Energy spectrum and structure of one-dimensional few-electron Wigner crystals with and without coupling to light in cavity

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Explicitly Correlated Gaussian basis is used to calculate the energies and wave functions of one dimensional few-electron systems in confinement potentials created by external potentials or coupling to light in cavity. The appearance and properties of Wigner crystal-like structures are discussed. It is shown that one dimensional Wigner crystals can be formed by coupling electrons to light due to the dipole self-interaction term in the light-matter Hamiltonian, provided an additional extremely weak confining potential is present.

I. INTRODUCTION

A Wigner crystal is a solid phase of electrons, predicted by Eugene Wigner in 1934. If an electron gas has a low enough density in a uniform, neutralizing background, the system can crystallize through the formation of an electron lattice, driven by Coulomb interaction.

Experimental study of Wigner crystals is hindered by the fact that low electron densities have to be reached in the presence of defects and impurities. Nevertheless, Wigner crystals have been experimentally demonstrated in liquid Helium2 and semiconductor heterostructures.3 These experiments have led to intense theoretical work focusing on energetics and structures of Wigner crystals.

Recently, there is a renewed interest in Wigner crystals after experimentally imaging them in Moire superlattices4 and one-dimensional (1D) systems.5,6 These new systems emerge as a highly conducive platform to study strong electronic correlations as well as topology. The most interesting experimental example of 1D Wigner crystals is found in carbon nanotubes. In this experiment, the signatures of N=1 to N=6 electron crystals are clearly identified.

In this work, we will investigate the role of the electronic correlations and long range Coulomb interactions in the formation of the 1D Wigner crystals using explicitly correlated basis functions that are especially suitable to represent the wave functions of few-electron systems. One-dimensional Wigner crystals have been studied using the bosonisation method, with an effective Hamiltonian and the configuration interaction (CI) approach (see a recent review highlighting other approaches). In this paper we complement these works with a more accurate approach that includes the full Coulomb Hamiltonian, using correlated basis functions to avoid the convergence issues of CI calculations, and addressing the structure of spin configurations.

The Wigner crystals are formed in external confining potentials. An alternative possibility to confinement is the use of electrons interactions with cavity photons. The dipole self-polarization term, \( \frac{1}{2} (\vec{\lambda} \cdot \vec{R})^2 \) (where \( \vec{\lambda} \) is the interaction strength and \( \vec{R} \) is the dipole moment), of the light-matter interaction Hamiltonian creates a harmonic oscillator-like confinement. We will show that coupling a very weakly confined few-electron system to light in cavity leads to tightly localised Wigner crystal structures. Such systems have not yet been experimentally discovered, but carbon nanotubes have been studied in microwave cavities, and coherent spin states in carbon nanotubes coupled to cavity photons have been investigated. Other 1D systems confined in parabolic potentials or 1D optical lattices in cavity have also been studied.

1D systems have been used as test cases mimicking more complicated dynamics because numerical solutions are easier in 1D. This interest is intensified with the investigation of light-matter coupling, where the representation of the coupled light-matter wave function requires the high dimensional product of spatial and photon bases. Restricting the nuclear or electronic motion to 1D makes model calculations feasible. Our calculations might help to improve these 1D model calculations and extend them to more complicated cases.

The ground state energies and wave functions will be calculated using Explicitly Correlated Gaussian (ECG) basis functions. The basis parameters have been optimized using the stochastic variational approach (SVM). The advantage of the approach is that the matrix elements are analytically available and it produces very accurate energies and wave functions. This method has been used to describe excitonic complexes and two and three-dimensional quantum dots.

We will compare our results to density functional theory (DFT) calculations. Spin-polarized DFT calculations have often been used to analyze the structure and energetics of two-dimensional confined electron systems and Wigner crystals. In this work, we will investigate how well the DFT densities approximate the accurate few-particle results. The advantage of the DFT is that it can easily be extended for larger systems while our ECG approach scales with \( N! \) due to the explicit antisymmetrization of the \( N \) electron wave function, which reduces the application to small systems.
II. FORMALISM

A. Few-electron system in an external confining potential in 1D

The Hamiltonian of an N electron system interacting with a Coulomb interaction and confined in an external potential Vc reads as

\[ H_c = -\frac{1}{2} \sum_{i=1}^{N} \frac{\partial^2}{\partial r_i^2} + \sum_{i<j}^{N} V(x_i, x_j) + \sum_{i=1}^{N} V_c(x_i), \]  

(2.1)

where \( x_i \) is the coordinate of the \( i^{th} \) electron, and atomic units are used. Due to the singular nature of the Coulomb potential, a soft Coulomb potential will be used

\[ V(x_i - x_j) = \frac{1}{\sqrt{(x_i - x_j)^2 + 1}}, \]  

(2.2)

and the confining potential is either quadratic \( V_c(x) = \frac{1}{2} \omega^2 x^2 \), or quartic \( V_c(x) = \frac{1}{4} \omega^2 x^4 \). Similar potentials are used in Ref.\cite{55}.

The wave function is a Gaussian shifted into position \( s_i \). By optimizing the center \( s_i \) and the width \( \beta_i \), one can describe the position of particle \( i \). The

\[ e^{-\beta_i (x_i - s_i)^2} \]  

(2.4)

function is a Gaussian shifted into position \( s_i \). By optimizing the center \( s_i \) and the width \( \beta_i \), one can describe the position of particle \( i \). The

\[ e^{-\frac{1}{2} \sum_{i < j}^N \alpha_{ij}(x_i - x_j)^2} \]  

(2.5)

part can be used to represent the correlation between particles \( i \) and \( j \). The \( N \) electron wave function then can be written as

\[ \Psi(\vec{x}) = \sum_{k=1}^{K} c_k \psi_k(\vec{x}), \]  

(2.6)

where \( K \) is the dimension of the basis. The linear coefficients, \( c_k \), can be determined by diagonalization, and the nonlinear ones are optimized by SVM. In the SVM, the nonlinear parameters are optimized by randomly generating a large number of candidates and selecting the ones that give the lowest energy\cite{55,36}. The size of the basis can be increased by adding the best states one by one and a \( K \) dimensional basis can be refined by replacing states with randomly selected better basis functions. This approach is very efficient in finding suitable parameters in high dimensional spaces.

B. Few-electron system in 1D coupled to photons in cavity

In this case the Hamiltonian is given by

\[ H = H_e + H_{ph} = H_e + H_p + H_{ep} + H_d. \]  

(2.7)

\( H_{ph} \) describes the electron-photon interaction and \( H_e \) is the same electronic Hamiltonian as in the previous section. The electron-photon interaction can be described by using the Pauli-Fierz (PF) non-relativistic QED Hamiltonian. The PF Hamiltonian can be rigorously derived\cite{33,52,55} by applying the Power-Zienau-Woolley gauge transformation\cite{50}, with a unitary phase transformation on the minimal coupling (\( p \cdot A \)) Hamiltonian in the Coulomb gauge

\[ H_{ph} = \frac{1}{2} \sum_{\alpha=1}^{M} \left[ \frac{\partial^2}{\partial p_\alpha^2} + (\omega_\alpha p_\alpha - \lambda_\alpha X)^2 \right], \]  

(2.8)

where \( X = \sum_{i=1}^{N} q_i x_i \) is the dipole operator (\( q_i = -1 \) is the electron charge). This Hamiltonian describes \( M \) photon modes with elongation \( p_\alpha \), frequency \( \omega_\alpha \), and polarization \( \lambda_\alpha \). The sum can be decomposed into sum of a photonic part \( H_p \), dipole self-interaction \( H_d \), and \( H_{ep} \) that describes the light–matter interaction in the electric-dipole form. The photonic part is

\[ H_p = \sum_{\alpha=1}^{M} \left( -\frac{1}{2} \frac{\partial^2}{\partial p_\alpha^2} + \frac{\omega_\alpha^2}{2} p_\alpha^2 \right) = \sum_{\alpha=1}^{M} \omega_\alpha \left( \hat{a}_\alpha^+ \hat{a}_\alpha + \frac{1}{2} \right), \]  

(2.9)

where \( \hat{a}_\alpha = \sqrt{\frac{\omega_\alpha}{2}} \left( p_\alpha - \frac{\partial}{\partial \omega_\alpha} \right) \) is the annihilation operator, and \( \hat{a}_\alpha^+ = \sqrt{\frac{\omega_\alpha}{2}} \left( p_\alpha + \frac{\partial}{\partial \omega_\alpha} \right) \) is the creation operator. With the introduction of the creation and annihilation operators, the photon states \( |n_\alpha \rangle \) can be generated by multiple applications of the creation operators on the vacuum state \( |n_\alpha \rangle = (\hat{a}_\alpha^+)^n |0 \rangle \), and all other photon operations can be done by using \( \hat{a}_\alpha \) and \( \hat{a}_\alpha^+ \). The interaction term is

\[ H_{ep} = -\sum_{\alpha=1}^{M} \omega_\alpha p_\alpha \lambda_\alpha X = -\sum_{\alpha=1}^{M} \sqrt{\frac{\omega_\alpha}{2}} (\hat{a}_\alpha + \hat{a}_\alpha^+) \lambda_\alpha X. \]  

(2.10)

Note that \( \hat{a}_\alpha \) and \( \hat{a}_\alpha^+ \) only connect photon state \( |n_\alpha \rangle \) to \( |n_\alpha \pm 1 \rangle \), and the matrix elements of the dipole operator \( X \) are only nonzero between spatial basis functions of angular momentum \( l \) and \( l \pm 1 \). The strength of the electron-photon interaction is described by the effective coupling parameter

\[ g_\alpha = |\lambda_\alpha| \sqrt{\frac{\omega_\alpha}{2}}. \]  

(2.11)

The dipole self-interaction is

\[ H_d = \frac{1}{2} \sum_{\alpha=1}^{M} (\lambda_\alpha X)^2, \]  

(2.12)
which describes how the polarization of the electrons acts back on the photon field. The importance of this term for the existence of a ground state is discussed in Ref. 52.

We will only consider one photon mode and the wave function in this case will be defined as

$$\Psi(\vec{x}) = \sum_n \sum_{k=1}^{K_n} c_k \psi^n_k(\vec{x})|n\rangle,$$  \hspace{1cm} (2.13)

where $\psi^n_k$ is the spatial basis function belonging to an $n$ photon state and $|n\rangle$ is the photon state. The summation over $n$ includes photon states that significantly lower the energy. $K_n$ is the dimension of the basis belonging to photon state $|n\rangle$.

The necessary matrix elements can be analytically calculated for both the spatial and the photon parts. Note that the basis functions in Eq. (2.13) do not have definite angular momentum quantum numbers. During the optimization, the symmetry of the Hamiltonian will dictate the selection of basis functions with appropriate symmetry. For example, if the Hamiltonian is spherically symmetric (which is not true in the present case due to the interaction with the photons), then the wave function converges to $L = 0$ angular momentum for the lowest state. In principle, one can use Wigner rotation matrices to project out good angular momentum functions, but in our present case many angular momentum states will be coupled with the photons and we will let SVM to select the proper ground state.

C. Density functional approach

In DFT, the Hamiltonian is defined as

$$H_e = -\frac{1}{2} \frac{d^2}{dx^2} + V_H[\rho(x)] + V_{ex}[\rho(x)] + V_c(x),$$  \hspace{1cm} (2.14)

where $V_{ex}$ is the exchange-correlation potential and $V_H$ is the Hartree potential. The local density approximation (LDA) is used for the exchange-correlation potential\textsuperscript{57} and the Hartree potential is defined as

$$V_H[\rho(x)] = \int \int \rho(x')V(x-x')dx',$$  \hspace{1cm} (2.15)

where $V$ is the soft Coulomb potential defined in Eq. (2.2). The solution of the eigenvalue problem of the DFT Hamiltonian

$$H_e \phi_i(x) = c_i \phi_i(x)$$  \hspace{1cm} (2.16)

gives the Kohn-Sham orbitals and the density is calculated as

$$\rho(x) = \sum_{i=1}^N \phi_i(x)^2.$$  \hspace{1cm} (2.17)

In this case we solve the eigenvalue equation on a numerical grid with 400 grid points and 0.1 a.u. grid spacing.
FIG. 2: Electron density of the three electron system. Top $S=1/2$, bottom $S=3/2$, left $\omega = 1$ a.u., right $\omega = 0.1$ a.u. The solid curve is calculated by ECG; the dashed line is by DFT.

FIG. 3: Electron density of the four electron system. Top $S=0$, middle $S=1$, bottom $S=2$, left $\omega = 1$ a.u., right $\omega = 0.1$ a.u. The solid curve is calculated by ECG; the dashed line is by DFT.
III. RESULTS AND DISCUSSION

A. Electrons in a harmonic confinement

The DFT and ECG results are compared in Figs. 1-5 for N=2-6 particle systems with different spin configurations. The ECG results are well converged and can be considered as benchmark calculations, the DFT calculations seem to provide good approximations to the electron density in certain cases. We have tried two different confinement potentials. The first potential, \( \omega = 1 \) a.u., is strong and confines the electrons into a [-5,5] a.u. box (high electron density). The second one, \( \omega = 0.1 \) a.u., confines the electrons into a [-20,20] a.u. box. We also have calculations for \( \omega = 0.01 \) which roughly correspond to a [-80,80] a.u. box but the results are not significantly different from the \( \omega = 0.1 \) a.u. results. Besides the quadratic confinement, we have also tested quartic confinement, but we did not observe any important change in the tendencies.

The two electron density (Fig. 4) does not show two peaks for strong confinement for \( S = 0 \), but the two peaks appear for the weaker case. In the spin-polarized \( S = 1 \) case we have two peaks for strong and weak confinements because the Pauli and the Coulomb repulsion together are strong enough to localize the electrons. The localization is naturally more significant in the weak confinement case, which is shown by the increased distance and the lower density between the density peaks. The two peak structure does not disappear when the strength of the confinement increases; for \( \omega = 20 \) a.u. the electrons are squeezed into a [-1,1] a.u. interval, but the two peaks are present in the spin-polarized case. The reason is simple: in the case of very strong confinement, the single particle
states of the confining potential determine the structure of the system and the Coulomb contribution is negligible. The two spin-polarized electrons have to occupy different orbitals, the first is the ground state and the second is the first excited state. The ground state is node-less, the first excited state has one node and is more extended in space than the ground state. The density, the sum of the square of the two wave functions, will always have two peaks coming from the first excited state.

The contributions of the kinetic, Coulomb, and confinement part to the total energy are shown in Table I. For very strong confinement ($\omega = 20 \text{ a.u.}$) the lowest single particle energy of the harmonic confinement is $E_0 = \frac{1}{2} \hbar \omega = 10 \text{ a.u.}$, and the energy of the first excited...
state is \( E_1 = \frac{3}{2} \hbar \omega = 30 \text{ a.u.} \). As we have discussed above, for \( S = 0 \) the two electrons can occupy the lowest state, and the calculated kinetic energy 9.99 a.u. and the confinement energy 10.01 a.u. (for a harmonic oscillator, the kinetic and potential energy contributions are equal according to the virial theorem) show that this is the case. For the spin-polarized case the electrons occupy the first two states and the energy contribution is equal to 20 a.u. for the kinetic and harmonic part. The Coulomb contribution is nearly equal in both the \( S = 0 \) and \( S = 1 \) cases, but it is very small compared to the kinetic and harmonic contributions. For \( \omega = 1 \text{ a.u.}, E_0 = 0.5 \text{ a.u.}, \) and \( E_1 = 1.5 \text{ a.u.}, \) the single particle dominance is much less, the kinetic and confinement energy contributions are not equal to 0.5 a.u. (\( S = 0 \)) and 1 a.u. (\( S = 1 \)), and the Coulomb energy is significant compared to the other terms. For weaker confinements the Coulomb energy becomes the largest term (about half of the total energy) and the kinetic energy becomes very small.

Similar arguments are true for spin-polarized states with \( N=3,4,5,6 \) electron number cases shown in Figs. 2 and 5. In particular, each spin-polarized case with \( N \) particles exhibits \( N \) density peaks regardless of the confinement, for a similar reason as in the two electron case. For example, for \( N=6 \) the first 6 states with increasing number of nodes are occupied, each contributing to the density. However, the number of density peaks does not necessarily agree with the number of particles in mixed-spin systems and cannot be readily determined in a simple way. As before, the electron density is more localized in the stronger confinements in most cases. Quartic or other forms of confinement do not change the shapes too much and the nodal structure is still the same. This 1D picture is significantly different from the 2D or 3D cases where several single particle states are degenerate and the electrons can be placed in different spatial configurations.

Both the 3 and 4 electron systems can show a single peak (see Figs. 2 and 5) in mixed-spin cases if the confinement is strong. The two density peaks in the \( S = 0, \omega = 1 \) case of \( N = 4 \) can be easily explained. There are two electrons with up spins and two with down spins and the distinguishable particles can occupy the same spatial regions. In the \( S = 1, \omega = 1 \) case of \( N = 4 \), there is one peak with two shoulders. In this case, most likely an up-down electron pair occupies the middle region, and the two remaining electrons with spin up are on the outer region forming the shoulders.

The structure in \( N = 5 \) and \( N = 6 \) cases can be understood using similar arguments to the \( N = 3,4 \) cases. One can also think of these as a structure formed by an \( N = 3 \) or \( N = 4 \) system by adding two electrons. For example, the middle peak in the \( S = 3/2, \omega = 1 \text{ a.u.}, \) \( N = 5 \) case is very similar to the \( S = 1/2, \omega = 1 \text{ a.u.}, N = 3 \) density, with two electrons added forming the outer shoulders. The same is true for \( S = 2, \omega = 1 \text{ a.u.}, N = 6 \) comparing with \( S = 1, \omega = 1 \text{ a.u.}, N = 4 \).

The DFT and ECG densities are in very good agreement for \( \omega = 1 \). For weaker confinements the agreement is not as good, probably because the LDA is not a good approximation for low densities where the Coulomb interaction plays a more pronounced role. For spin-polarized systems the DFT density remains close to the ECG even for weaker confinements.

Table I shows the energy of the \( N=2-6 \) systems for ECG and DFT. Besides general trends no agreement is expected, and the DFT with LDA is not close to accurate ECG energies for small atoms like H, He, or Li either. The general trends, however, are similar. For example, energy orders of different spin states are predicted to be the same by ECG and DFT, especially for strong confinements. One particular failure of DFT is the negative energy for the \( N = 2, S = 1 \) case and this clearly shows that one needs to go beyond LDA. Due to the shell structure, the energies of different spin states are very different in cases of strong confinements, but for weak confinements the energies are nearly degenerate.

### B. Electrons in a cavity

In figures 7-10 we further present our results of ECG calculations for \( N=2-4 \) electron Wigner crystals formed and controlled by light-matter coupling. In these systems we use a weak harmonic oscillator confining potential (\( \omega = 0.1 \text{ a.u.} \)). Although this confinement allows the density to spread out far away from the center, the interaction of these systems with light strongly squeezes the density toward the center.

We test the systems for three different \( \omega \)’s (photon frequency) and different coupling strengths. The first strong coupling \( \lambda = 1 \) confines the system into a [-5,5] a.u. box; the second moderate coupling \( \lambda = 0.1 \) confines the system into a [-10,10] a.u. box; and the weakest \( \lambda = 0.01 \) forces the system into a roughly [-12,12] a.u. box. In this case we do not make comparison with DFT because the LDA based DFT does not produce meaningful results. Only selected spin states are included, as

| \( \omega \) | \( T \) | \( V \) | \( V_c \) | \( E \) |
|---|---|---|---|---|
| S=0 | 0.01 | 0.007 | 0.032 | 0.025 | 0.069 |
| 1.0 | 0.44 | 0.76 | 0.57 | 1.77 |
| 20.0 | 9.99 | 0.97 | 10.01 | 20.97 |
| S=1 | 0.01 | 0.007 | 0.032 | 0.025 | 0.069 |
| 1.0 | 0.92 | 0.54 | 1.09 | 2.55 |
| 20.0 | 20.0 | 0.94 | 20.00 | 40.94 |

**Table I**: Energy contributions (in atomic units) for a two electron system as a function of the confinement strength. \( T \) is the kinetic energy, \( V \) is the Coulomb energy, \( V_c \) is the confinement contribution, and \( E \) is the total energy.
others show similar density distributions.

Note that in this case we are not merely dealing with a harmonic confinement as in the previous section, but as the wave function in Eq. (2.13) shows, the electrons are confined in different photon number spaces coupled to each other. The electron density is the sum of the electron density calculated in the orthogonal photon number spaces. An example is shown in Fig. 8 for a case of a single electron. The figure shows the probability of different photon number spaces, the fraction of the norm of the wave function belonging to different $|n\rangle$ in Eq. (2.13). In this one electron case the coupling is relatively strong; high photon spaces are coupled and less than fifty percent of the density is in the zero photon space.

Fig. 7 shows the electron density of an $N = 2$ system as a function of $\omega_p$ and $\lambda$. The coupling between different photon spaces is controlled by $g$ (see Eq. (2.11)), and the strength of confinement in a given photon space is determined by $\lambda$. For a given $\lambda$ value the dependence on $\omega_p$ is relatively small. For a given $\omega_p$ the positions and structures of the peaks are strongly dependent on $\lambda$. One significant difference between the harmonic confinement and the photon coupled case (Figs. 1 and 8) is that the density is much smaller between the peaks in the latter case.

Figs. 8 and 9 show a similar dependence on $\omega_p$ for a given $\lambda$. The confinement is determined by $\lambda$ and the density distributions have almost identical widths and peak positions. By increasing $\omega_p$, the peak structure may become less emphasized for non-spin-polarized cases (E.g. for $N = 4 S = 0$ case only two or three peaks manifest for larger $\omega_p$ or $\lambda$). Similar to harmonic confinement, the number of the density peaks still matches with the number of electrons in spin-polarized cases.

For a given $\omega_p$, the dependence on $\lambda$ is strong (Figs. 7,9). Larger $\lambda$ values make more compact systems. Overall, the $\lambda$ dependence seems to be very similar in all cases. Photon spaces with small photon number ($n=0,1,2$) contain almost all the electron densities even for stronger $\lambda$. The dependence of the densities and energies on the photon frequency is moderate. The strong dependence on $\lambda$ is due to two reasons. First, as Eq. (2.11) shows the coupling is proportional to $\lambda$. Second and more importantly the dipole self-interaction strength grows as $\lambda^2$. The latter fact also explains that for a given $\lambda$ and changing $\omega$ (see Figs. 7,8 and 9), the spread of the density is nearly identical and only the relative heights of the peaks change. The dipole self-interaction term is responsible for squeezing the density toward the center.

These systems would not be bounded harmonically without an external confining potential. The photons couple to the electrons through the center of mass coordinate of the system (see Eqs. (2.10) and (2.12)). The total wave function of the electrons can be factorized as a wave function of relative motion (depending on the relative coordinate) and the wave function of the center of mass motion (depending on $X$ only). If there is no confinement, then the relative motion is governed by the repulsive Coulomb interaction and the system dissociates. The strength of the confinement, however, plays very little role. Fig. 10 shows three and four electron systems with a very weak confining potential for the spin polarized ($S=3/2$ and $S=2$) cases. Without coupling, the density spreads out to 40 a.u. The coupling squeezes the density and the electrons form a tightly localized Wigner crystal. These three and four electron densities are very similar to the $\omega = 0.1$ a.u. cases shown in Figs. 8 and 9.

IV. SUMMARY

1D few-electron systems are investigated using ECG basis functions. All matrix elements are analytically calculated and the basis parameters are optimized to generate flexible basis and accurate wave functions. $N=2-6$ electron systems with different spin states are studied.

Two different confinements are considered. In the first case, an external potential is used to localize the electrons. In the second case, there is a weak confining potential but the electrons are coupled to light and the dipole self-polarization determines the confinement. 1D Wigner crystal-like structures appear in both cases and there is a similar tendency in the shape of the density as the confinement strength changes.

In spin-polarized cases the number of density peaks is equal to the number of electrons because the shell structure, created by the confining potential, dominates. For non spin-polarized cases the number of peaks depends on the confinement strength and the total spin.

We have shown that the Wigner crystal structure is not suppressed by strong confinement. In the strong confinement regime, the Coulomb interaction becomes negligible compared to the kinetic energy and the confinement. But in this region in 1D a shell structure is overwhelming and the nodes of the wave functions define the crystal-like peaks in the density.

Simpler models like DFT based calculations can capture the Wigner crystal structure in certain cases, especially for spin-polarized systems. Better exchange-correlation potentials can potentially extend the range of applications of the DFT based approach to other cases. The advantage of the DFT is that it is easily applicable to much larger electron systems. The densities calculated by ECG can be used to create better exchange-correlation potentials for these 1D systems.

We have considered electrons with (soft) Coulomb interaction in this work, but other systems with repulsive interactions, such as degenerate Fermi gases in confinement or cavities, would be expected to show similar structures.

Wigner crystals in systems confined by external potentials have already been observed. The experimental realization of the light coupled systems might be possible by using nanotubes or optical lattices in cavities.
| $\omega$ | $E_{\text{ECG}}$ | $E_{\text{DFT}}$ |
|---|---|---|
| 2e$^-$ | | |
| S=0 | 0.1 | 0.392 | 0.005 |
| | 1.0 | 1.774 | 1.111 |
| S=1 | 0.1 | 0.396 | -0.1 |
| | 1.0 | 2.554 | 1.827 |
| 3e$^-$ | | |
| S=0.5 | 0.1 | 1.009 | 0.256 |
| | 1.0 | 4.481 | 3.385 |
| S=1.5 | 0.1 | 1.016 | 0.246 |
| | 1.0 | 6.078 | 4.872 |
| 4e$^-$ | | |
| S=0 | 0.1 | 1.877 | 0.982 |
| | 1.0 | 7.808 | 6.261 |
| S=1 | 0.1 | 1.887 | 0.846 |
| | 1.0 | 8.589 | 7.005 |
| S=2 | 0.1 | 1.894 | 0.837 |
| | 1.0 | 11.024 | 9.293 |
| 5e$^-$ | | |
| S=0.5 | 0.1 | 2.999 | 1.678 |
| | 1.0 | 12.490 | 10.443 |
| S=1.5 | 0.1 | 2.985 | 1.671 |
| | 1.0 | 14.069 | 11.955 |
| S=2.5 | 0.1 | 3.020 | 1.663 |
| | 1.0 | 17.379 | 15.064 |
| 6e$^-$ | | |
| S=0 | 0.1 | 4.362 | 2.822 |
| | 1.0 | 17.733 | 15.164 |
| S=1 | 0.1 | 4.357 | 2.715 |
| | 1.0 | 18.566 | 15.919 |
| S=2 | 0.1 | 4.336 | 2.716 |
| | 1.0 | 20.911 | 18.221 |
| S=3 | 0.1 | 4.413 | 2.716 |
| | 1.0 | 25.099 | 22.167 |

**TABLE II**: Total energy $E$ (in atomic units) for few-electron systems as a function of the external confinement strength $\omega$. 
FIG. 6: Photon number as a function of the photon space for a single electron system with $\lambda = 0.1$ a.u., and $\omega_p = 0.1$ a.u.

FIG. 7: Electron density of the two electron $S = 1$ system coupled to light. Left $\lambda = 0.1$ a.u., right $\omega_p = 1$ a.u.

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FIG. 8: Electron density of the three electron system coupled to light. Top $S = 1/2$, bottom $S = 3/2$; left $\lambda = 0.1$ a.u., right $\omega_p = 1$ a.u.

FIG. 9: Electron density of the four electron system coupled to light. Top $S = 0$, bottom $S = 2$; left $\lambda = 0.1$ a.u., right $\omega_p = 1$ a.u.

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FIG. 10: Electron density of the four (left) and three (right) electron systems coupled to light. The solid line shows the density for $\lambda = 1$ a.u., $\omega_p = 0.5$ a.u. and $\omega = 0.001$ a.u., the dashed line shows the density without coupling.
