

Reduced Potential Energy Matrix and Perturbed Reduced Potential Energy Matrix

	state index	energy function	configurations from state 1			configurations from state 2			configurations from state M			
			x_1^1	...	$x_1^{N_1}$	x_2^1	...	$x_2^{N_2}$	x_M^1	...	$x_M^{N_M}$	
sampled states	1	$U_1(\cdot)$	$U_1(x_1^1)$	\cdots	$U_1(x_1^{N_1})$	$U_1(x_2^1)$	\cdots	$U_1(x_2^{N_2})$	$U_1(x_M^1)$	\cdots	$U_1(x_M^{N_M})$	$= A_{M,N}$
	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots	\ddots	\vdots	\vdots	\ddots	\vdots	
	M	$U_M(\cdot)$	$U_M(x_1^1)$	\cdots	$U_M(x_1^{N_1})$	$U_M(x_2^1)$	\cdots	$U_M(x_2^{N_2})$	$U_M(x_M^1)$	\cdots	$U_M(x_M^{N_M})$	
perturbed states	1	$U'_1(\cdot)$	$U'_1(x_1^1)$	\cdots	$U'_1(x_1^{N_1})$	$U'_1(x_2^1)$	\cdots	$U'_1(x_2^{N_2})$	$U'_1(x_M^1)$	\cdots	$U'_1(x_M^{N_M})$	$= B_{L,N}$
	\vdots	\vdots	\vdots	\ddots	\vdots	\vdots	\ddots	\vdots	\vdots	\ddots	\vdots	
	L	$U'_L(\cdot)$	$U'_L(x_1^1)$	\cdots	$U'_L(x_1^{N_1})$	$U'_L(x_2^1)$	\cdots	$U'_L(x_2^{N_2})$	$U'_L(x_M^1)$	\cdots	$U'_L(x_M^{N_M})$	