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S.G. Louie

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Steven G. Louie

Department of Physics
University of California

and

Materials Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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Correlated Wavefunction Quantum Monte Carlo Approach to Solids

Steven G. Louie

Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720, U.S.A.

Abstract. A method for calculating the electronic and structural properties of solids using correlated wavefunctions together with quantum Monte Carlo techniques is described. The approach retains the exact Coulomb interaction between the electrons and employs a many-electron wavefunction of the Jastrow-Slater form. Several examples are given to illustrate the utility of the method. Topics discussed include the cohesive properties of bulk semiconductors, the magnetic-field-induced Wigner crystal in two dimensions, and the magnetic structure of bcc hydrogen. Landau level mixing is shown to be important in determining the transition between the fractional quantum Hall liquid and the Wigner crystal. Information on electron correlations such as the pair correlation functions which are not accessible to one-electron theories is also obtained.

1. Introduction

A major issue in calculating accurately the properties of solids from first principles is the treatment of electron-electron interactions or electron correlation effects. With very few exceptions [1-3], modern *ab initio* electronic structure calculations for solids treat this problem using some sort of self-consistent field schemes such as the Hartree-Fock (HF) or the local density functional (LDA) methods. These methods have been successfully applied to study the properties of many materials, but they have also encountered difficulties because of the approximate exchange-correlation functions used. In this paper, we describe some recent advances in using correlated many-electron wavefunction together with quantum Monte Carlo techniques to calculate materials properties. This approach allows treatment of electron-electron interactions in condensed matter systems going beyond self-consistent field schemes.

The present approach [1] employs a wavefunction of the Jastrow-Slater form and the exact Coulomb interaction between valence electrons. We discuss several applications briefly in this short review. For bulk semiconductors, calculations have been carried out for the electronic and structural properties yielding results in excellent agreement with experiment. The method has further been applied to compute quantities such as the electron pair correlation functions and single-particle orbital occupancy which are not accessible in standard self-consistent-field theories.

For the two-dimensional (2D) electron system, we applied the approach to investigate the phenomenon of Wigner electron crystallization. Recent experimental evidence [4,5] indicate that this elusive crystal is perhaps finally observed in 2D electron and hole systems at semiconductor heterojunctions in the fractional quantum Hall regime. The

ground-state energy of a triangular Wigner crystal has been calculated as a function of carrier density, carrier mass, and applied magnetic field. The effects of exchange, correlations, and Landau level (LL) mixing are investigated. Our results show that LL mixing effects significantly alter the critical LL filling factor ν_c for the liquid-solid transition in the regime of experimental parameters.

As a final example, we discuss the magnetic structure and equation of state of bcc solid hydrogen. This is studied as a prototypical Mott system with the long-range Coulomb interaction.

2. Correlated Wavefunction Variational Quantum Monte Carlo Approach

The use of correlated wavefunctions for many-electron systems dated back to the early days of quantum mechanics. The basic idea is to evaluate the ground-state properties of a system using the exact Hamiltonian but with a variational many-electron wavefunction. In the past, for condensed matter systems, various additional approximations had to be introduced to make the evaluation of the wavefunction and various physical quantities tractable. With the advance of Monte Carlo integration algorithms and modern computers, it is now possible to perform calculations on various systems without these further approximations.

In the present studies, the Hamiltonian is of the form

$$H = \sum_{i=1}^N \left\{ \frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}_i) + \frac{1}{2} \sum_{j \neq i} \frac{e^2}{r_{ij}} \right\} \quad (1)$$

where the last term is the exact Coulomb interaction between the electrons. For valence electron properties, the second term which describes the interaction with the cores may be accurately approximated by norm-conserving ionic pseudopotentials [1]. The many-electron wavefunction employed is of the form of an exponential correlation factor, the Jastrow factor, multiplying a Slater determinant of single particles:

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \exp \left\{ \sum_{i=1}^N \chi(\mathbf{r}_i) - \sum_{i < j} u(\mathbf{r}_{ij}) \right\} D(\mathbf{r}_1, \dots, \mathbf{r}_N) \quad (2)$$

where N is the number of electrons in the system. A single particle term χ and a two-particle term u are retained in the Jastrow factor. The two-particle term correlates the motion of the particles so that two electrons may avoid each other dynamically, and the one-particle term allows a relaxation of the charge density distribution in the presence of the multiple-particle correlations. In the calculations, variational parameters enter into χ and u . The exact form of these correlation terms will depend on the system under consideration. However, physical arguments may often be used to constrain their general behaviors [1]. For accurate solid-state properties, simulation cell containing hundreds of electrons with periodic boundary conditions is required. Thus, it is necessary to use Metropolis Monte Carlo integration algorithms [6] in evaluating various physical quantities.

The correlated wavefunction VQMC method has shown to be a viable approach to the studies of electron correlation effects in solids. Calculations have been carried out for the

cohesive and structural properties and correlation functions in various systems [1,3,7,8]. A particularly interesting and important recent application of this approach, which is not easily feasible in other *ab initio* schemes, has been the study of the effects of high magnetic fields [9].

3. Cohesive Properties and Electron Correlations in Solids

A first application of the method described in Sec. 2 to crystals was to the covalent solids. The binding energy and structural properties of carbon- and silicon-based crystals [1] were calculated using simulation cells with periodic boundary conditions containing up to 216 electrons (or 54 atoms). The Slater determinant part of the wavefunction was formed with single-particle orbitals obtained in a LDA calculation with *ab initio* norm-conserving pseudopotentials. A two-particle term of the form $u(r_{ij}) = A[1 - \exp(-r_{ij}/F)]/r_{ij}$ was used with A and F spin-dependent variational parameters. A single-particle term with one variational parameter which permits the valence charge density distribution to relax was also included.

Figure 1 shows the calculated total energy of silicon as a function of lattice constant. The theoretical results are also fitted to a Murnaghan equation of state. A calculated equilibrium lattice constant of $5.40 \pm 0.04 \text{ \AA}$ and a bulk modulus of $108 \pm 10 \text{ GPa}$ are obtained, in very good agreement with the experimental values of 5.43 \AA and 99 GPa , respectively. Similarly accurate results for the structural parameters have been obtained for diamond. The calculated cohesive energies of diamond, graphite, and silicon are presented in Table I. The correlated wavefunction results are in excellent agreement with experiment [10]. In general, Hartree-Fock (HF) calculations significantly underestimate the cohesive energy whereas the LDA calculations tend to overestimate the cohesive energy, typically by 15 - 20% or more. Electron correlation effects, thus, play a very

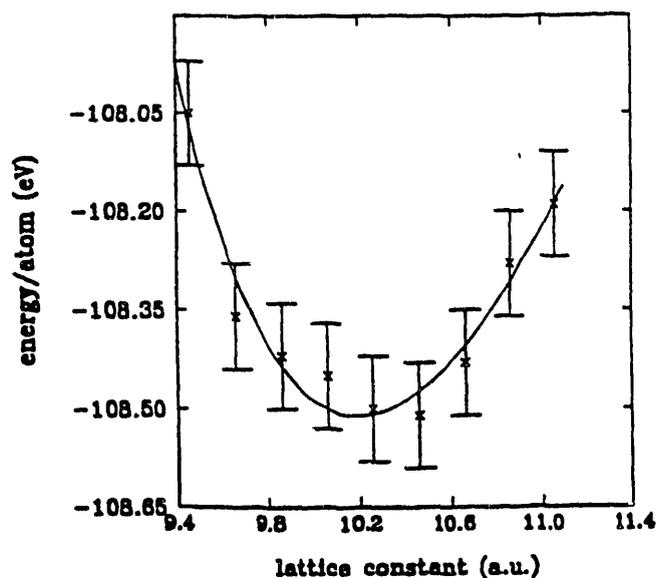


Fig. 1. Calculated energy of silicon (dots) together with a fit to the Murnaghan equation of state (line).

Table I. Calculated cohesive energies (in eV).

	LDA	VQMC	Experiment ^a
Diamond	8.63	7.45(7)	7.37
Graphite	8.65	7.40(7)	7.39
Silicon	5.29	4.81	4.7±0.1

a) Ref. 10

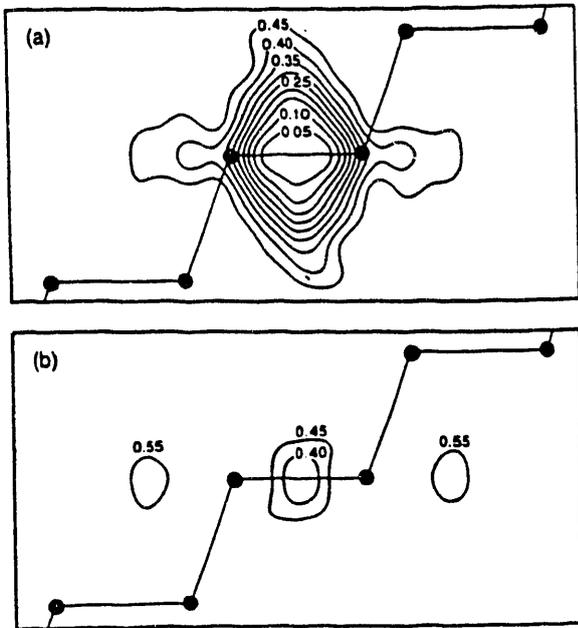


Fig. 2. Pair-correlation function in diamond for (a) parallel spin and (b) opposite spin with one electron at the bond center.

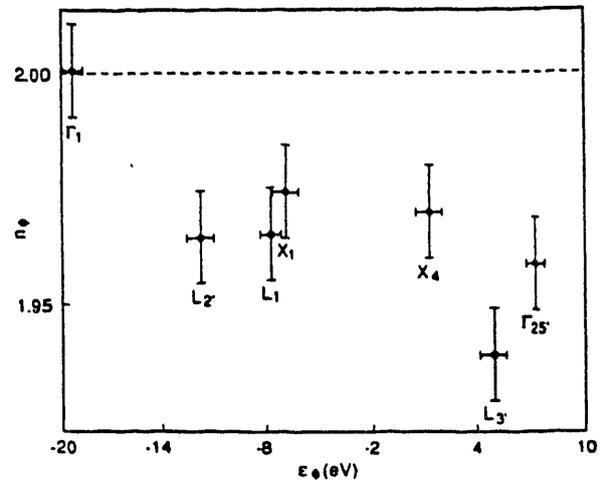


Fig. 3. Occupation of states in diamond below the Fermi level vs the single-mode-approximation energy of the state.

significant role in determining the crystal cohesive energy. For example, the valence electron correlation energy is calculated to be 4.1 eV per atom in diamond but only 2.4 eV for the isolated carbon atom. In general, the correlated wavefunction VQMC calculations yield 90 - 95% of the correlation energy as compared to experiment.

With the wavefunction given in Eq. (2), it is straightforward to compute during the Monte Carlo sampling various quantities such as the single-particle orbital occupation number, the quasiparticle excitation energies within a Feynman single mode approximation, and the electron pair correlation functions [7]. For example, the pair correlation function $g_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2)$ may be evaluate through the relation

$$g(x_1, x_2)n(x_1)n(x_2) = N(N - 1) \int |\psi(r_1 = x_1, r_2 = x_2, \dots, r_N)|^2 dr_3 \dots dr_N \quad (3)$$

where n is the electron number density and spin indices are suppressed. Figure 2 illustrates the calculated pair correlation functions in diamond. Our results for $g_{\alpha\beta}$ of diamond and silicon show that, unlike the uniform electron gas case, g is indeed highly anisotropic and is a sensitive two-point function of \mathbf{r}_1 and \mathbf{r}_2 . Both $g_{\uparrow\uparrow}$ and $g_{\uparrow\downarrow}$ are very rich in structure. For example, as seen in Fig. 2, the correlation hole, $h_{\uparrow\downarrow}(\mathbf{r}) = g_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}) - 1/2$, for \mathbf{r}_1 located at the bond center of diamond has a density distribution which is distinctly related to the structure and covalent character of the material. It is negative near \mathbf{r}_1 , the bond center, as expected, but $h_{\uparrow\downarrow}$ is positive only in the nearby low density antibonding/interstitial regions and not in the neighboring bond centers reflecting the covalent nature of diamond. Since the pair correlation function is intimately related to the

exchange-correlation energy density, information such as those contained in Fig. 2 may be used to gain microscopic understanding of electron correlations in solids.

The occupation number of a single-particle orbital ϕ_i is the i th diagonal element of the matrix

$$n(i, j) = N \int \phi_i^*(\mathbf{r}_1) \psi(\mathbf{r}_1, \mathbf{r}_2, \dots) \psi^*(\mathbf{r}_1', \mathbf{r}_2', \dots) \phi_j(\mathbf{r}_1') d\mathbf{r}_1 d\mathbf{r}_1' d\mathbf{r}_2 \dots \quad (4)$$

The matrix $n(i, j)$ again may be calculated by Monte Carlo evaluation. The quasihole energies within the Feynman single-mode approximation [11] are given by $\epsilon_i = \langle \psi | c_i^\dagger [H, c_i] | \psi \rangle / n(i, i)$, where c_i^\dagger and c_i are the single-particle creation and annihilation operators for the state ϕ_i , and $[H, c_i]$ is the commutator of the many-body Hamiltonian with the annihilation operator. This approximation depends for its success on the renormalization of the quasiparticle peak in the spectral distribution being negligible.

Some calculated single-particle orbital occupation numbers of the LDA orbitals (which have been shown to be virtually identical to the quasiparticle wavefunction [13]) versus corresponding quasihole energy for diamond are shown in Fig. 3. Complete occupation of a state would give an occupation number of 2. The results show the expected trend of lower occupation as one goes nearer the Fermi level, but the trend is not monotonic. The theoretical bandwidth is 25.4 ± 0.8 eV, in good agreement with the x-ray photoemission spectroscopy measurement [12] of 24.2 ± 1 eV but somewhat larger than other quasiparticle calculations [13].

4. Wigner Crystallization in the Fractional Quantum Hall Regime

In this section, we discuss the effects of exchange, correlations, and Landau level mixing to the ground-state energy of a triangular electron crystal in a perpendicular magnetic field [9]. In 1934, Eugene Wigner pointed out that, in the jellium model, electrons will crystallize at sufficiently low densities owing to the Coulomb repulsion which tends to localize the electrons. This quantum phase transition as a function of density at $T = 0$ has yet to be observed in three dimensions. However, there are several recent experiments [4,5] indicating that in the fractional quantum Hall regime, because of the strong localizing effect of the external applied magnetic field, Wigner crystallization is perhaps finally observed in 2D electron and hole systems at semiconductor heterojunctions.

The 2D electron or hole gas in a strong magnetic field, realizable experimentally in a MOSFET or a semiconductor heterojunction, exhibits a rich variety of phenomena [14]. By varying the carrier density, the carrier effective mass, and the strength of the external magnetic field, a very intricate phase diagram is expected. Among the various possible phases are the incompressible quantum Hall liquid phase and the Wigner crystal phase. Although the experimental evidence for the Wigner crystal phase are still being scrutinized, the observed re-entrant behavior to an insulating phase near Landau level filling factor $\nu = 1/5$ for n-type samples [4] and near $\nu = 1/3$ for p-type samples [5] of GaAs/AlGaAs junctions of comparable carrier densities have been interpreted as evidence for pinned Wigner crystals.

Exchange-correlation effects in 2D systems are fundamentally affected by the presence of a strong perpendicular magnetic field. For example, at fractional filling factors, particles can and prefer to correlate with each other to lower the interaction energy at no cost to the

kinetic energy owing to the high degeneracy of the Landau levels. The presence of a strong B field introduces a new length, the magnetic length given by the radius of the Larmor orbit $l_B^2 = \hbar c/eB$, and a new energy, the cyclotron frequency $\omega_c = eB/m^*c$, into the problem. Both quantities are independent of the carrier density. Crystallization is expected when l_B is less than the inter-electron distance d , that is, in the regime of $\nu < 1$. Landau level mixing is expected to be important when the electron-electron interaction energy $E_{\text{coul}} = e^2/\epsilon d$ is comparable to or larger than the inter-LL spacing $\hbar\omega_c$. There are, therefore, three important materials parameters in determining the ground state: the density n , the effective mass m^* , and the applied B field. The system is characterized by two independent dimensionless quantities which are the filling factor ν which is a function of n and B and the electron gas parameter r_s which is a function of n and m^* . There have been many studies on B-field induced Wigner crystals in 2D [14-18]. Most of these were carried out, however, within the Hartree-Fock approximation. With few exceptions [18], only the lowest Landau level is considered.

In our simulation, the usual periodic boundary conditions cannot be directly applied for electrons in a strong applied B field due to the aperiodic vector potential in the Hamiltonian. For example, in the symmetric gauge $\mathbf{A} = (-yB/2, xB/2)$ for a uniform field. The appropriate translational symmetry may be recovered by introducing the concept of rational fields [19] and noting that the physics of the system should be gauge invariant and that a finite translation in the present case is equivalent to a gauge transformation. These symmetry properties allow us to perform simulation with modified periodic boundary conditions in a magnetic field.

Our trial wavefunctions for the Wigner crystal are still in the general Jastrow-Slater form of an exponential correlation factor multiplying a function of the single-particle orbitals. The single-particle orbitals are chosen to be Gaussians localized about the lattice sites:

$$\phi_j(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \frac{\beta}{l_B} \sum_{\mathbf{T}} \exp \left\{ -\frac{\beta^2}{4l_B^2} (\mathbf{r} - \mathbf{R}_j - \mathbf{T})^2 + \frac{i}{2l_B^2} [x(\mathbf{R}_j^y + \mathbf{T}^y) - y(\mathbf{R}_j^x + \mathbf{T}^x)] \right\} \quad (5)$$

Here β is a variational parameter involving LL mixing and to be optimized. For $\beta = 1$, Eq. (5) corresponds to a wavefunction in the lowest LL localized on a lattice site \mathbf{R}_j with the proper phase factors resulting from the use of a symmetric gauge at the origin. (The \mathbf{T} 's in Eq. (5) are translation vectors of the simulation cells associated with the periodic boundary conditions used.) All calculations reported are done for spin-aligned electrons with a 100-electron simulation cell. Tests show that the resulting finite effects are smaller than the statistical noise in the results.

We first summarize the results from wavefunctions which are made up of functions only from the lowest Landau level with either exchange or correlations included and then discuss next the effects of LL mixing. This first part of the discussion serves to make contact with earlier work and to establish the validity of the correlated wavefunction VQMC method. Our exchange-only (or HF) results are obtained by using a wavefunction which is just a Slater determinant of the single-particle orbitals given above with $\beta = 1$. The correlation-only results are calculated for distinguishable particles (again, with $\beta = 1$ for the orbitals) with the Jastrow correlation factor derived from the consideration of the magnetophonons similar to the work of Lam and Girvin [16]. In the large field limit, this Jastrow factor may be written as an analytic function of the complex variables which describe the position of the particles in 2D. Hence, in both calculations, there is no mixing

in of higher LL's into the ground-state wavefunction by construction, and the kinetic energy per electron is trivially given by $\hbar\omega_c/2$.

The exchange-only and correlation-only results with no LL mixing are presented in Fig. 4 by the curves with the triangle and square symbols, respectively. Previously, the most accurate energies for the 2D electron system in a strong magnetic field in the exchange-only approximation were calculated from the viewpoint of charge density waves (CDW) [15] rather than the explicit Wigner crystal wavefunction used here. Our present HF results are extremely close to the CDW results. Thus, little is gained by the explicit self-consistency procedure used in the CDW approach.

Our correlation-only results with no LL mixing are the same as those obtained by Lam and Girvin [16] who used a special k-point sampling scheme in calculating the energy rather than the VQMC method. In this approximation, the Wigner crystal is considered as distinguishable particles correlated by the magnetophonons. Thus, although it contains correlation effects, exchange interaction is ignored. As noted in Ref. 16, at $\nu = 1/2$, the correlation-only result is, in fact, higher in energy than the HF result due to the rather large exchange interaction at this filling factor. However, a comparison of the Hartree, the exchange-only, and the correlation-only energies in the lowest LL approximation shows that correlation effects dominate over exchange in the range of $\nu \lesssim 1/3$. The energies for the Laughlin state taken from Ref. 17 are given by the dashed curve with the hexagon symbols in Fig. 4. Thus, within the lowest LL approximation, the cross-over from the liquid state to the solid state is $\nu_c \approx 1/6.5$ as found by Lam and Girvin.

Now let us discuss the effects of Landau level mixing. Our work is motivated by the recent experimental work on the 2D hole systems [5] which indicates the occurrence of a Wigner crystal phase around $\nu = 1/3$. This earlier transition from that of the electron case is ascribed to a larger LL mixing due to the heavier hole mass in GaAs. Even for the electron systems, the electron interaction energy is comparable to the cyclotron frequency. Relevant measure of the importance of LL mixing is the ratio $E_{\text{coul}}/\hbar\omega_c = \nu r_s/2$. A higher value for the ratio indicates a strong LL mixing. For typical 2D electron systems $r_s \sim 2$, but for the 2D hole system investigated, $r_s \sim 13 - 25$ depending on the assumed hole effective mass [5,20].

Admixture of higher LL orbital to the ground state allows a lowering of the interaction energy at the expense of the kinetic energy. Because of the Coulomb repulsion between electrons on neighboring sites, it is energetically favorable to have (1) a charge density distribution more localized than the one given by single-particle orbitals in the lowest Landau level and (2) a nonanalytic correlation term u in the Jastrow factor which optimizes the dynamical short-range avoidance of two electrons. These are the driving mechanisms for Landau level mixing. We put in these two effects by optimizing the energy with respect to the parameter β in Eq. (5) and by adding to the magnetophonon correlation factor a term of the form $u(r) = A[1 - \exp(-\sqrt{r}/F - 1/2 r/F)]/\sqrt{r}$ where r is the distance between two electrons. Both deviation of β from 1 in the single-particle orbitals and the additional term in the Jastrow exponent correspond to admixture of higher LL's into the wavefunction, and one needs to evaluate both the kinetic and interaction energies. The changes in energy and in the localization of the electrons due to LL mixing can be quite large in the range of $\nu = 1/2 - 1/5$ depending on the value of r_s . For example, at $\nu = 1/3$, with just an optimization in the parameter β , we find an increase in density at the lattice site by $\delta\rho(0)/\rho(0) = 70\%$ and an lowering in energy by $\delta E/(E - \hbar\omega_c/2) = -4.4\%$ at $r_s = 20$ whereas at $r_s = 2$ the same two quantities are 10% and -0.8%, respectively. With the LL-mixing Jastrow factor, the total energy is lowered even further.

The final results with full LL mixing and magnetophonon correlations for the case of $r_s = 20$ are given in Fig. 4 as the solid curve. The parameters used in the calculation correspond roughly to those in the experiment on the 2D hole systems [5]. We see that there is a dramatic lowering in energy by allowing LL mixing in the range of ν of experimental interest. At $r_s = 20$, LL mixing effects are, in fact, larger than those of intralevel exchange-correlation effects. And as seen in Fig. 4, the Wigner crystal energy curve lies entirely below the Laughlin wavefunction energies at $r_s = 20$ for the whole range of ν considered. This is not an accurate comparison of the energy of the two phases because the Laughlin wavefunction [17] does not include higher LL's. There is, however, a recent VQMC calculation [21] on the fractional quantum Hall liquid using a Laughlin-like wavefunction but included LL mixing. The calculations were carried out on a sphere with a LL-mixing correlation term in the Jastrow factor. Their results for the case of $r_s = 20$ are presented in Fig. 4 by the cross symbols. As expected, LL mixing does not affect the liquid phase as much as the solid phase. Comparison of the two calculations shows that the liquid-solid transition occurs near $\nu = 1/3$. Thus, our results give quantitative support to the observation that, because of LL mixing effects, 2D hole systems at GaAs/AlGaAs interface crystallize at a larger ν than 2D electron systems at comparable densities.

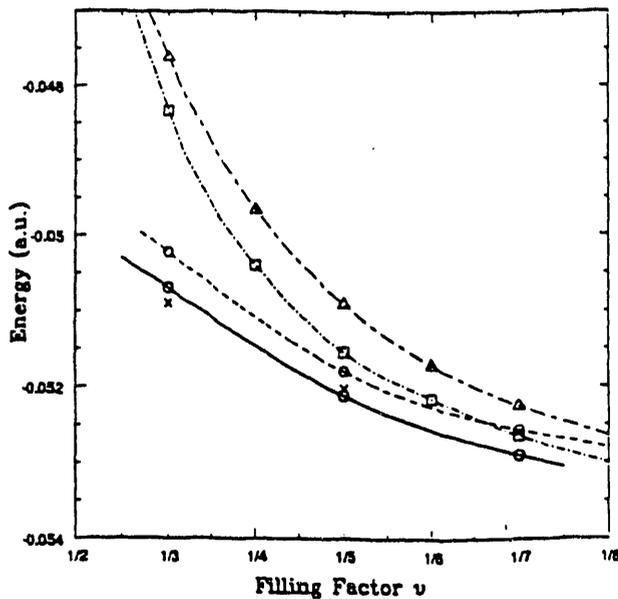


Fig. 4. Calculated Wigner electron crystal energy $E - \hbar\omega_c/2$ using exchange only with no LL mixing (Δ), correlations only with no LL mixing (\square), correlations with LL mixing for $r_s = 20$ (---). The energy of the Laughlin liquid (Ref. 17) is given by the dashed curve, and the energies for the liquid with LL mixing (Ref. 21) are given by the crosses.

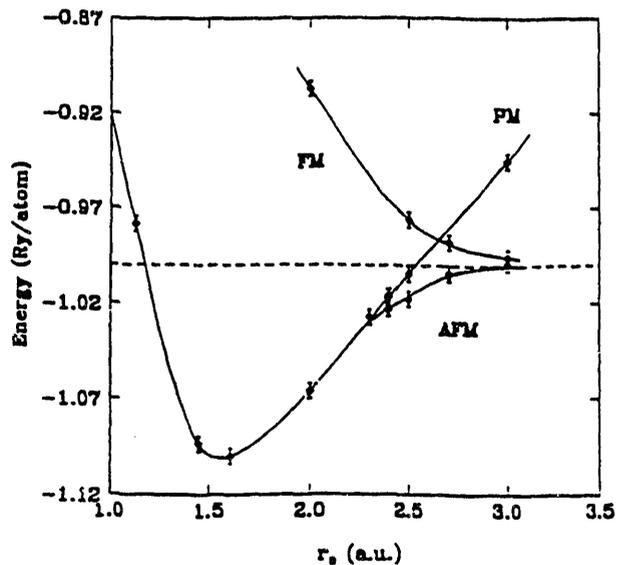


Fig. 5. Energy vs. density for three magnetic structures of bcc hydrogen. The dashed line is the energy of an isolated hydrogen atom.

5. Magnetic Structure of BCC Hydrogen

The present approach has also been applied to study the equation of state and magnetic structure of bcc solid hydrogen [8,22]. Various forms of the wavefunction have been used to investigate the relative stability of the paramagnetic (PM) state, the antiferromagnetic (AFM) state, and the ferromagnetic (FM) state as a function of the lattice constant. The calculations were carried out at densities between Wigner-Seitz radius of $r_s = 1.0$ to 3.0 a.u.

The results of the 54-atom simulation cell calculations [8] are presented in Fig. 5. Most of the interesting features occur between $r_s = 2.0$ and $r_s = 3.0$. An earlier LDA study [23] suggested that both the magnetic and metal-insulator transitions occur in this region. Our results show that the fully FM phase is unbound at all densities which is analogous to the unbound hydrogen molecule in a spin-triplet electronic state. Among the magnetic structures considered, the PM phase is the ground state for r_s less than 2.2, and its energy rises above the fully FM phase at $r_s = 2.7$. Contrary to some previous work [23,24], we did not find any indication of a stable partial-FM phase at the densities considered.

Our results show a transition from PM to AFM phase at $r_s = 2.2$. At this density the system also undergoes a metal-insulator transition with an energy gap opening up in the excitation spectrum. The present transition density of $r_s = 2.2$ is significantly different from previous LDA [23] or self-interaction corrected LDA [24] calculations. Also, as for other materials, the cohesive energy is significantly overestimated in the LDA calculation. For example, at $r_s = 3.0$, the LDA calculations found that the AFM phase is bound by 15 mRy/atom while our VQMC results show that the binding is less than 1 mRy/atom.

6. Summary

We have described a correlated wavefunction variational quantum Monte Carlo method for calculating the total energy and related properties of solids. Highly accurate cohesive and structural properties, as well as quantities such as the electron pair correlation functions, have been obtained for carbon- and silicon-based crystals. The energetics of the magnetic-field-induced Wigner crystal in 2D in the fractional quantum Hall regime has also been investigated. Landau level mixing effects are shown to be very important in the range of density and magnetic field strength of experimental interest. The results provide an explanation for the recent observation of a re-entrant insulating transition near $\nu = 1/3$ for 2D hole systems at GaAs/AlGaAs interfaces. We also investigated the magnetic structure and metal-insulator transition in bcc hydrogen as a function of density. The present approach is shown to be quite versatile and provides a viable new avenue for computing the properties of and studying the electron-electron interactions in a variety of solid-state systems.

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