

1 Молекула водорода

Гамильтониан

$$\begin{aligned}\hat{H}_{H_2} = & -0.042\hat{\sigma}_{0000} + 0.178(\hat{\sigma}_{3000} + \hat{\sigma}_{0300}) - 0.243(\hat{\sigma}_{0030} + \hat{\sigma}_{0003}) \\ & + 0.171\hat{\sigma}_{3300} + 0.123(\hat{\sigma}_{3030} + \hat{\sigma}_{0303}) + 0.168(\hat{\sigma}_{3003} + \hat{\sigma}_{0330}) + 0.176\hat{\sigma}_{0033} \\ & + 0.045(\hat{\sigma}_{3113} - \hat{\sigma}_{3311} - \hat{\sigma}_{1133} + \hat{\sigma}_{1331}).\end{aligned}\quad (1)$$

Гамильтониан для обучения

$$\hat{H} = h_1\hat{\sigma}_{0123} + h_2\hat{\sigma}_{0213} + h_3\hat{\sigma}_{0330} + h_4\hat{\sigma}_{1023} + h_5\hat{\sigma}_{1100} + h_6\hat{\sigma}_{1230} + h_7\hat{\sigma}_{1313},$$

$\hat{\sigma}_{0000}$	$\hat{\sigma}_{0123}$	$\hat{\sigma}_{0213}$	$\hat{\sigma}_{0330}$	$\hat{\sigma}_{1023}$	$\hat{\sigma}_{1100}$	$\hat{\sigma}_{1230}$	$\hat{\sigma}_{1313}$
$\hat{\sigma}_{0123}$	$\hat{\sigma}_{0000}$	$\hat{\sigma}_{0330}$	$\hat{\sigma}_{0213}$	$\hat{\sigma}_{1100}$	$\hat{\sigma}_{1023}$	$-\hat{\sigma}_{1313}$	$-\hat{\sigma}_{1230}$
$\hat{\sigma}_{0213}$	$\hat{\sigma}_{0330}$	$\hat{\sigma}_{0000}$	$\hat{\sigma}_{0123}$	$i\hat{\sigma}_{1230}$	$-i\hat{\sigma}_{1313}$	$-i\hat{\sigma}_{1023}$	$i\hat{\sigma}_{1100}$
$\hat{\sigma}_{0330}$	$\hat{\sigma}_{0213}$	$\hat{\sigma}_{0123}$	$\hat{\sigma}_{0000}$	$-i\hat{\sigma}_{1313}$	$i\hat{\sigma}_{1230}$	$-i\hat{\sigma}_{1100}$	$i\hat{\sigma}_{1023}$
$\hat{\sigma}_{1023}$	$\hat{\sigma}_{1100}$	$-i\hat{\sigma}_{1230}$	$i\hat{\sigma}_{1313}$	$\hat{\sigma}_{0000}$	$\hat{\sigma}_{0123}$	$i\hat{\sigma}_{0213}$	$-i\hat{\sigma}_{0330}$
$\hat{\sigma}_{1100}$	$\hat{\sigma}_{1023}$	$i\hat{\sigma}_{1313}$	$-i\hat{\sigma}_{1230}$	$\hat{\sigma}_{0123}$	$\hat{\sigma}_{0000}$	$i\hat{\sigma}_{0330}$	$-i\hat{\sigma}_{0213}$
$\hat{\sigma}_{1230}$	$-\hat{\sigma}_{1313}$	$i\hat{\sigma}_{1023}$	$i\hat{\sigma}_{1100}$	$-i\hat{\sigma}_{0213}$	$-i\hat{\sigma}_{0330}$	$\hat{\sigma}_{0000}$	$-\hat{\sigma}_{0123}$
$\hat{\sigma}_{1313}$	$-\hat{\sigma}_{1230}$	$-i\hat{\sigma}_{1100}$	$-i\hat{\sigma}_{1023}$	$i\hat{\sigma}_{0330}$	$i\hat{\sigma}_{0213}$	$-\hat{\sigma}_{0123}$	$\hat{\sigma}_{0000}$