Momentum distribution of electrons in parabolic quantum dots

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We investigate the momentum distribution of interacting electrons confined in a two-dimensional parabolic quantum dot for varying values of the interaction strength and for different number of electrons. We use an optimized Jastrow-type wave function for the ground state in which the Slater determinant part has been calculated using density-functional theory and evaluate the ground-state momentum distribution using the Fermi hypernetted-chain equations. We discuss the effects of interactions on the momentum distribution and reveal the existence of a shell structure in momentum space in analogy with what happens to the spatial density profile. The momentum distribution can thus be used as a further tool to investigate the effects of the interaction in parabolic quantum dots.

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I. INTRODUCTION

In the past few years, the interest in the properties of electronic nano-structures has continued to increase, motivated by the possibilities of technological applications. Exploiting the type and geometry of semiconductor heterostructures, experimentalists can devise systems with reduced dimensionality. One of the most studied nano-devices is the so-called semiconductor quantum dot (QD) which has been proposed as a building block for future devices as well as a device for itself. In particular, heterostructures of GaAs/AlGaAs are frequently used to construct QDs which confine from a few to thousands of electrons in two-dimensional parabolic potentials.[1] Due to the high degree of experimental controllability of the confining potentials and to the possibility of trapping low number of particles, QDs has been considered in many respects as artificial atoms[2,3] and, therefore, many studies carried out on real atoms has been naturally extended to QDs.

As a first step toward a better understanding of QDs, many research efforts have been focused on the investigation of the ground-state structure and the transport properties of electrons in such devices (for a general review see, e.g., Refs. 4 and 5); common examples being the measurement of the addition energy spectra[6–8] and the study of Hund's rule.[9–11] The ground-state density profile and energy of the electrons has been calculated by means of exact diagonalization techniques[12,13] for few-particle systems and within Hartree, Hartree-Fock, and density-functional (DFT) theories[14,15] in a broader range of particle number. Furthermore, the single-particle and collective excitation modes have been evaluated using random-phase approximation,[16] time-dependent DFT[17,18] and Green's functions techniques.

On the other hand, the experimental and theoretical study of the momentum distribution (MD) of electrons has attracted little attention so far,[19–21] though its knowledge provides additional information on the interplay between correlation and confinement effects and on the structure of the many-body ground state. In particular, it is well known that the electron MD is proportional to the dynamic structure factor at large momentum transfers.[22] Experimentally, the MD can be accessed by means of Compton scattering, where the cross-section is proportional to the projection of the electron MD onto the scattering vector,[23,24] and by positron annihilation spectroscopy as recently illustrated for CdSe QDs in Ref. 21. Theoretically, Saniz *et al.*[20] have studied the Compton profile of noninteracting electrons confined in a three-dimensional spherical well and found an increase of the width of the MD around the Fermi momentum for decreasing dot radii.

In the present work we investigate the MD of few electrons confined in a two-dimensional parabolic QD as a function of the strength of the Coulomb repulsion and number of electrons. We adopt a many-body wave function of the Jastrow form and calculate the mean values of one- and two-body operators using the Fermi hypernetted-chain (FHNC) integral equations.[25,26] We find that the width of the MD diminishes on increasing repulsions, while the value of Compton cross section at $k=0$ increases. The dependence of the MD on the particle number is evinced by the appearance of a shell structure analogue to the shell structure present in the spatial density profile of confined systems see, e.g., Ref. 6.

The article is organized as follows. In Sec. II we introduce the Hamiltonian describing electrons in a QD and the definition of mean values of relevant operators in the ground state. We then briefly summarize the FHNC/0 procedure to calculate one- and two-body density matrices. The results for the MD of $N=6$, 12, and 20 electrons in QDs are presented in Sec. III. Section IV contains the summary and main conclusions of our work.

II. THE THEORY

A parabolic QD is described by the Hamiltonian of a system of N electrons with effective band mass m interacting via the Coulomb potential $v(r)=e^2/(\kappa r)$ and confined in an external potential $V_{\text{ext}}(r)=m\omega_0^2 r^2/2$. Introducing the usual field operator $\hat{\Psi}_\sigma^\dagger(\mathbf{r})$, which creates an electron at position $\mathbf{r}$ with spin σ, the Hamiltonian in second quantization can be written as

$$H = \sum_{\sigma} \int d^2\mathbf{r}\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(r)\right)\hat{\Psi}_{\sigma}(\mathbf{r}) + \frac{1}{2}\sum_{\sigma\sigma'} \int d^2\mathbf{r}d^2\mathbf{r}'\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\hat{\Psi}^{\dagger}_{\sigma'}(\mathbf{r}')v(|\mathbf{r}-\mathbf{r}'|)\hat{\Psi}_{\sigma'}(\mathbf{r}')\hat{\Psi}_{\sigma}(\mathbf{r}). \quad (1)$$

Choosing as unit of length the harmonic-oscillator length $\ell_0=\sqrt{\hbar/(m\omega_0)}$ and as unit of energy the harmonic-oscillator quantum $\hbar\omega_0$, the QD physics is governed by the number of electrons and the dimensionless parameter

$$\lambda = \frac{e^2/(\kappa\ell_0)}{\hbar\omega_0} = \frac{\ell_0}{a_B^{\star}}, \quad (2)$$

where $a_B^{\star}=\kappa\hbar^2/(me^2)$ is the effective Bohr radius. In addition, the Hamiltonian Eq. (1) is invariant under rotations along the z axis and commutes with the z-component S_z of the total spin, we thus consider circularly symmetric ground states with definite S_z, and in particular focus on states with $S_z=0$. Finally, we choose parameters suitable for a two-dimensional electron gas confined in a GaAs quantum well, i.e., $m=0.067$ bare electron masses and $\kappa=12.4$. With this choice $a_B^{\star}\approx 9.8$ nm and the effective Hartree energy is $e^2/(\kappa a_B^{\star})\approx 11.9$ meV.

A. Ground-state properties

The MD $n(k)$ can be obtained by Fourier transforming the one-body density matrix $\rho_{(1)}(\mathbf{r},\mathbf{r}')=\Sigma_{\sigma}\langle\psi_0|\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\hat{\Psi}_{\sigma}(\mathbf{r}')|\psi_0\rangle$ as follows:

$$n(k) = \frac{1}{N}\int d^2\mathbf{r}d^2\mathbf{r}'e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\rho_{(1)}(\mathbf{r},\mathbf{r}'), \quad (3)$$

where $|\psi_0\rangle$ is the N-electron ground state. Furthermore, the knowledge of the ground-state density $n(r)=\rho_{(1)}(\mathbf{r},\mathbf{r})$ and of the two-body distribution function $\rho_{(2)}(\mathbf{r},\mathbf{r}')=\Sigma_{\sigma\sigma'}\langle\psi_0|\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\hat{\Psi}^{\dagger}_{\sigma'}(\mathbf{r}')\hat{\Psi}_{\sigma'}(\mathbf{r}')\hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})|\psi_0\rangle$ allows us to calculate the ground-state energy $E_0=\langle\psi_0|H|\psi_0\rangle$ as

$$E_0 = N\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\hbar^2k^2}{2m}n(k) + \int d^2\mathbf{r}n(r)V_{\text{ext}}(r) + \frac{1}{2}\int d^2\mathbf{r}d^2\mathbf{r}'\rho_{(2)}(\mathbf{r},\mathbf{r}')v(|\mathbf{r}-\mathbf{r}'|). \quad (4)$$

One way to evaluate the energy E_0 and density profile of the ground-state $n(r)$ is using DFT, but to access other expectation values one should go beyond simple DFT. For example, a practical scheme to calculate the two-body distribution function starting from the accurate knowledge of the one-body properties has been proposed in Ref. 27. In atomic systems, the MD has been obtained using a combination of Hellmann-Feynman's theorem and DFT.[28–30] In this work we evaluate the MD from a suitable Jastrow-type many-body wave function.

B. Jastrow wave function and Fantoni-Rosati FHNC approach

The inclusion of correlations in the many-body state of a system is accomplished by going beyond the mean-field approximation of the wave function. The early work of Jastrow[31] introduced a simple way to take into account two-body correlations and served as a starting point for the systematic construction of correlated wave functions. In the context of electrons in QDs, Jastrow-type wave functions has been used, e.g., to investigate the transition to a Wigner regime with increasing magnetic field[32] and to calculate the energy and conditional probability density in variational Monte Carlo (VMC) schemes.[33,34]

In the present work, we use the FHNC integral equations in the Fantoni-Rosati formulation[25] to evaluate the ground-state properties of QDs using a Jastrow-type wave function. The ground-state wave function reads

$$\psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \left(\prod_{i<j=1}^{N} f(|\mathbf{r}_i-\mathbf{r}_j|)\right)\Phi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N), \quad (5)$$

where $\Phi_0(\mathbf{r}_1,\ldots,\mathbf{r}_n)$ is a Slater determinant of N single-particle wave functions and the Jastrow factor $f(r)$ is a short-ranged correlation function that we take of the following simple form

$$f(r) = 1 + \alpha e^{-\beta\mathbf{r}^2}, \quad (6)$$

which ensures the fulfilment of the cluster property;[26] however, this Jastrow factor does not satisfy the cusp condition.[35,36] In Eq. (6) α and β are variational parameters which are determined by minimizing the ground-state energy Eq. (4).

In the same spirit of the classical cluster expansion in statistical mechanics,[37] a perturbation expansion has been developed[38,39] to calculate one- and two-body properties in the ground-state Eq. (5). The quantities of interest can be expressed by a series of diagrams where the perturbation parameter is the so-called correlation factor $h(r)\equiv f^2(r)-1$. The diagrams are topologically classified in linked and unlinked and it can be shown that only linked diagrams enter the evaluation of expectation values.[40,41] Furthermore, the linked diagrams can be divided into reducible and irreducible ones. For homogeneous Fermi fluids the translation invariance ensures that the reducible diagrams cancel out[40] and this allows the construction of the chain equations. This is not true in finite systems where vertex corrections were introduced[42] in order to recover the chain equations. A further classification distinguishes between nodal, composite, and elementary diagrams. In this work we use the FHNC/0 approximation, which corresponds to neglecting the elementary diagrams. The FHNC/0 is a summation scheme which allows to add up the diagrammatic series by means of an iterative process[25] in which one uses a limited set of nodal and composite diagrams as building blocks. These summations can be recasted in a set of integral equations which are solved in a self-consistent way (for the whole set of equations see the Appendices of Refs. 43 and 44).

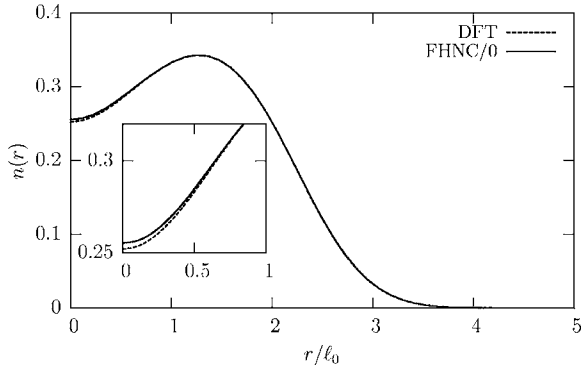

FIG. 1. Density profile $n(r)$ (in units of ℓ_0^{-2}) as a function of r/ℓ_0 for a QD with $N=6$ electrons at $\lambda=1.89$. The FHNC/0 result is compared with DFT. In the FHNC/0 calculation we have considered $\alpha=-0.14$ and $\beta=0.30/\ell_0^2$. The inset shows a detail of the density profiles.

To summarize, starting from the Jastrow wave function Eq. (5) one can evaluate the ground-state energy, the two-body distribution function and the MD[45] by means of a set of integral equations known as FHNC/0. Other approaches have also been developed to evaluate ground-state properties starting from a Jastrow wave function by functional optimization of the energy in the space defined by Jastrow-type wave functions for arbitrary $f(r)$ and Φ_0. This method has been originally derived for the study of uniform-density nuclear matter[46] and then applied to other many-body systems, e.g., the electron gas.[47] Further generalization has been done in the case of inhomogeneous systems[48] and applications have been done in both nuclear[49] and atomic[50] physics.

III. RESULTS

In this section we present the results for the MD calculated in the FHNC/0 approximation where the mean-field wave function $\Phi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ in Eq. (5) is constructed with the Kohn-Sham[51] orbitals obtained in a DFT calculation using the exchange-correlation potential of Tanatar and Ceperley,[52] as described in Ref. 27. This choice ensures a good quality of the density profiles as illustrated in Fig. 1, where we compare the predictions of DFT and FHNC/0 for a system with $N=6$ and $\lambda=1.89$.[56] The FHNC/0 density profile differs very little from the DFT counterpart, which, as previously noticed,[11,27] is in excellent agreement with Monte Carlo data.

Even though the effects on the density profiles are rather small, we shall show that FHNC/0 yields non-negligible corrections to the MD calculated in DFT. In Fig. 2 we compare the profile of the electron MD's obtained in DFT and FHNC/0 schemes. At large momentum k the DFT and FHNC/0 calculations are in good agreement, but neither yields the asymptotic power-law behavior of the MD that would be implied by the cusp condition.[53] However, at small k, the FHNC/0 calculation incorporates long-range corrections through the resummation of the nodal diagrams.[54] In the inset of Fig. 2, we report the mean value $\langle k^{-1}\rangle$ which corresponds to the value of the Compton cross-section at $k=0$[55] and thus can be directly measured.

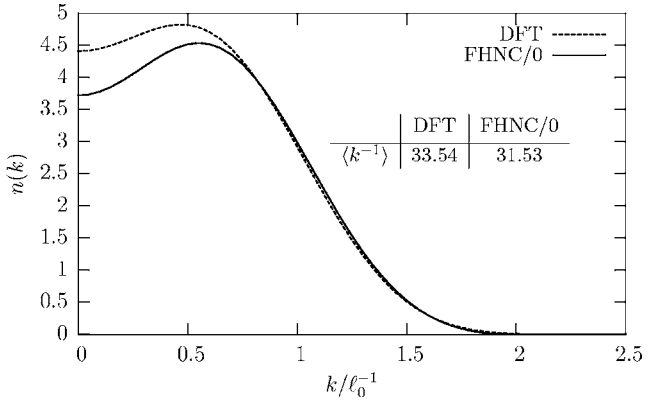

FIG. 2. Momentum distribution $n(k)$ (in units of ℓ_0^2) as a function of k/ℓ_0^{-1} for a QD with $N=6$ and $\lambda=1.89$. The FHNC/0 result is compared with DFT. The inset shows the corresponding mean values $\langle k^{-1}\rangle$ (in units of ℓ_0).

In the following we analyze the effects on the electron MD of varying the interaction strength. To this purpose we define the Fermi momentum k_F following Ref. 20 as the momentum at which $\partial n(k)/\partial k$ attains its absolute minimum. The behavior of $n(k)$ and $\partial n(k)/\partial k$ at varying λ is depicted in Figs. 3 and 4, respectively. We observe that on increasing the strength of the interaction the MD narrows. This behavior is expected from the broadening of the density profile in real space.[27] The value of $\langle k^{-1}\rangle$ is a very sensitive measure of the variation of the MD and, as shown in the inset of Fig. 3, increases monotonically with λ. Therefore, it can be used to discriminate between different interaction strengths. The above trend of $n(k)$ is also reflected in a more pronounced minimum of $\partial n(k)/\partial k$ at k_F for larger λ. However, due to the confinement and the relatively small interaction strength, the width of the minimum does not change much with varying the interaction. This is at variance to what found in Ref. 20 where on increasing the size of the QD while keeping constant the average density, $\partial n(k)/\partial k$ approaches the homogeneous electron gas limit, i.e., a delta function centered at k_F. In our case the number of electrons is kept constant and therefore the sole increase of the width of $n(r)$ does not lead to the homogeneous electron gas limit.

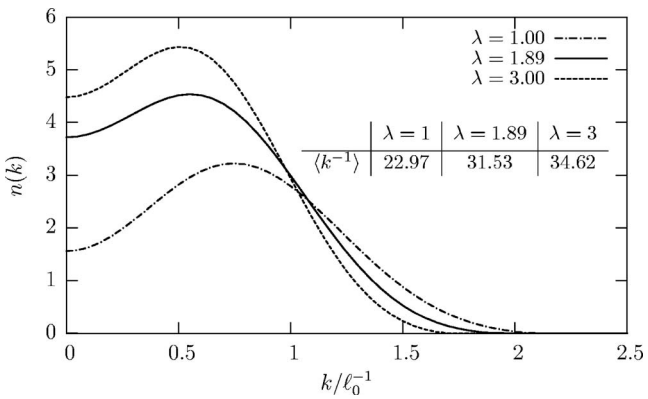

FIG. 3. Momentum distribution $n(k)$ (in units of ℓ_0^2) as a function of k/ℓ_0^{-1} for a QD with $N=6$ electrons and several interaction strengths λ. The inset shows the corresponding mean values $\langle k^{-1}\rangle$ (in units of ℓ_0).

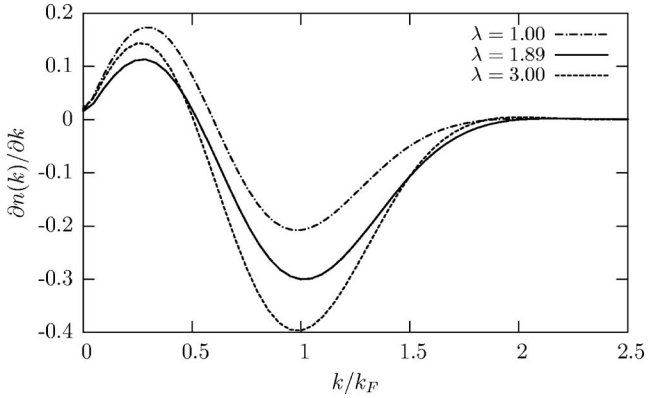

FIG. 4. The derivative of the momentum distribution with respect to the momentum $\partial n(k)/\partial k$ (in units of ℓ_0^3) as a function of k/k_F for a QD with $N=6$ electrons at varying λ.

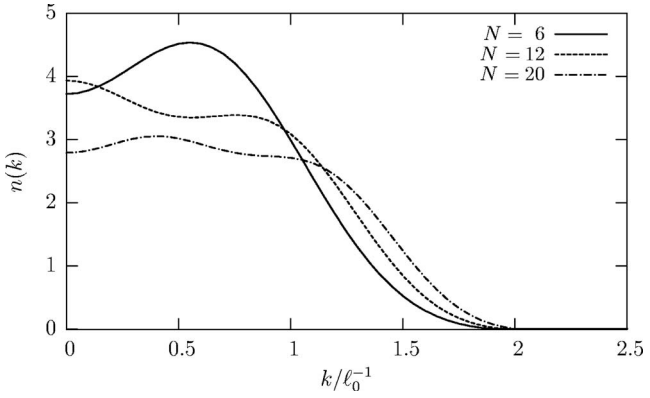

FIG. 5. Momentum distribution $n(k)$ (in units of ℓ_0^2) as a function of k/ℓ_0^{-1} for a QD at $\lambda=1.89$ with varying number of electrons.

Finally, we investigate the dependency of the MD at varying electron number. Figure 5 shows the MD of $N=6$, 12, and 20 electrons in a QD with $\lambda=1.89$. We observe the formation of a shell structure analogously to what happens in real space due to the high degeneracy of the single-particle energy levels. In a parabolic potential the noninteracting electron MD has the same form as the spatial density profile. The presence of interactions tends to wash out the oscillations on $n(k)$ as can be inferred from Fig. 3, but these are still visible at $\lambda=1.89$. The number of extremes of $n(k)$ are strictly related to the number of shell which are filled. In the $N=6$ case, where two shell are totally occupied, we observe two structures, one minimum at $k=0$ and a maximum around $k=0.55\ell_0^{-1}$. For $N=12$ and 20 the number of structures correspond to three and four filled shells, respectively. We also notice that as the number of particles increases the amplitude of the oscillations decreases.

IV. CONCLUSIONS

We have calculated the momentum distribution of interacting electrons confined in a parabolic quantum dot. We used a Jastrow-type many-body wave function to describe the ground state of the system and evaluated the momentum distribution by means of the Fermi hypernetted-chain equations in the Fantoni-Rosati formulation. The momentum distribution obtained from a Slater determinant built with Kohn-Sham orbitals and a parameter-optimized Jastrow factor shows a remarkable difference with the momentum distribution calculated in DFT at low momenta. This discrepancy could be directly observed in a Compton scattering experiment.

Finally, we have shown the existence of a shell structure on the momentum distribution resembling that present in the spatial density profile. The main effects of the electron interactions are to narrow the momentum distribution and to weaken the amplitude of the shell structure.

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