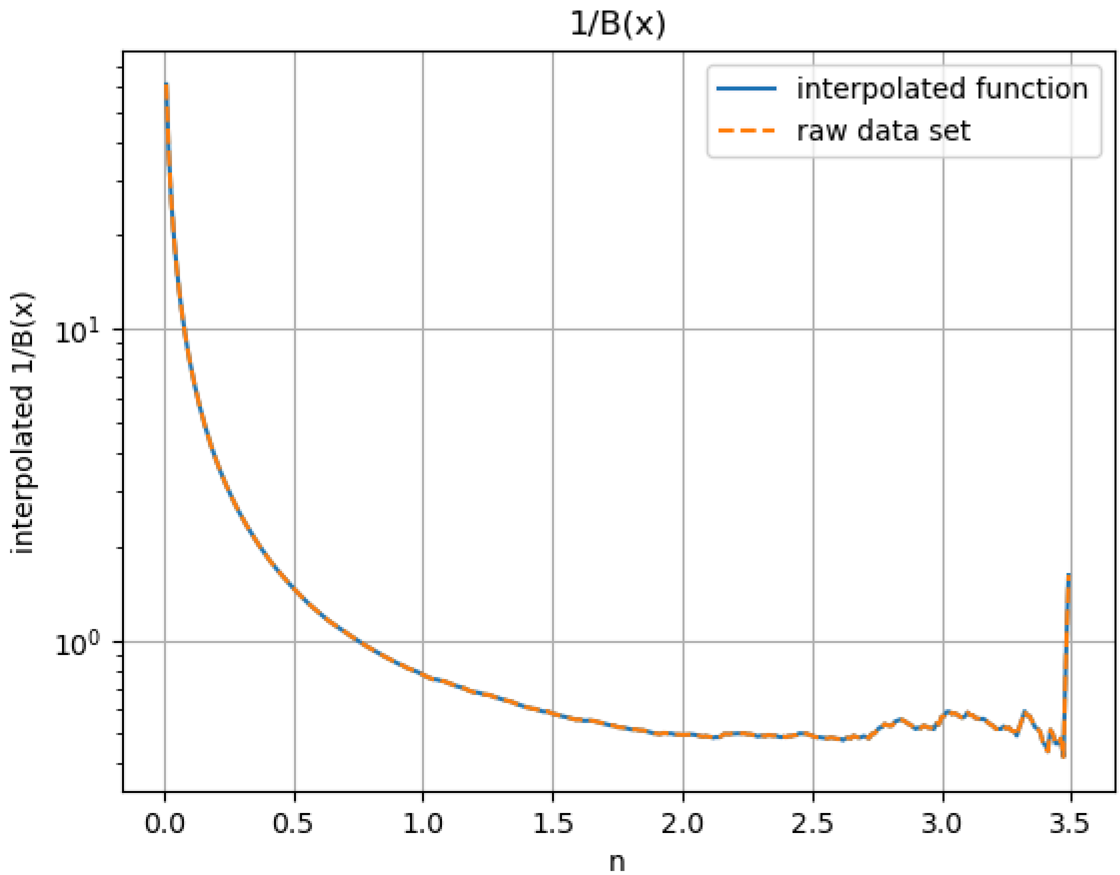
In [34]:
```
integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

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 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()
```

```
4.519590988151761e-08
```



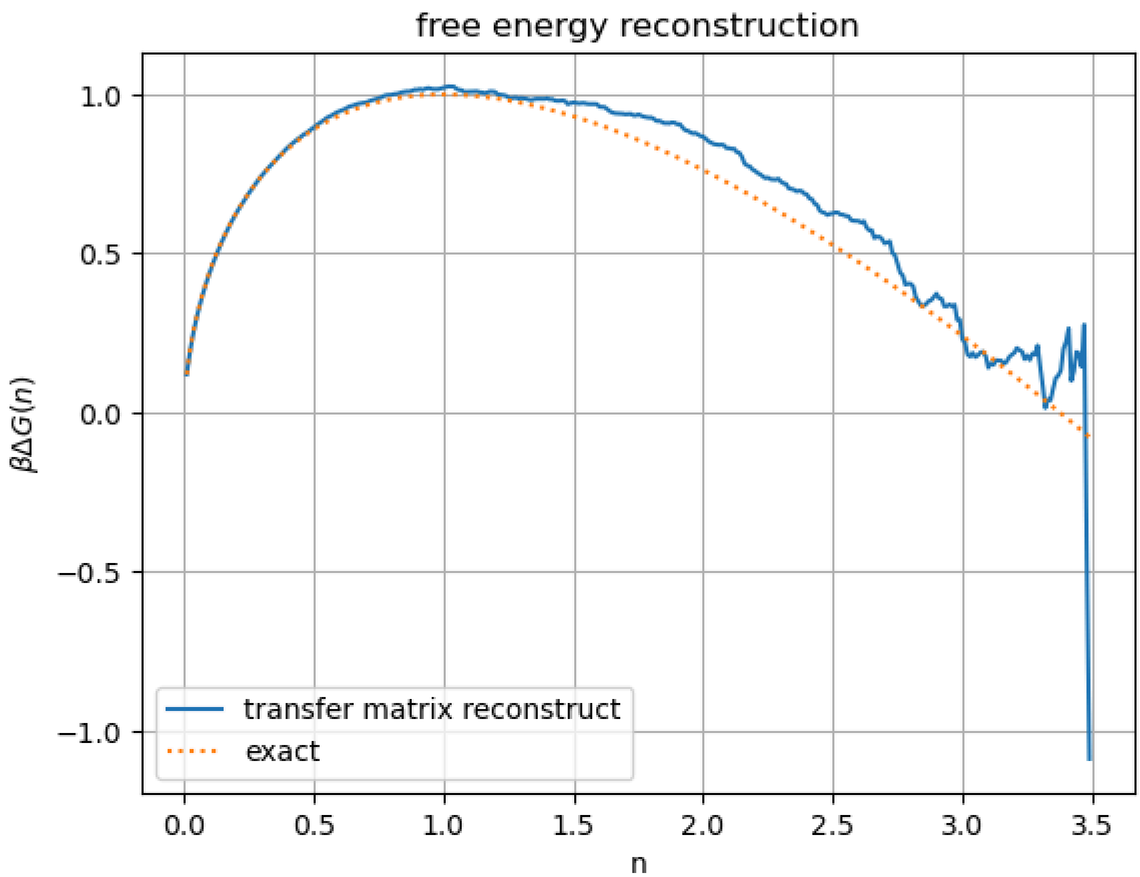
In [35]:

```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
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') # 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()
```



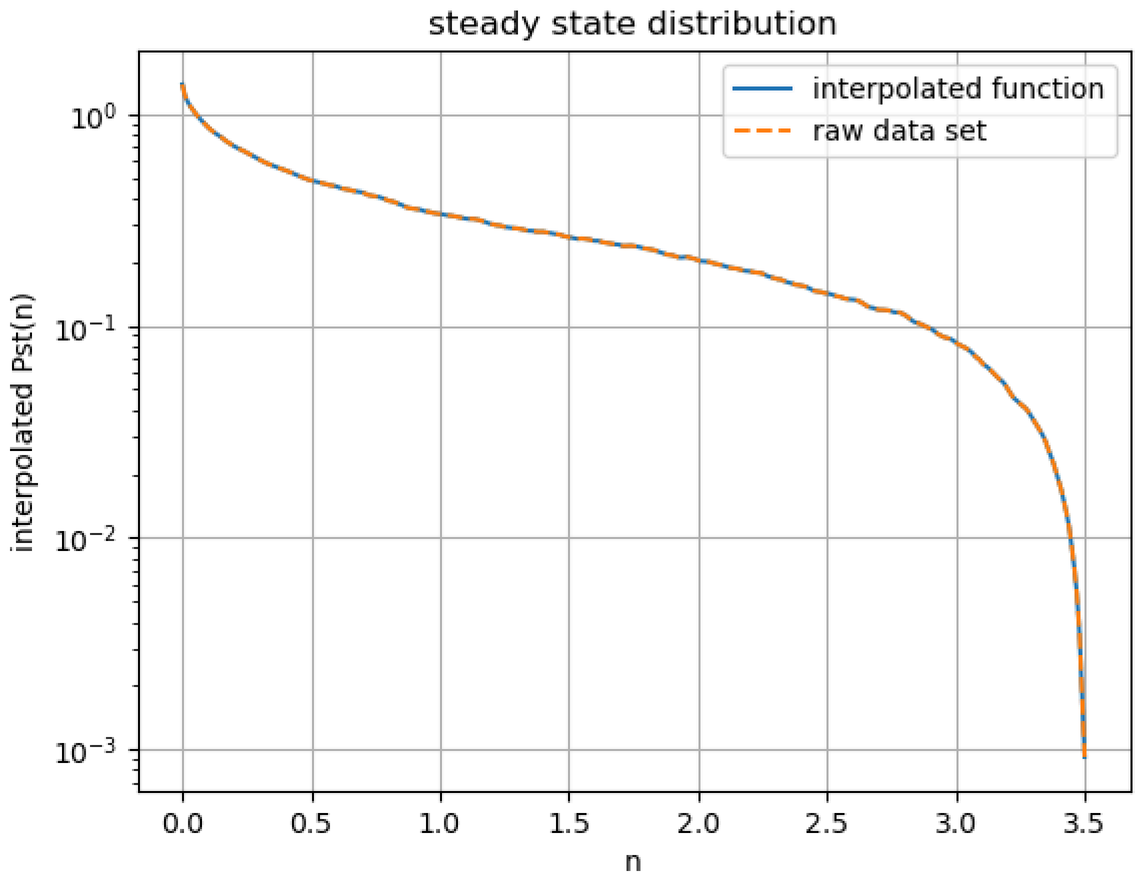
In [36]:
```
integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

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 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_715167/3486299942.py:6: IntegrationWarning: The maximum numbe
r 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])
0.0006448207799047978
```



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

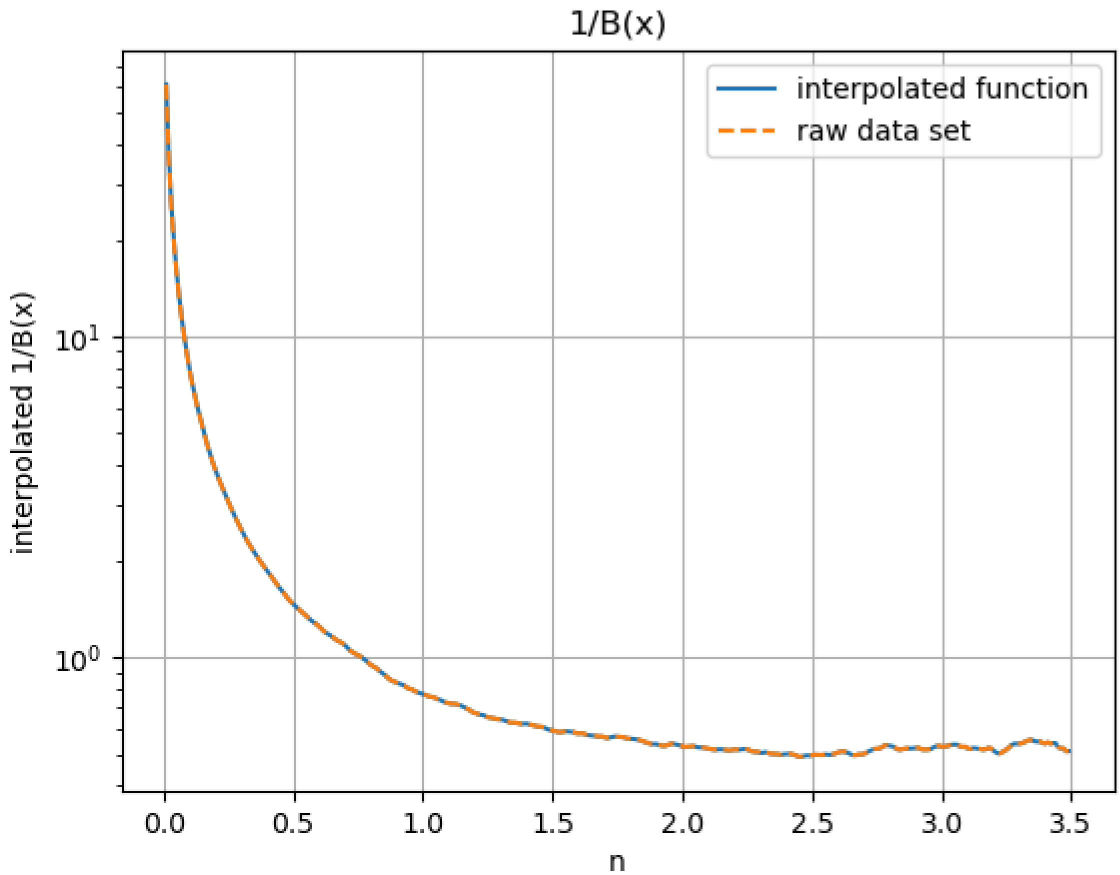
In [37]:
```
interp_simu_Pst_func = interp1d(simu_x_arr, Pst_n, kind='cubic', fill_value=
# interp_Pst_func = PchipInterpolator(b_arr, Pst_arr)

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]:

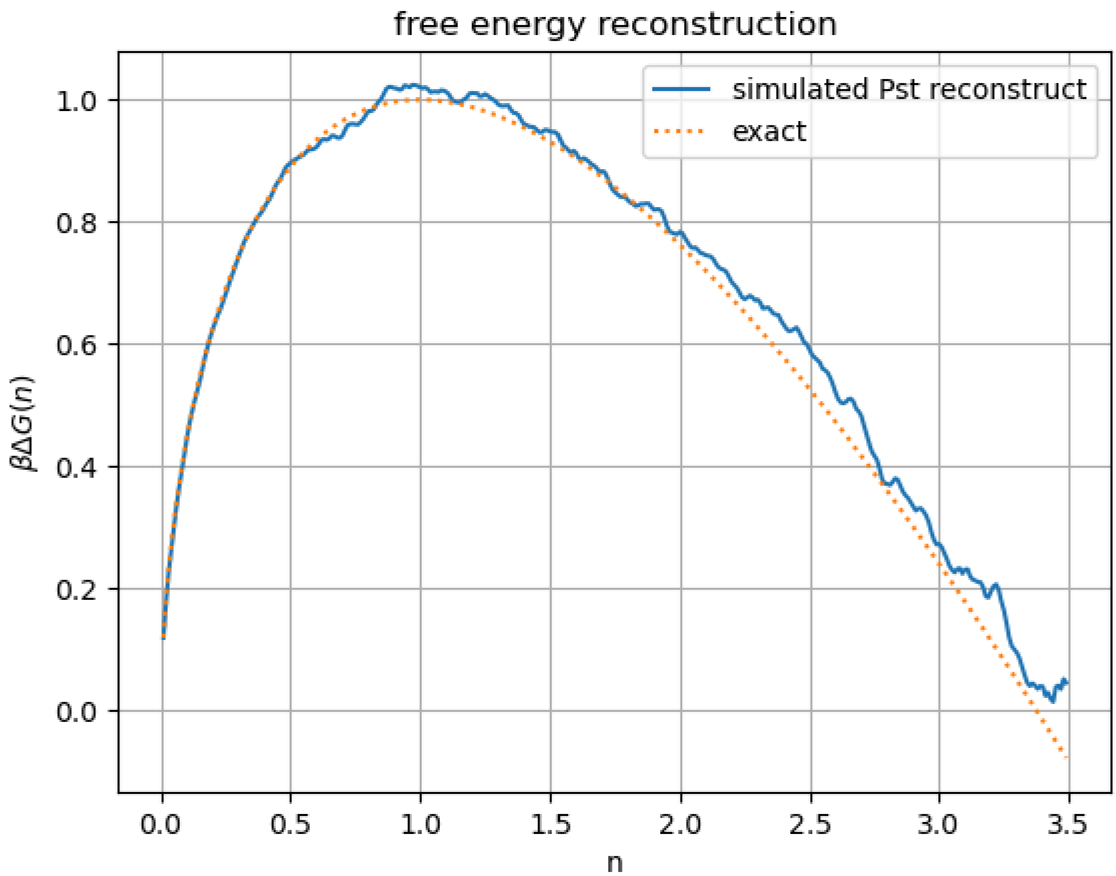
```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
simu_Bx_arr = np.zeros(N-2)
integral_Pst_arr = np.zeros(N-2)
for i in range(N-2):
    integral_Pst_arr[i], _ = quad(interp_simu_Pst_func, simu_x_arr[1+i], sim
    simu_Bx_arr[i] = -1.0/Pst_n[1+i]*(integral_Pst_arr[i]-(mfpt_arr[-1]-mfpt

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

plt.semilogy(simu_x_arr[1:-1], interp_simu_invertBx_func(x_arr[1:-1]), label
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_715167/3951444635.py:5: IntegrationWarning: The maximum numbe
r 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])
```



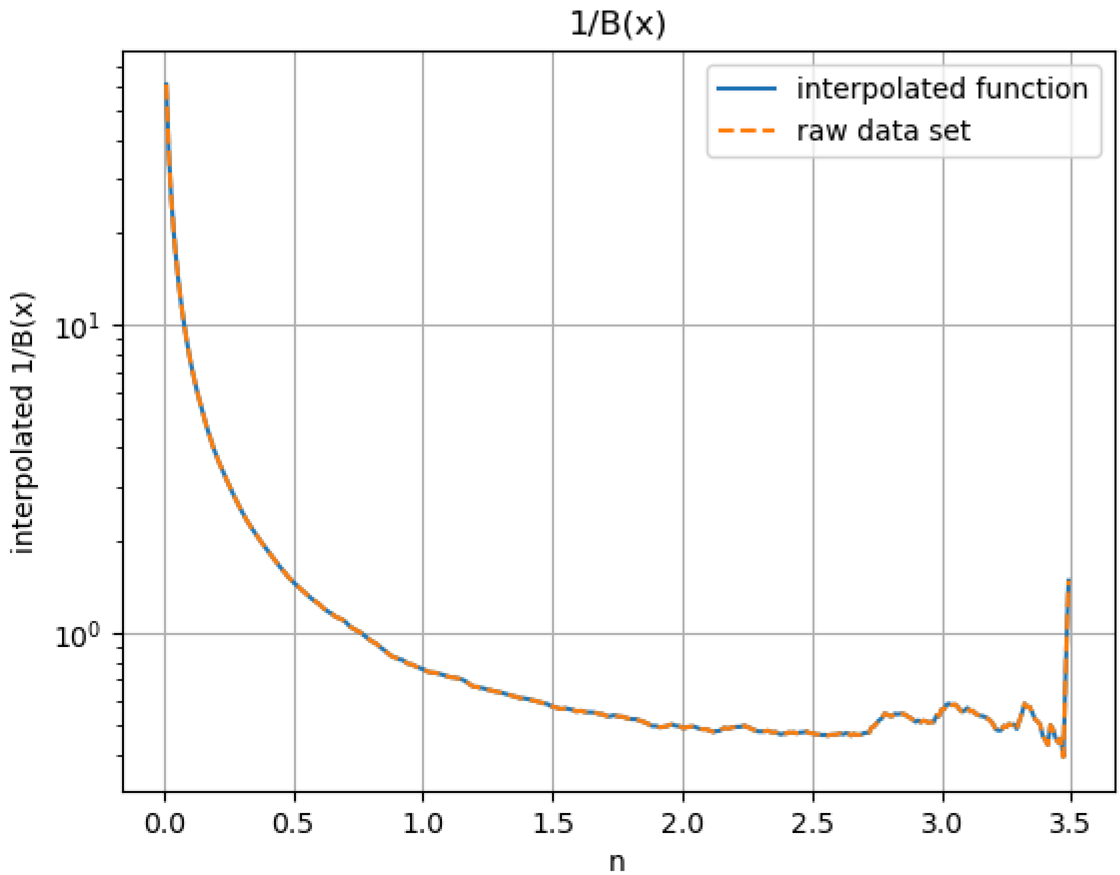
In [39]:
```
integral_invertBx_arr = np.zeros(N-2)
beta_Grec2_arr = np.zeros(N-2)

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_715167/4156853672.py:6: IntegrationWarning: The maximum numbe
r 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])
0.0017887756247244187
```



In [40]:
```
# Except for the absorbing boundary Pst(b) = 0, D(x)=0, also avoid at reflec
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], sim
    simu_Bx_arr[i] = -1.0/Pst_n[1+i]*(integral_Pst_arr[i]-(mfpt_simu_arr[-1]

interp_simu_invertBx_func = interp1d(simu_x_arr[1:-1], 1.0/simu_Bx_arr, kinc

plt.semilogy(simu_x_arr[1:-1], interp_simu_invertBx_func(x_arr[1:-1]), label
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_715167/1053423012.py:5: IntegrationWarning: The maximum numbe
r 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])
```

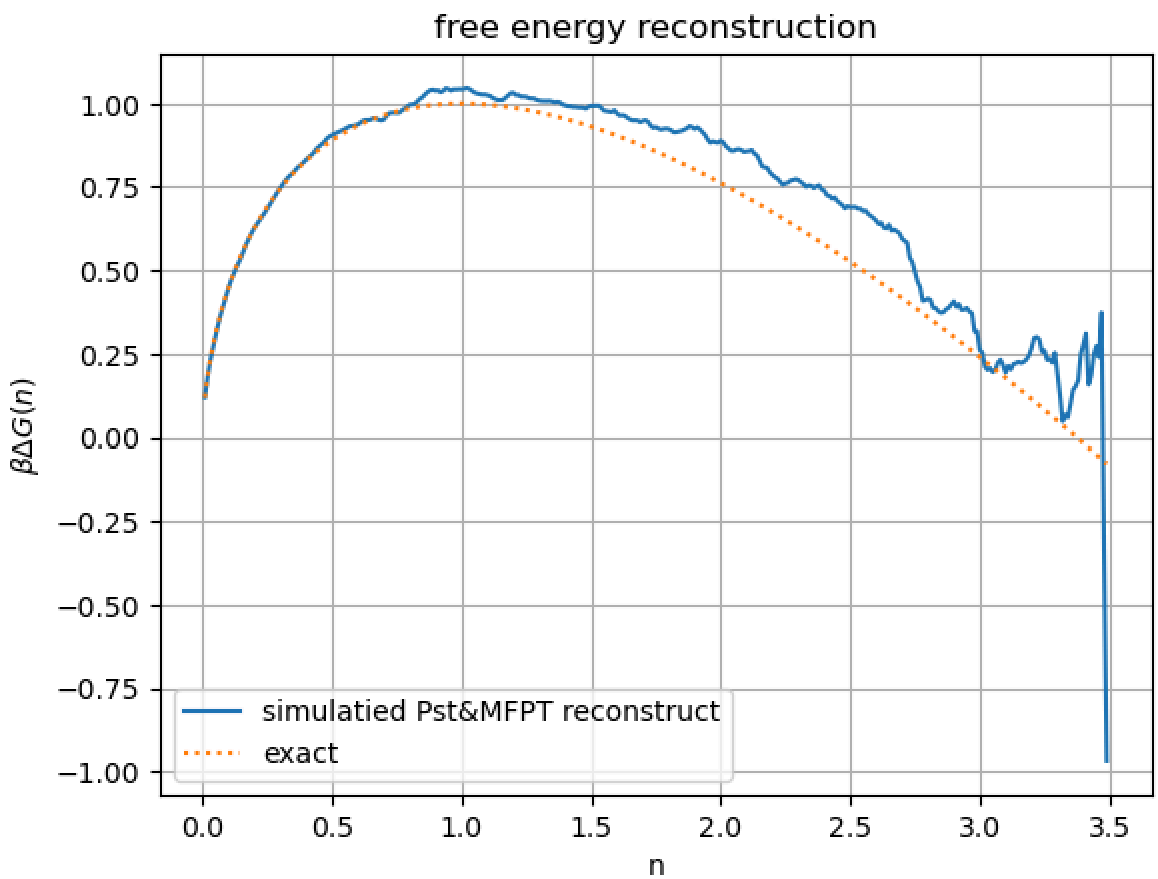


In [41]:

```
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
    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="simulatied Pst&MFPT recons
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_715167/2326235107.py:6: IntegrationWarning: The maximum numbe
r 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])
0.0018742845017403198
```



In [ ]:

In [ ]: