New Stochastic Method for Systems with Broken Time-Reversal Symmetry: 2D Fermions in a Magnetic Field

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We present a stochastic method able to deal with complex Hermitian Hamiltonians where time reversal invariance is broken explicitly. We fix the phase of the wave function and show that the equation for the modulus can be solved by quantum Monte Carlo techniques. Then, any choice for its phase provides a variational upper bound for the ground state energy of the system. We apply the *fixed-phase* method to the 2D electron gas in the presence of a magnetic field with generalized periodic boundary conditions, where we study the transition between an incompressible $\nu = 1/m$ Laughlin liquid and a Wigner crystal.

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In spite of the significant effort devoted to develop stochastic methods to study many-fermion systems, there are no rigorous solutions. Furthermore, with the exception of variational approaches, all methods to date are restricted to systems with time-reversal symmetry. However, many interesting physical processes (particles in an external magnetic field or in a rotating frame) involve explicit breaking of this symmetry. In this Letter, we present a general procedure to circumvent the latter problem. Though the method turns out to be of broad applicability we will illustrate it by the study of fermions in the presence of magnetic fields.

The fractional quantum Hall effect (FQHE) [1] involves 2D interacting electrons under the influence of high perpendicular magnetic fields and, where particle correlations are crucial to stabilize the ground state of the system. Of particular importance is the determination of the phase boundary between a Laughlin liquid (LL) [2] and a Wigner crystal (WC) [3] as a function of the particle density and Landau-level filling factor ν. A transition has been suggested based upon recent experimental observations of a reentrant insulating-FQHE-insulating behavior around ν=1/5 and ν=1/3 for electron and hole systems, respectively [4].

We are concerned with the study of the ground state ($T = 0$) properties of a 2D quantum system, defined by the spin-free many-body Hamiltonian

$$\widehat{\mathbb{H}} = \sum_{i=1}^{N} \frac{\mathbf{\Pi}_i^2}{2m^*} + \sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \Lambda \quad , \tag{1}$$

where $\mathbf{\Pi}_i = \mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)$. Λ is a constant potential which ensures the global charge neutrality of the system (neutralizing background) of N fermions of mass m^* and charge $-e$. The vector potential $\mathbf{A}$, whose curl is the external magnetic field $\mathbf{B}$, is given by $\mathbf{A}(\mathbf{r}) = (-B\,y,\, 0)$ $[\mathbf{A}(\mathbf{r}) = (-By/2,\, Bx/2)]$ in the Landau (symmetric) gauge.

The approach developed in the present Letter uses diffusion Monte Carlo (DMC) methods which can determine ground state properties of many-particle systems and are not, in principle, constrained to a variational ansatz. It is based on the observation that the N-particle Schrödinger equation in Euclidean time (imaginary time t) can be interpreted as a diffusion and branching process [5]. All implementations to date have required the wave function to be real in order to use sampling methods. However, the many-body Hamiltonian $\widehat{\mathbb{H}}$ involves interacting fermions in the absence of time-reversal symmetry, implying that its eigenfunctions must be complex valued.

In order to overcome this limitation we introduce the *fixed-phase* method [6]. The first step is to write the scalar N-particle state $\Phi(\mathcal{R}) = |\Phi(\mathcal{R})| \exp[i\varphi(\mathcal{R})]$, with $|\Phi|$ and φ real functions. Here $\mathcal{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N)$ denotes a point in the $2N$-dimensional configuration space. The real and imaginary parts of the many-body Schrödinger equation, $\widehat{\mathbb{H}}\Phi = E\Phi$, yield, respectively, two coupled equations (in atomic units):

$$\widehat{H}\,|\Phi(\mathcal{R})| = \left[\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2} + V(\mathcal{R})\right] |\Phi(\mathcal{R})| = E\,|\Phi(\mathcal{R})|\,, \tag{2}$$

$$\sum_{i=1}^{N} \nabla_i \cdot \left\{ |\Phi(\mathcal{R})|^2 \left[\nabla_i\, \varphi(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)\right] \right\} = 0, \tag{3}$$

where the effective potential $V(\mathcal{R})$ is given by

$$V(\mathcal{R}) = \sum_{i>j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{i=1}^{N} \left[\nabla_i\, \varphi(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)\right]^2 + \Lambda. \tag{4}$$

We have mapped a fermionic problem into a bosonic one for $|\Phi|$, but with the additional complication that we have to solve simultaneously two multidimensional differential equations. An alternative way of looking at this transformation is to regard it as a gauge transformation whose effect is to add a vector potential $[\nabla_i \varphi(\mathcal{R})]$ to the Hamiltonian, giving rise to a fictitious magnetic field. The essence of the *fixed-phase* method consists in making a choice for φ and solving *exactly* the bosonic problem for $|\Phi|$ using DMC. It is easily seen that the method provides a variational bound for the energy and, for a prescribed trial phase φ_T, the *lowest* energy consistent with this phase. For real symmetric Hamiltonians the *fixed-phase*

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method reduces to the *fixed-node* approximation [5] when we make the choice $\varphi = \pi\,[1 - \Theta(\Phi_T/|\Phi_T|)]$, where Θ is the unit step function. In this way Eq. (2) is solved in domains of the configuration space delimited by the nodes of the trial state Φ_T where hard wall boundary conditions are imposed.

We can transform the time-dependent Schrödinger equation for $|\Phi|$ in Euclidean time t to a master equation for the *importance-sampled* distribution $P(\mathcal{R},t) = |\Phi_T(\mathcal{R})|\,|\Phi(\mathcal{R},t)|$,

$$\frac{\partial P(\mathcal{R},t)}{\partial t} = \sum_{i=1}^{N} \nabla_i \cdot \left[\frac{1}{2}\nabla_i P(\mathcal{R},t) - \mathbf{F}_i(\mathcal{R})\,P(\mathcal{R},t)\right] - [E_{\rm loc}(\mathcal{R}) - E_T]\,P(\mathcal{R},t), \tag{5}$$

where $\Phi_T(\mathcal{R}) = |\Phi_T(\mathcal{R})|\exp[i\varphi_T(\mathcal{R})]$ is a trial function used to *guide* the random walk, $\mathbf{F}_i(\mathcal{R}) = \nabla_i \ln|\Phi_T|$ is the *drift velocity*, $E_{\rm loc}(\mathcal{R}) = |\Phi_T|^{-1}\,\hat{H}\,|\Phi_T|$ is the local energy, and E_T is a suitable trial energy which shifts the zero of the energy spectrum. At sufficiently long times $P(\mathcal{R}, t\to\infty) \to |\Phi_T(\mathcal{R})|\,|\Phi_0(\mathcal{R})|$, where $|\Phi_0|$ is the lowest energy state, compatible with the phase φ_T, which has a component in $|\Phi_T|$. In order to get this stationary distribution, E_T must be adjusted to be equal to the fixed-phase ground state energy E_0, given in turn by $E_0 = \lim_{t\to\infty}\langle E_{\rm loc}(\mathcal{R})\rangle_{P(\mathcal{R},t)}$. The modulus of the trial state, $|\Phi_T(\mathcal{R})|$, affects the convergence and statistical fluctuations of the stochastic averages. To solve Eq. (5) we use methods similar to Refs. [5,7].

It is well known [8,9] that assigning boundary conditions to quantum systems in a closed manifold is a subtle matter. For particles moving on the surface of a flat torus in presence of a magnetic field, consistent boundary conditions for the many-body state (Φ_T) and vector potential ($\mathbf{A}$) imply that both have to change by a "large" gauge transformation in order to allow a nonzero quantized external flux (these are generalized periodic boundary conditions). Hence, Φ_T must be a quasiperiodic function under a uniform translation of the system by a lattice vector $\mathbf{L} = n_1\mathbf{L_1} + n_2\mathbf{L_2}$,

$$\Phi_T(\{\mathbf{r}_j + \mathbf{L}\}) = \exp\left(i\,\boldsymbol{\theta}\cdot\mathbf{L} - i\sum_{j=1}^{N}\Delta_j(\mathbf{L})\right)\Phi_T(\{\mathbf{r}_j\}), \tag{6}$$

where $\mathbf{L_1}\wedge\mathbf{L_2}$ defines the principal region of the torus, n_1, n_2 are arbitrary integers, $\boldsymbol{\theta}$ is a twist angle vector which includes the effect of the electric field, $\Delta_j(\mathbf{L})$ is the gauge function given by $\Delta_j = x_j L_y/\ell^2$ [$\Delta_j = (x_j L_y - y_j L_x)/2\ell^2$] in the Landau (symmetric) gauge, and $\ell = 1/\sqrt{B}$ is the magnetic length. Note that even if toroidal boundary conditions lead to quasiperiodic states, the quantities in Eq. (5) ($|\Phi_T|$, $\mathbf{F}_i$) are genuine periodic functions on the torus. This fact simplifies the Monte Carlo sampling procedure.

Thus, we are left with the task of exploring the set of nonequivalent phases $\{\varphi_T\}$ and of determining the minimum of the functional $E_0\,[\varphi_T]$. Of course, we do not pretend to scan the space of all possible phases but just use some conventional choices for φ_T. There are some mathematical constraints that can be imposed on φ_T, for instance, we would like to conserve the symmetries of the Hamiltonian unless some of them are spontaneously broken (like in the WC phase). In any case, it is obvious that a phase that satisfies Eq. (3) (*continuity equation*) for the exact $|\Phi(\mathcal{R})|$ will lead to the exact solution of the many-fermion problem. Thus, trial functions Φ_T that satisfy the *continuity equation* are good candidates for the phase. Consider trial functions of the form

$$\Phi_T(z_1, z_2, \ldots, z_N) = F(\{z_i\})\,\exp\left[-\Omega(\{z_i, z_i^*\})\right], \tag{7}$$

where $F(\{z_i\})$ is an analytic (holomorphic) function of $\{z_i\}$, and $\Omega(\{z_i, z_i^*\}) = \sum_{j=1}^{N}|z_j|^2/4\ell^2$ in the symmetric gauge or $\Omega(\{z_i, z_i^*\}) = \sum_{j=1}^{N} y_j^2/2\ell^2$ in the Landau gauge. Particle positions are written in complex coordinate representation $z_j = x_j + iy_j$. It is straightforward to prove [10] that the above conditions on Φ_T imply

$$\nabla_i \cdot \left\{|\Phi_T(\mathcal{R})|^2\,[\nabla_i\,\varphi_T(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)]\right\} = 0, \tag{8}$$

$$\nabla_i \cdot [\nabla_i\,\varphi_T(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)] = 0, \tag{9}$$

and

$$E_{\rm loc}(\mathcal{R}) = \frac{N}{2\ell^2} + \sum_{i>j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \Lambda. \tag{10}$$

Notice that Eq. (8) is just the desired second equation, Eq. (3), except that the exact Φ is replaced by the trial Φ_T. Thus for this class of functions, Eq. (3) is approximately satisfied analytically. Furthermore, the last equation shows that the local energy needed in the sampling is given by an extremely simple form. These results are independent of the manifold in which particles move, i.e., of the boundary conditions.

There are two independent parameters characterizing the 2D electron gas in the presence of a magnetic field at $T = 0$: the Wigner-Seitz radius $r_s = 1/\sqrt{\pi\rho}$, which measures interparticle spacing in units of the Bohr radius (ρ is the areal density), and the Landau level filling factor $\nu = 2\ell^2/r_s^2$. It is the interplay between these two parameters that will determine the zero temperature phase diagram. As ν is decreased or r_s is increased the 2D system is expected to undergo a first order transition between a LL and a WC.

In the following we will assume that the spin degrees of freedom are frozen by the magnetic field and that no electric field is present; i.e., we will consider the physical situation where Zeeman energies are so large that electrons moving on the surface of the torus [$\mathbf{L_1} = (L_1, 0), \mathbf{L_2} = (0, L_2)$] with boundary angle $\boldsymbol{\theta} = \mathbf{0}$ are completely spin polarized.

The unnormalized $\nu = 1/m$ Laughlin state, Φ_m, with toroidal boundary conditions has the form referred to in Eq. (7) with (Landau gauge) [11]

TABLE I. $E_0-\omega_c/2$ in units of $1/\ell$ for different electron densities r_s and filling factors ν. The first column refers to the energy of the Laughlin wave function Φ_m, while the remaining four correspond to the fixed-phase φ_m result. In all cases we have used generalized periodic boundary conditions.

		r_s			
ν	Laughlin	1	10	20	30
1/3	-0.4099(2)	-0.4112(2)	-0.4150(2)	-0.4179(2)	-0.4201(2)
1/5	-0.3277(1)	-0.32799(9)	-0.32902(9)	-0.32999(9)	-0.3308(1)
1/7	-0.2810(1)	-0.28118(7)	-0.28164(8)	-0.28214(9)	-0.28262(9)

$$F(\{z_i\}) = \exp[ikZ]\left[\vartheta_1\left(\frac{\pi(Z-Z_l)}{L_1}\middle|\tau\right)\right]^m \prod_{1\le i<j\le N}\left[\vartheta_1\left(\frac{\pi(z_i-z_j)}{L_1}\middle|\tau\right)\right]^m , \tag{11}$$

where ϑ_1 is the first odd elliptic theta function [12],

$$\tau = i\frac{L_2}{L_1}, \quad Z=\sum_{j=1}^{N} z_j, \quad k=\frac{\pi N m}{L_1}, \quad Z_l = N\frac{L_1 - iL_2}{2}$$

(all center-of-mass zeros at the same point). Because of the scaling properties of the Laughlin states with r_s, its kinetic and potential energies will satisfy the virial relation.

As a first check we use the Metropolis algorithm to compute the expectation value of the potential energy. The values are quoted in the first column of Table I where energies are expressed in units of $1/\ell$. We have verified that, up to the sizes considered in our study ($N \sim 400$), finite-size effects are smaller than the statistical error and it turns out, when compared to the results of Ref. [13], that the energy is insensitive to boundary conditions.

At this point, we start our *fixed-phase* computation with the Laughlin phase $\varphi_m = -i\ln[\Phi_m/|\Phi_m|]$. We begin with an ensemble of N_c=200 configurations $\mathcal{R}_i$ ($i=1,\ldots,N_c$) distributed according to $P(\mathcal{R},t=0) = |\Phi_m|^2/\|\Phi_m\|^2$, then diffuse with drift each configuration as $\mathcal{R}_i' = \mathcal{R}_i + \Delta t\,\mathbf{F}(\mathcal{R}_i) + \aleph$, where $\aleph$ is a normally distributed random variable and the role of $\mathbf{F}$ is to guide the random walk towards regions of phase space where the trial function is larger. The total number of configurations is stabilized when E_T equals the mean value of the local energy, which in the large time limit equals the best upper bound to the true ground state energy. The results of this computation (E_0) are shown in Table I for $N=45$ spin-polarized electrons in a square Bravais lattice.

In Fig. 1 we compare (in effective a.u.) the fixed-phase (FP) total energy to the Laughlin (L) and Price *et al.* recently proposed Jastrow-Slater wave function (PPH) for r_s=20. It is clear from the figure that we get a substantial lowering of the liquid energies, which is relevant for studies of the liquid-solid transition.

Figure 2 shows the mixed estimator pair correlation functions defined as $g(r) = [2/\rho(N-1)] \times\langle\sum_i^N\sum_{j\neq i}^N \delta(r-r_{ij})\rangle_{P(\mathcal{R},t\to\infty)}$ for ν=1/7 at different r_s's. The physical picture that emerges is clear, as r_s increases (lower electron densities) more correlation is gained because of a more effective Landau level mixing.

Let us now consider a Wigner crystal state using a phase which breaks explicitly the continuous translational and rotational invariance. To this end, we will consider the simplest trial state: a determinantal wave function

$$\Phi_W = \hat{\mathcal{A}}\prod_{i=1}^{N}\phi_i(\mathbf{r}_i), \tag{12}$$

where $\hat{\mathcal{A}}$ is the antisymmetrization operator and ϕ_i

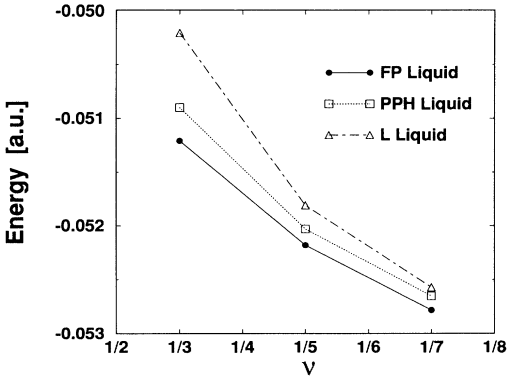

FIG. 1. $E_0-\omega_c/2$ in effective atomic units for the Laughlin liquid at r_s=20. FP stands for *fixed phase*, PPH is the variational state proposed by Price *et al.*, and L corresponds to the Laughlin wave function. The size of the symbols is proportional to the statistical uncertainty and lines are just a guide to the eye.

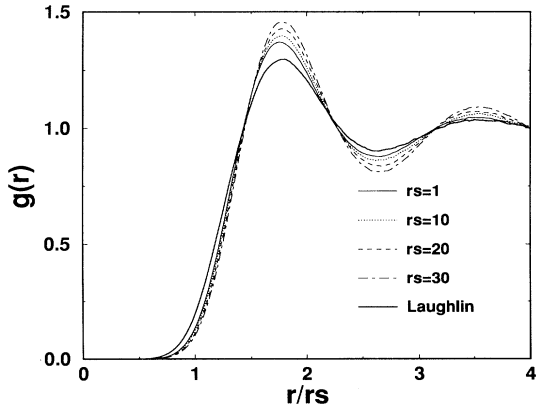

FIG. 2. Mixed estimator pair correlation functions, $g(r)$, at ν=1/7. We also show the one that corresponds to the Laughlin wave function.

single-particle states given by (symmetric gauge) [14,15]

$$\phi_i(\mathbf{r}) = \frac{\beta}{\sqrt{2\pi\ell^2}} \sum_{\mathbf{L}} \exp\left(\frac{-1}{4\ell^2}\left[\beta^2(\mathbf{r}-\mathbf{R}_i-\mathbf{L})^2 - 2i\,(\mathbf{r}\wedge\mathbf{R}_i + \mathbf{r}\wedge\mathbf{L} + \mathbf{R}_i\wedge\mathbf{L})_z\right]\right), \tag{13}$$

with β a variational parameter which fixes the width of the orbital and $\mathbf{R}_i$ points of a regular 2D triangular lattice.

It turns out that, under the assumption of nonoverlapping states $\langle\phi_i|\phi_j\rangle = \delta_{ij}$, the total energy $\langle\Phi_W \mid \widehat{\mathbb{H}}\Phi_W\rangle_\beta$ can be evaluated analytically [10] and minimized with respect to β. The result of this calculation for r_s=20 is shown in Fig. 3 (HFLM) where we compare it to the Lam and Girvin's magnetophonon wave function results (LG) [14].

We have assessed the importance of exchange in the total energy by using the determinantal wave function Φ_W. It is evident that in the low density regime particle exchanges do not affect the total energy (which is mainly Hartree) because of the rapid Gaussian falloff. In particular, we have checked that this is the case for $r_s = 20$. Thus, in order to apply the FP method, we have considered the phase that corresponds to the even simpler unsymmetrized Φ_W state. Our results are described in Fig. 3 for $N = 56$ particles enclosed in a rectangular torus which is commensurate with a triangular lattice. Again, we have verified that finite-size effects are smaller than the statistical uncertainties. It is apparent from the figure that for this simple choice of phase no transition to a WC is observed at $r_s = 20$ in the range of ν's considered.

In a recent paper Zhu and Louie [15] used the variational Monte Carlo method to study the magnetic-field-induced WC in the FQHE regime. The energies they get for the solid phase ($r_s = 20$) are shown in Fig. 3 with the best energy available at the time for the liquid [13] and concluded there would be a transition to the WC for ν=1/5. Our improved energies for the liquid show that further work must be done to show definitively which phase is stable at ν=1/5. We are currently investigating improved FP calculations using phases which include magnetophonon correlations.

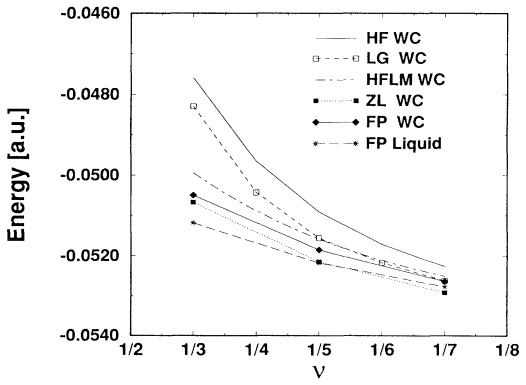

FIG. 3. $E_0 - \omega_c/2$ for the Wigner crystal at r_s=20 resulting from different approximations. Comparison with our FP liquid energy (from Fig. 1) is also given. HF: Eq. (13) for β=1; LG: Lam and Girvin; HFLM : HF for optimized β; ZL: Zhu and Louie.

In conclusion, we have presented a stochastic method able to deal with complex hermitian Hamiltonians. The method uses as a key ingredient a trial phase that plays the role of singular gauge function in the unitary transformation that maps the original fermion problem into a boson one for the modulus of the wave function. We applied these ideas to the 2D electron gas in a magnetic field using two nonequivalent phases: one for the liquid and another for the solid. The present ideas can be easily extended to path integral methods to study the effect of temperature in the stability of the different states of the 2D electron gas. Other possible applications of the *fixed-phase* method include systems with rotational symmetry and fixed angular momentum or systems in a rotating frame.

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