# Formulation and Application of the Quantum Monte Carlo Method to Fractional Quantum Hall Systems

### Sei Suzuki[1] and Tatsuya Nakajima[2]

[1] *Department of Basic Science, University of Tokyo, Tokyo, 153-8902, Japan*
[2] *Department of Physics, Tohoku University, Sendai, 980-8578, Japan*

Two-dimensional electron gas (2DEG) in a strong magnetic field is known as a system which shows various phenomena resulting from the electronic interaction. In particular, the fractional quantum Hell (FQH) effect has attracted much theoretical and experimental attention from this point of view. To investigate such strongly-correlated systems theoretically, numerical studies play a significant role. For example, the exact diagonalization and density matrix renormalization group (DMRG) methods have been used for the study of FQH systems as the ones directly accessible to the ground state. However, the exact diagonalization can study static and dynamic properties only for small systems, while it is not so easy to obtain dynamical information by the DMRG. Thus we apply the quantum Monte Carlo (QMC) method to this system in the present work.

The QMC method has been used for several quantum many-body systems. It can investigate both static and dynamical properties of systems larger than those applicable in the exact diagonalization. However, this method is inherently involved with the so-called negative-sign problem. Thus we need to overcome (at least, or moderate) the negative-sign nuisance in order to make the best use of the method. In this study , we formulate the QMC method to the FQH system that is free of the sign problem and report some numerical results.

We consider interacting electrons confined on a spherical surface with a magnetic monopole located at the center of the sphere. For simplicity, we neglect the spin degrees of freedom and assume that all the electrons occupy the lowest Landau level. Then single-particle states are specified by the $z$-component, $m$, of angular momentum whose amplitude is $s$, where $2s$ is the number of flux quanta piercing the sphere. $m$ ranges from $-s$ to $s$. The Hamiltonian can be written in the quadratic form of the density operator and its time reversal:

$$\mathcal{H} = -\sum_{K=0}^{2s} \chi_K \sum_{N=-K}^{K} \rho_{KN}\tilde{\rho}_{KN} + C_0\,\rho_{00},$$

$$\rho_{KN} \equiv \sum_{m_1,m_2} \langle KN|m_1m_2\rangle(-1)^{s+m_2}\, a_{m_1}^\dagger a_{-m_2}, \quad \tilde{\rho}_{KN} = (-1)^K\,\rho_{KN}^\dagger,$$

where $a_m$ is an annihilation operator of electron, $\langle KN|m_1m_2\rangle$ the Clebsch-Gordan coefficient, and $C_0$ is a constant. The coupling constant $\chi_K$ is related with the Haldane pseudopotential $V_J$ as

$$\chi_K = \sum_{J=0}^{2s} T_{KJ}V_J, \quad T_{KJ} = (-1)^{2s-J+K+1}(2s-J)\begin{Bmatrix} s & s & J \\ s & s & K \end{Bmatrix}, \tag{1}$$

where the braces denote Wigner's $6j$ symbol. The transformation matrix $T$ satisfies $T^{-1} = T$, that is, $V_J = \sum_{K=0}^{2s} T_{JK}\chi_K$.

In the zero-temperature formalism, the expectation value of an observable $\mathcal{O}$ is given by $\langle\mathcal{O}\rangle = \lim_{\beta\to\infty}\langle\psi|e^{-\beta\mathcal{H}/2}\mathcal{O}e^{-\beta\mathcal{H}/2}|\psi\rangle/\langle\psi|e^{-\beta\mathcal{H}}|\psi\rangle$, where $|\psi\rangle$ is an arbitrary state not orthogonal to the ground state. The imaginary-time evolution operator $e^{-\beta\mathcal{H}}$ is decomposed to imaginary-time slices $e^{-\Delta\beta\mathcal{H}}\cdots e^{-\Delta\beta\mathcal{H}}$, and the Hubbard-Stratonovich (HS) transformation is performed for each slice. After all, the expectation value is expressed in the form of an auxiliary-field path integral. We evaluate it by means of the Monte Carlo method. The negative-sign problem is

nothing but the fact that the integrand function of the normalization denominator, $\langle\psi|e^{-\beta\mathcal{H}}|\psi\rangle$, is not always positive for any auxiliary-field configuration.

It can be shown that the sign problem can be avoided completely under the following conditions: (i) $2s$ is odd and the number of electrons, $N_e$, is even, (ii) the coupling constants in the Hamiltonian satisfy $\chi_K \geq 0$ for $K = 1, 2, \cdots, 2s$. The condition (i) can be satisfied, for example, in case of $2s = 3N_e - 3$ for the $\nu = 1/3$ Laughlin state, or $2s = 2N_e - 3$ for the Pfaffian state. However, the condition (ii) is not satisfied when the values for the Coulomb interaction are used for $V_J$ in Eqn.(1). Thus we control the value of $\chi_K$ (that is, that of $V_J$) by solving a linear programming problem for the satisfaction of the condition (ii). Namely, taking into account that only $V_J$ for odd $2s - J$ are physical for fermionic systems, we inquire for $\chi_K$ which minimizes

$$F(\chi_0, \chi_1, \cdots, \chi_{2s}) \equiv \sum_{2s-J:\text{odd}} \lambda_J (\sum_{K=0}^{2s} T_{JK}\chi_K - V_J)$$

under the conditions that $\chi_0 \leq 0$, $\chi_K \geq 0$ for $K = 1, 2, \cdots, 2s$, and $\lambda_J(\sum_{K=0}^{2s} T_{JK}\chi_K - V_J) \geq 0$ for odd $2s - J$. We note here that $\lambda_J$ controls the variance of pseudopotential $V_J$ from that for the Coulomb interaction for each $J$. Then obtained $\chi_K$ minimizes the variance satisfying the condition (ii).

Figure 1(a) shows an example of pseudopotentials free of the negative-sign problem. Although the optimized potential does not coincide completely with that for the Coulomb interaction, its monotonical dependence on $J$ is realized naturally. We note that optimized pseudopotentials can be obtained with less variance for the higher Landau levels or in the presence of finite-thickness effects.

In Figure 1(b), the energy expectation values are shown against the width of imaginary-time slice $\Delta\beta$. Although finite value of $\Delta\beta$ gives rise to numerical errors by the Suzuki-Trotter decomposition, the expectation value almost saturates for $\Delta\beta \leq 1/8$ $[1/(e^2/l_B)]$ ($l_B \equiv \sqrt{c/eB}$: the magnetic length) and converges to the groundstate energy (pointed by the arrow) for $\beta > 20$ $[1/(e^2/l_B)]$. The convergence is consistent with the fact the energy gap is about $0.1e^2/l_B$.
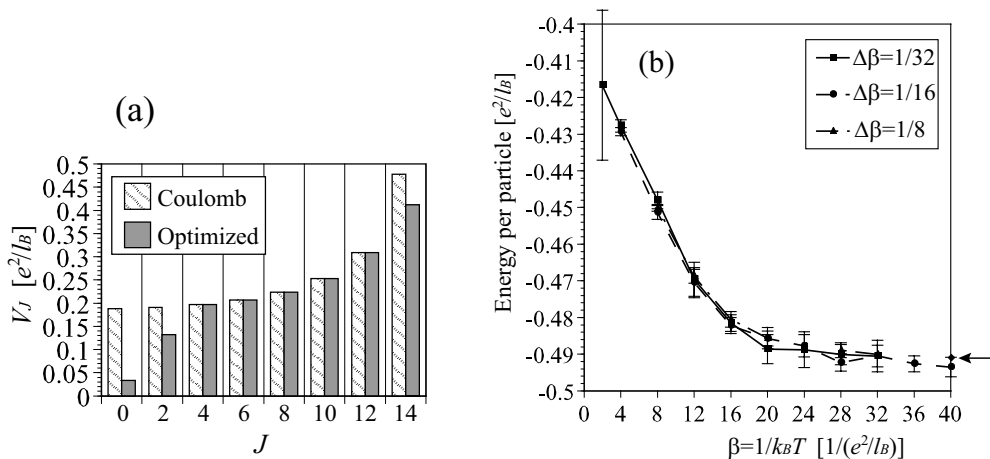


Figure 1: (a) Pseudopotentials for the Coulomb interaction and optimized negative-sign-free potential for $2s = 15$. Only the physical ($2s - J$: odd) components are shown. (b) Energy expectation value per particle vs. inverse temperature by the QMC calculation for $2s = 15$ and $N_e = 6$. Optimized potential in (a) was used, and the values used as imaginary-time slice width are $\Delta\beta = 1/8, 1/16$, and $1/32$ $[1/(e^2/l_B)]$. The groundstate energy obtained by the exact diagonalization is shown by an arrow at the right side.