Journal of Statistical Physics, Vol. 43, Nos. 5/6, 1986

Quantum Monte Carlo of Coupled Fermion Chains

David S. Kung[1]

KEY WORDS: Quantum Monte Carlo: fermion field theory; critical phenomena.

Computation involving fermions in more than one dimension presents a challenge to Monte Carlo simulations. One is either faced with calculation of the fermion determinant or the appearance of random walks that carry negative weights. The cancellations among positive and negative weights give rise to uncontrollable fluctuations. A new stochastic algorithm is proposed for treating quantum problems in which the matrix elements of the projection operator, $U(\beta) = e^{-\beta H}$, carries both positive and negative signs. The algorithm is a variant of the population scheme of the Projector Monte Carlo method.[1] We apply this algorithm to a double-chain fermion system where electron tunnelling across the chains gives rise to unavoidable negative matrix elements. As discussed in Ref. 1, the operator U is factorized into a probability P and a score S. $U(\beta) = U(\Delta\tau)^N$ is simulated by simultaneously evolving (in imaginary time) a population of states. The population, ϕ, consists of $N(\phi, L)$ copies of the state $|L\rangle$, so the total number of states in the population is $N_{\text{tot}} = \sum_L N(\phi, L)$. To proceed with an elemental time step, one operates on the state $|I\rangle$ a total of $N(\phi, I)$ independent times with the operator $U(\Delta\tau)$. One such application to $|I\rangle$ leads to a final state $|F\rangle$ with probability $P(F, I)$ and a score $S(F, I)$. The final score for the state $|F\rangle$ is given by

$$S(F) = \sum_I S(F, I)$$

We then compute the total absolute score

$$S_{\text{tot}} = \sum_F |S(F)|$$

[1] Department of Applied Physics, Stanford University, Stanford, California 94305.

0022-4715/86/0600-0873$05.00/0

and form the ratio

$$R(F) = S(f)/S_{\text{tot}}$$

The new integer population distribution for the next intermediate state ϕ' is given by $N(\phi', F)$, which is the nearest integer to $R(F) \times N_{\text{tot}}$. The ground state energy and correlation functions are measured with good accuracy for a system of modest size. Since this algorithm requires sorting through the individual states generated by the Monte Carlo, it is ultimately limited by the number of dominant states in the constituency of the ground state. However, with a few megabytes of core memory, two-dimensional interacting fermion systems of reasonable size are within reach.

REFERENCES

1. D. Kung, R. Blankenbecler, and R. Sugar, *Phys. Rev. B* **32**:3058 (1985).