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Full Papers

精确固定节面量子**Monte**：**Carlo**差值法

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摘要 本文提出了精确固定节面量子Monte Carlo差值法，这个新算法能够在精确固定节面量子Monte Carlo方法的基础上直接计算两个体系之间的能量差，且使计算结果的统计误差达到10-2

kJ/mol 数量级，获得电子相关能90%以上。我们把这个新算法应用于分子势能面的研究中，使用一个“刚性移动”模型，利用Jacobi变换使分子两个几何构型的能量计算具有很好的正相关性，因而能得到准确的能量差值，
于是精确的分子势能面就可以得到。这个新算法已经被使用到BH分子基态势能曲线和H_3分子势能面的研究。这个算法还可应用于分子光谱、化学反应能量变化值等领域的研究。

关键词 节面量子

分类号

Exact Fixed-node Quantum Monte Carlo: Differential Approach

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Abstract A differential approach for exact fixed-node quantum Monte Carlo calculation was proposed in this paper. This new algorithm can be used to directly compute the energy differential between two systems in exact fixed-node quantum Monte Carlo process, making the statistical error of calculation reduce to order of 10^{-2} kJ/mol and recover about more than 90% of the correlation energy. The approach was employed to set up a potential energy surface of a molecule, through a model of rigid move, and Jacobi transformation utilized to make energy calculation for two configurations of a molecule having good positive correlation. So, an accurate energy differential could be obtained, and the potential energy surface with good quality depicted. This novel algorithm was used to study the potential energy curve of the ground state of BH and the potential energy surface of H_3, and could be also applied to study other related fields such as molecular spectroscopy and the energy variation of chemical reactions.

Key words exact fixed-node quantum Monte Carlo differential approach correlation sampling potential energy surface

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