Binary Alloy Hubbard Model

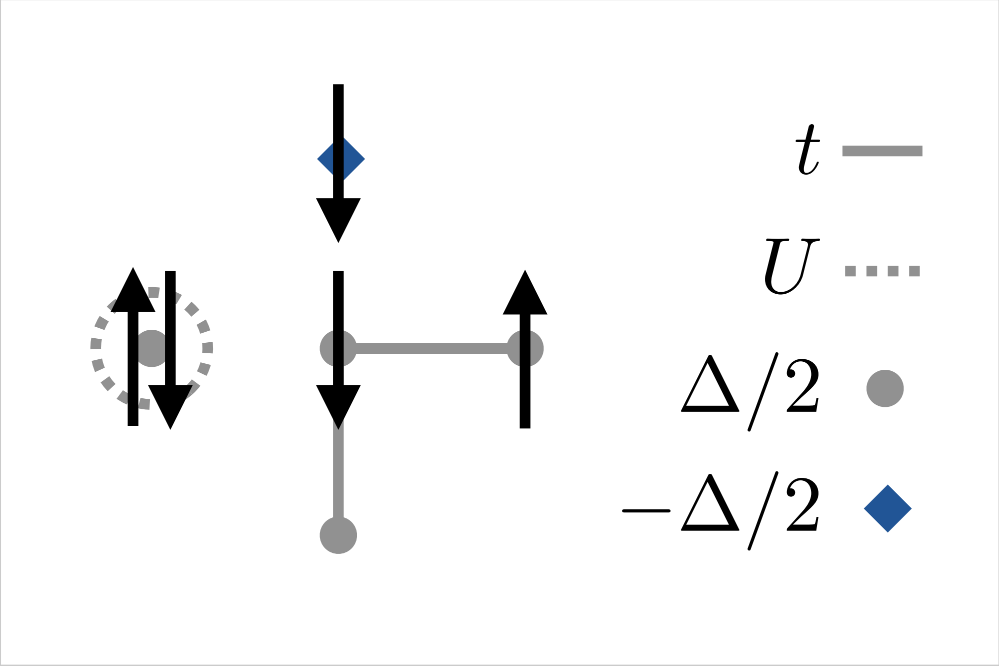
Results with Determinant Quantum Monte Carlo and Lanczos

Norman Paris, Andrew Baldwin, Richard Scalettar
University of California in Davis

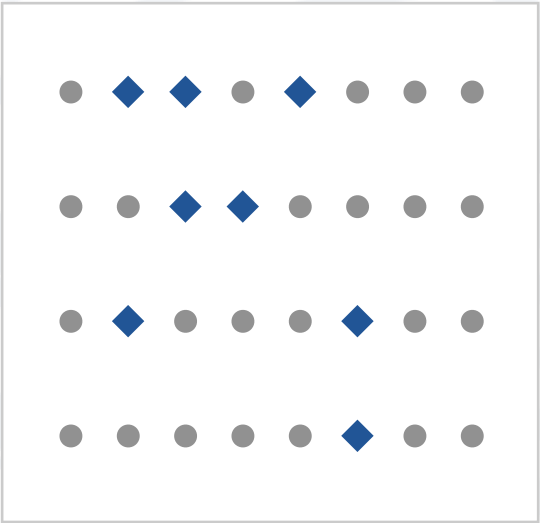
Binary Alloy Hubbard Model

$$H = -t \sum_{<l,j>\sigma} (c^\dagger_{j\sigma} c_{l\sigma} + c^\dagger_{l\sigma} c_{j\sigma}) + U \sum_l (n_{l\uparrow} - \frac{1}{2})(n_{l\downarrow} - \frac{1}{2}) + \sum_l (\epsilon_l - \mu)(n_{l\uparrow} + n_{l\downarrow})$$

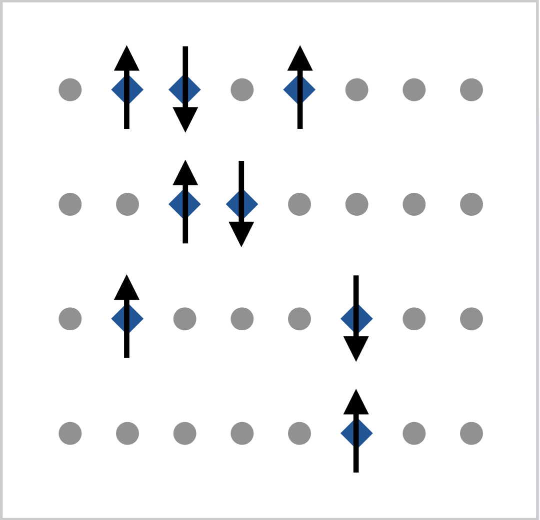
$$P(\epsilon_i) = x\delta(\epsilon_i + \Delta/2) + (1-x)\delta(\epsilon_i - \Delta/2) \qquad \Delta > U$$



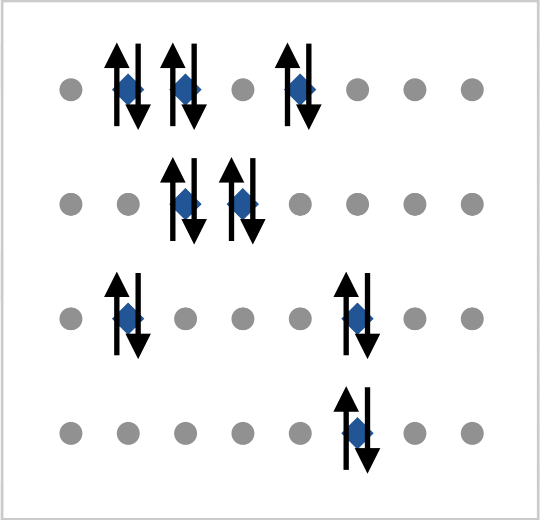
Inspired By:
Byczuk and Ulmke. arXiv:cond-mat/0411168
Byczuk, Hofstetter, and Vollhardt. P.R. B 69, 045112
Byczuk, Ulmke, and Vollhardt. P.R.L. 90 196403



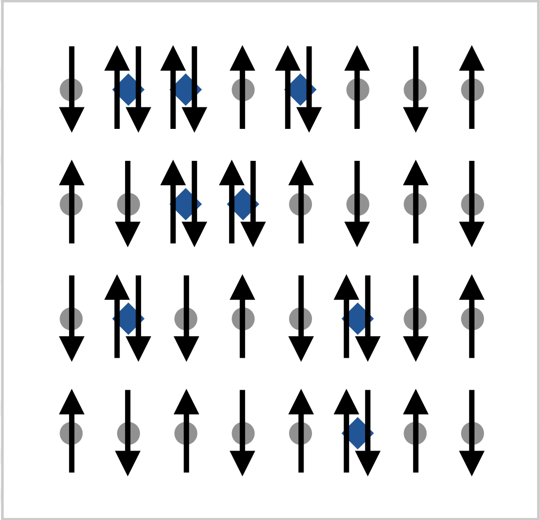
Alloy Mott Insulator | **Alloy Band Insulator** | **Alloy Mott Insulator**



$\rho = x$

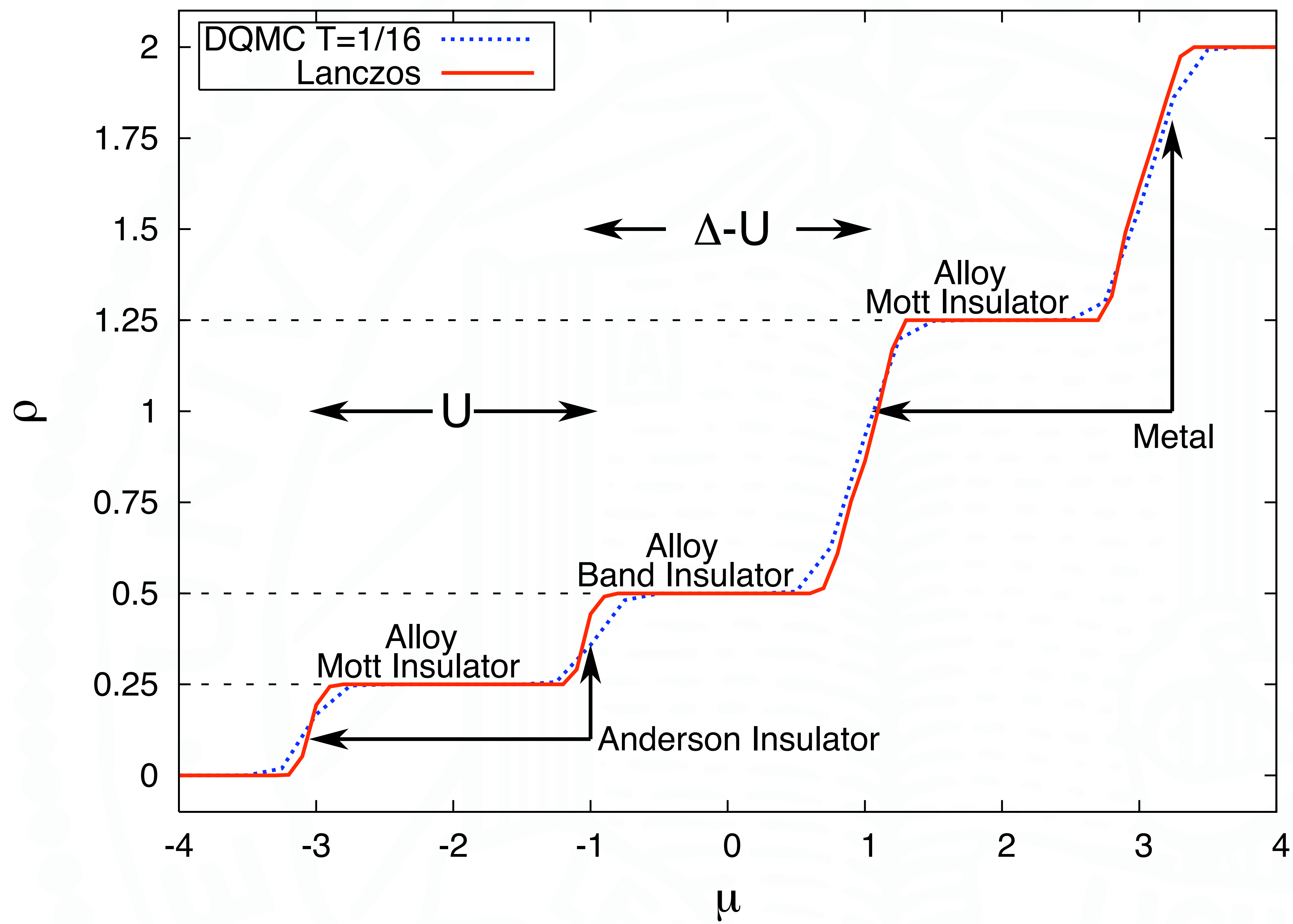


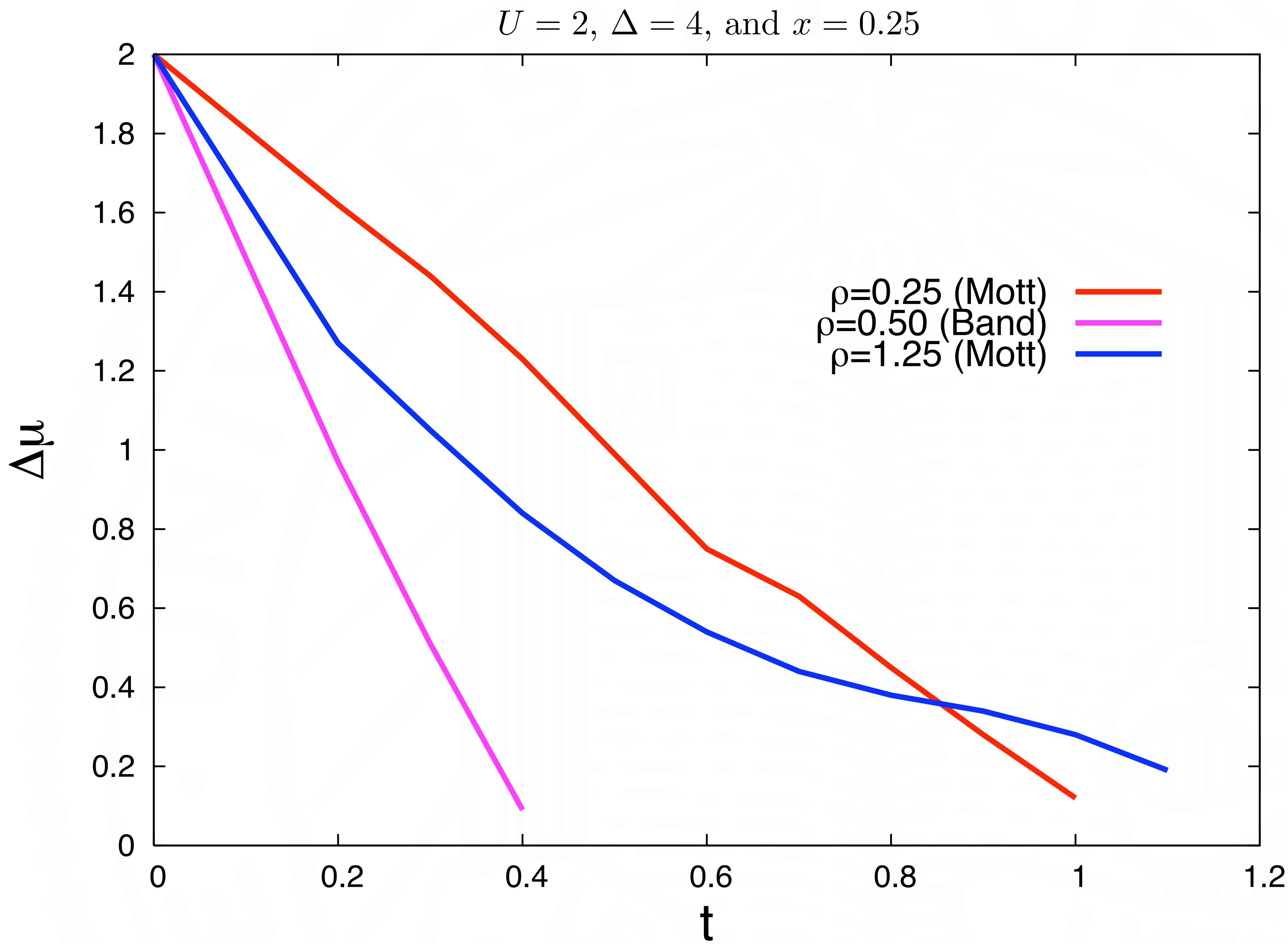
$\rho = 2x$



$\rho = 1 + x$

$t = 0.1$, $U = 2$, $\Delta = 4$, and $x = 0.25$



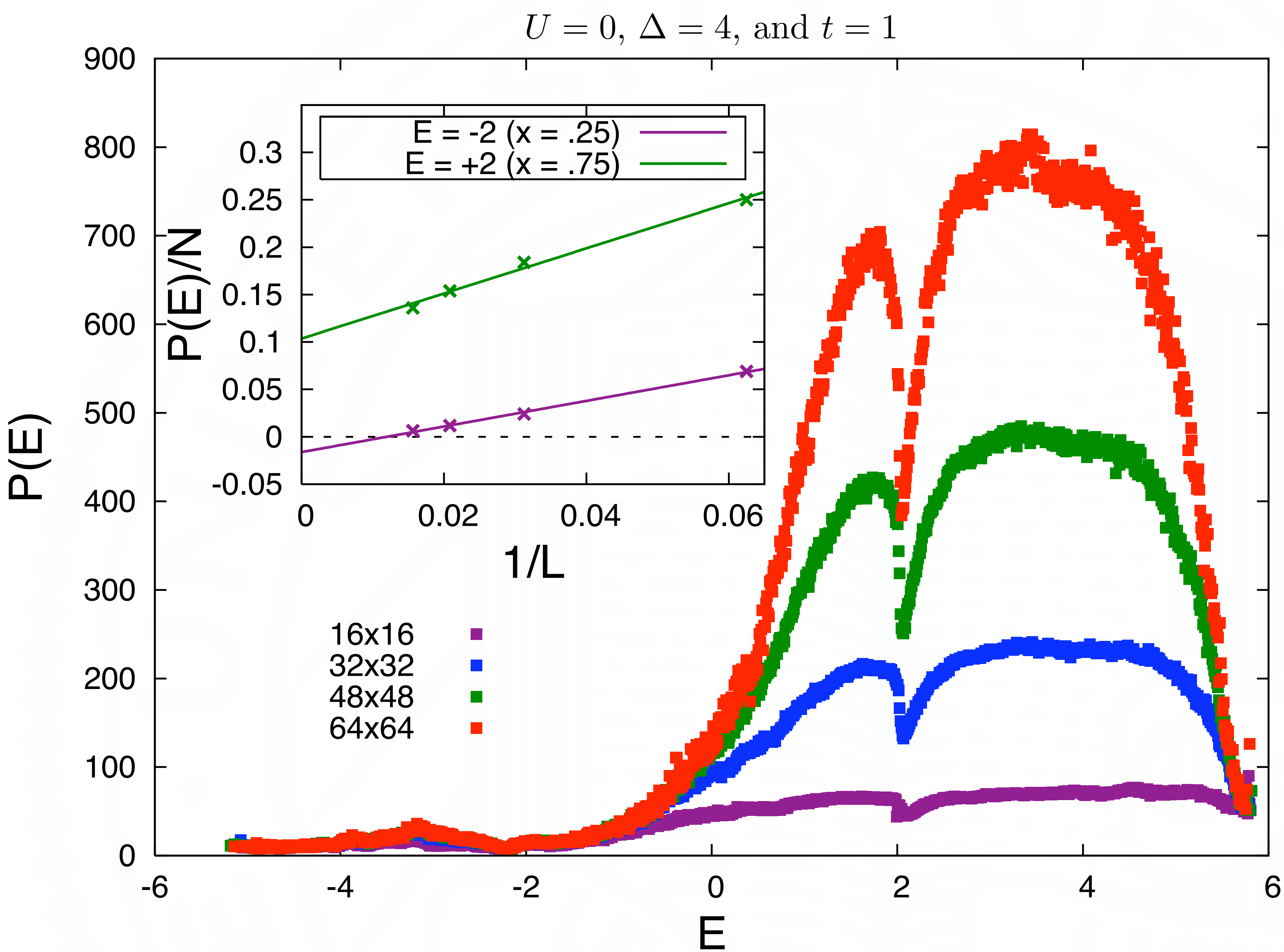


$U = 2$, $\Delta = 4$, and $x = 0.25$
ρ=0.25 (Mott)
ρ=0.50 (Band)
ρ=1.25 (Mott)
Δμ
t
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
1.2

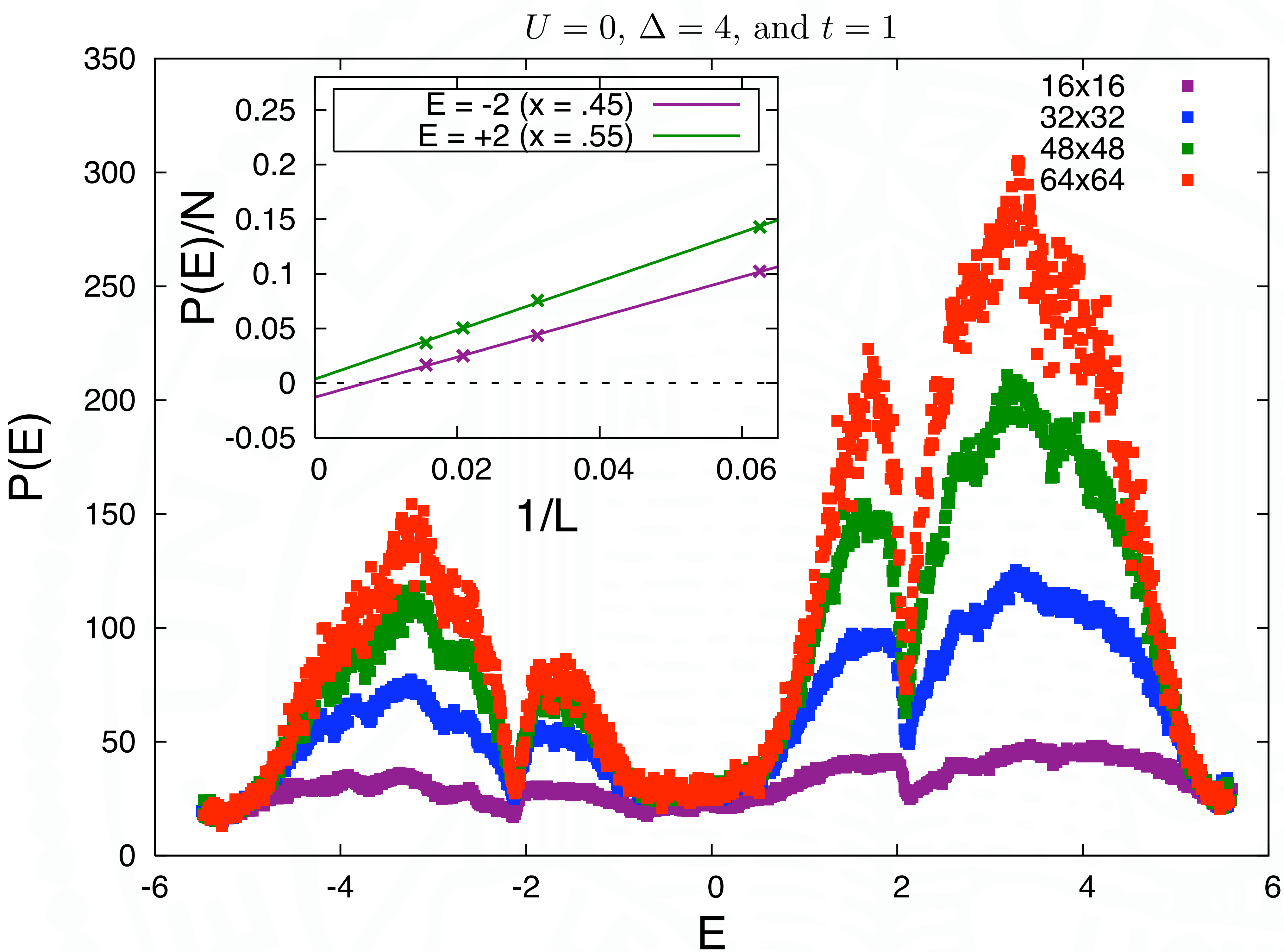
Participation Ratio

$$\mathcal{P}_n = \left(\sum_{i=1}^{N} |\langle\, i \,|\phi_n\rangle|^4 \right)^{-1}$$

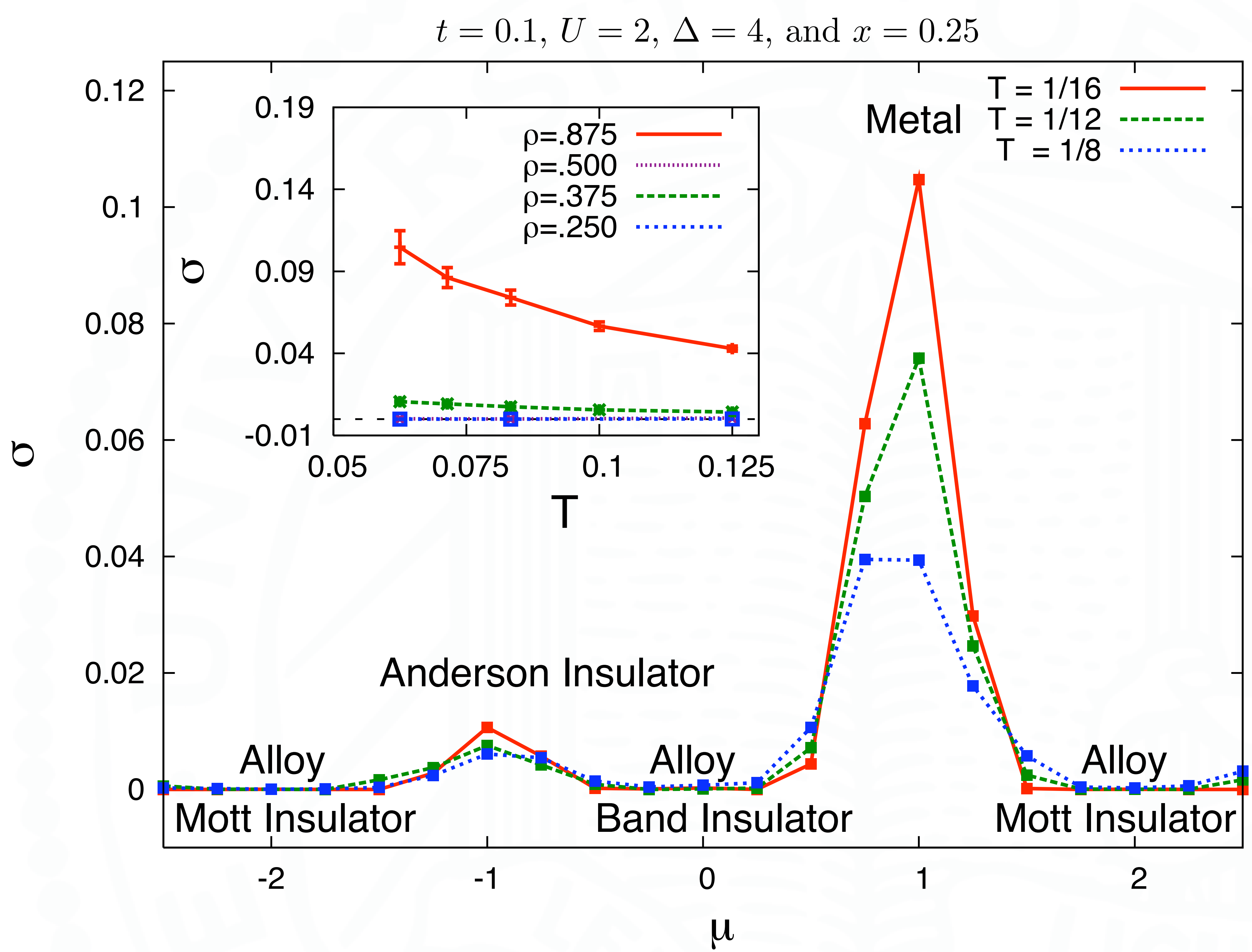
$$\begin{aligned} \mathcal{P}_n &= \quad 1 \quad \text{localized} \\ \mathcal{P}_n &= \quad N \quad \text{delocalized} \end{aligned}$$


$U = 0$, $\Delta = 4$, and $t = 1$
P(E)
E
900
800
700
600
500
400
300
200
100
0
-6
-4
-2
0
2
4
6
16x16
32x32
48x48
64x64
E = -2 (x = .25)
E = +2 (x = .75)
P(E)/N
1/L
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
0.02
0.04
0.06

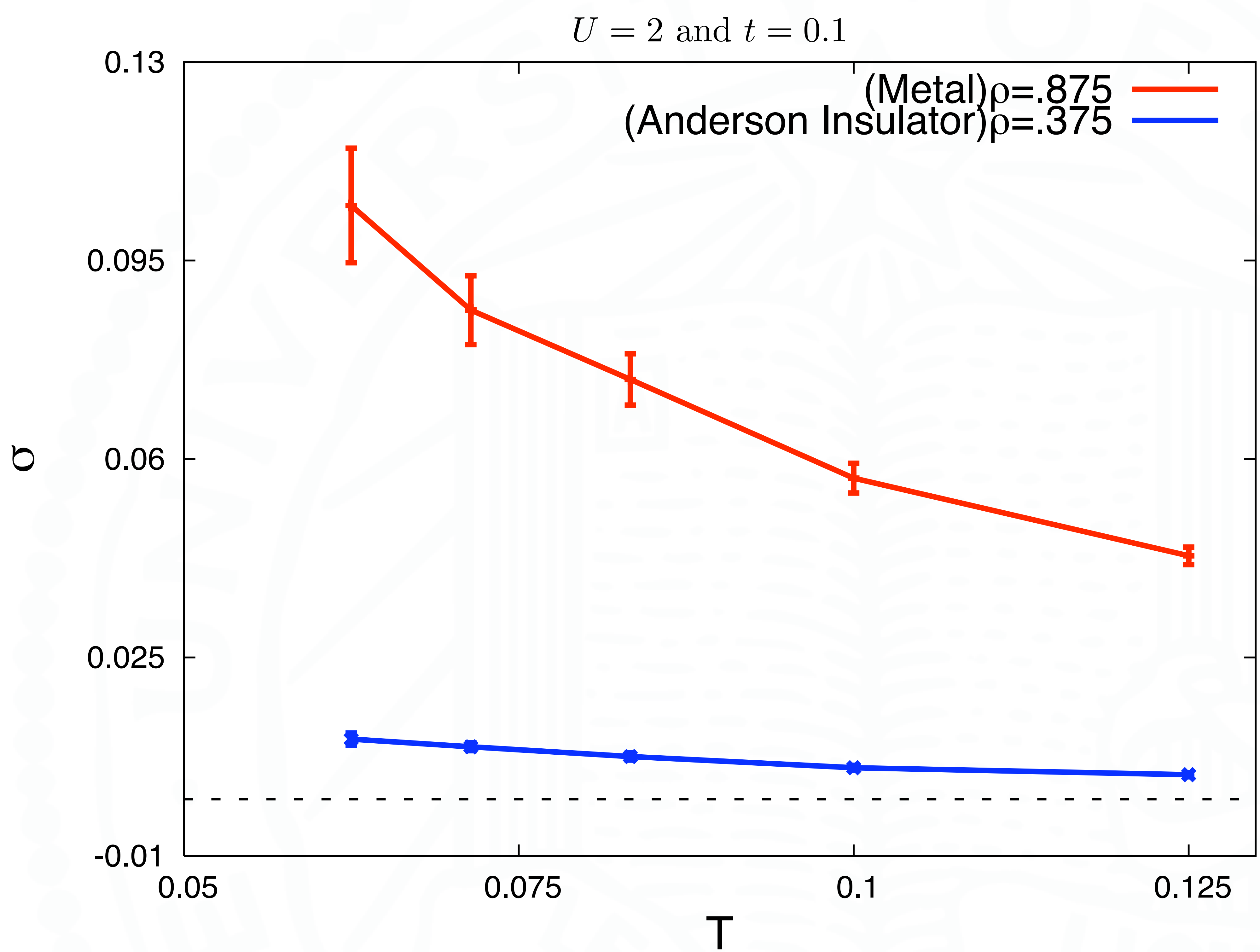
Participation Ratio at x=.45



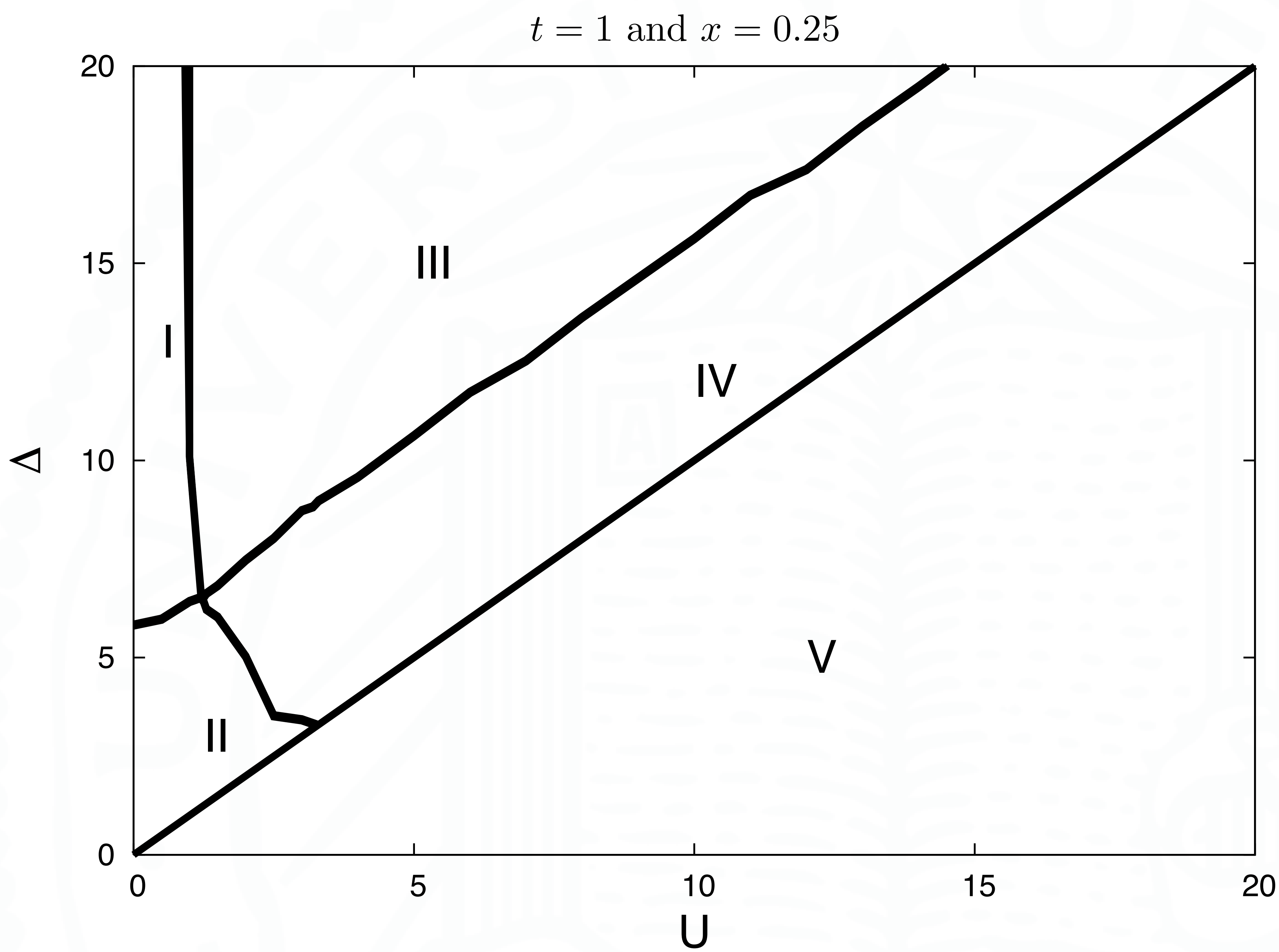
Conductivity vs. Chemical Potential



Conductivity vs. Temperature



Phase Diagram of U vs. Δ



I: Mott Insulator [ρ=0.25], II: Metallic, III: Band Insulator [ρ=0.50] and Mott Insulators [ρ=0.25 and ρ=1.25], IV: Mott Insulators [ρ=0.25 and ρ=1.25], V: U>Δ