

Spin magnetization of strongly correlated electron gas confined in a two-dimensional finite lattice

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The influence of disorder and interaction on the ground state polarization of the two-dimensional (2D) correlated electron gas is studied by numerical investigations of unrestricted Hartree-Fock equations. The ferromagnetic ground state is found to be plausible when the electron number is lowered and the interaction and disorder parameters are suitably chosen. For a finite system at constant electronic density the disorder induced spin polarization is cut off when the electron orbitals become strongly localized to the individual network sites. The fluctuations of the interaction matrix elements are calculated and brought out as favoring the ferromagnetic instability in the extended and weak localization regime. The localization effect of the Hubbard interaction term is discussed.

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I. INTRODUCTION

The combined effect of carrier interactions and Pauli principle leads to itinerant ferromagnetism in metals whenever the kinetic energy gain by parallel alignment of electronic spins is exceeded by the exchange energy of the antisymmetric wave function ([1]). The simplest model is the Hund's rule in atoms, where the energy is minimized when the fermionic wave function corresponds to the alignment of spins. Meanwhile the electron-spin correlations seems to be an important factor in the two-dimensional (2D) metal-insulator transition [2]. Measurements of the in-plane magnetoconductivity of a dilute 2D electron system in silicon heterostructures have shown the evidence for a zero-temperature quantum phase transition at critical density, indicating the existence of a ferromagnetic instability ([3],[4]). On the other hand a new method that measures the minute thermodynamic spin magnetization of a dilute 2D electron system in a silicon inversion layer favors the paramagnetic phase over the spontaneous magnetization [5].

The interaction strength between electrons is traditionally described by the 2D Wigner-Seitz radius, $r_s = 1/(\pi n_s a_B^2)^{1/2}$, where a_B is the Bohr radius and $n_s = n/L^2$ sheet density of electrons. As a function of r_s the ground state of the 2D electron gas can be, for instance, a Wigner crystal (in dilute limit, at $r_s \geq 35$ [6]), a ferromagnetic Fermi liquid with spontaneous magnetization or a paramagnetic Fermi liquid. An improved hypernetted-chain approximation was employed to study the 2D electron liquid at full Fermi degeneracy [7, 8]. The results indicate the paramagnetic phase as the ground state of the system until the Wigner crystallization density, even the separation with polarized states become minute (the energy difference with the ferromagnetic phase diminishes to milliRydbergs). In contrast, the transition from paramagnetic fluid phase to Wigner crystallization was recently studied for a 2D electron gas by

diffusion Monte Carlo simulations including the backflow corrections [9] showing the stability range of a polarized phase in-between. The earlier work including the backflow correlations did not find the polarization transition [10]. More recently a weakly first-order transition to a spin-polarized state was found to occur shortly before the Wigner crystallization [11].

Hubbard model is the simplest tool that can capture some of the salient properties of correlated systems. A delocalized Coulomb phase in 2D was observed in the calculations of by Waintal *et al.*[12] which showed the transition from the Anderson insulator towards an extended phase. Mean-field approximation considered in an unrestricted Hartree-Fock ansatz (UHF) was compared with constrained path quantum Monte Carlo method for repulsive Hubbard model at half-filling[13] and found both Anderson and Mott insulator phases. In a 3D system numerical mean-field studies by Tusch and Logan[14] at the unrestricted Hartree-Fock level revealed the phase diagram at half-filling. The phase diagram in a 2D system is studied by Hirsch[15] using a square lattice with nearest-neighbor hopping.

Nowadays there is also a growing interest in the spin polarization and Stoner instability of finite-size disordered systems [16],[17],[18],[19], [20]. In quantum dots, the singlet-triplet transitions even for weak interactions cause switching between states and a kink in the conductance [16]. For interaction strength below the Stoner criterion a nonzero spin ground state was found for an ensemble of small metallic grains in the Hartree-Fock approximation [19]. Close to the Stoner instability in a 2D metallic system there is an exponentially small probability for the appearance of local spin droplets[21]. The tendency of disorder to exhibit the magnetism of ground state was already pointed out in some recent works[18], [22],[23]. Meanwhile the fluctuations of the interaction matrix for different disorder ranges seem to have an important role in the spin polarization transition for finite

systems. At crossover between random matrix ensembles the correlations between different eigenvectors give rise to enhanced fluctuations of the interaction matrix elements (IME) in small metallic grains and semiconductor quantum dots [24]. When their fluctuations dominate a 2D random interaction model predicts an increased probability of a minimal spin for the ground state lowering in the tails of the energy band [17] and for a two-orbital model they also help in stabilizing a ground state with minimal spin [25].

Our goal in this work is to study the influence of disorder and interactions on the polarization of the ground state for a 2D finite lattice. We treat the interaction effects at the unrestricted Hartree-Fock level (UHF), neglecting the off-diagonal contribution of the Coulomb matrix. This approximation permits us to write an effective one-body Hamiltonian, suitable for calculating the conductances in the Landauer-Büttiker formalism [26]. We solve numerically the self-consistent set of equations for 2D systems with Hubbard interaction greater than the Coulomb interaction strength ($U_H \gg U$). For different disorder ranges we study the fluctuations of the interaction matrix elements and point out their role in the disorder induced spin polarization.

The rest of this paper is organized as follows. In the next section we outline the theoretical framework of unrestricted Hartree-Fock approximation and develop an effective Hamiltonian for the problem at hand. In Sec. III we present our results for the fluctuations in the interaction matrix elements in various disorder regimes. Section IV discusses the possibility of disorder enhanced spin polarization within our model. We close by listing our main conclusions in Sec. V.

II. THE UNRESTRICTED HARTREE-FOCK FORMALISM

We study a disordered rectangular lattice with n fermions on $L^2 = L_x \cdot L_y$ sites with vanishing boundary conditions imposed. If $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators of an electron at site i with spin σ , the Hamiltonian will be defined as follows:

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} \omega_i n_{i,\sigma} + U_{Hub} \sum_i n_{i\uparrow} n_{i\downarrow} + U \sum_{i \neq j, \sigma, \sigma'} \frac{n_{i,\sigma} n_{j,\sigma'}}{|i-j|} \quad (1)$$

where $n_{i,\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the occupation number operator, ω_i is the random Anderson disorder ($\omega_i \in [-W/2, W/2]$), U_{Hub} and U are the strength of the Hubbard and long-range Coulomb interaction, and t is the energy unit of the hopping integral (it will be considered equal to unity). For ω_i set to zero, the Hamiltonian of Eq. (1) is the extended Hubbard model, used for studying the correlated systems [27]. The Hubbard term was first introduced in [28] and the argument in favor of it is that only electrons

with opposite spins can occupy the same state (Pauli exclusion principle).

We write the Hamiltonian given in Eq. (1) in a basis formed by two sets of orthonormalized single-particle states $\phi_\alpha^\uparrow(i)$, $\phi_\alpha^\downarrow(i)$ with $\alpha \in [1, L^2]$ (unrestricted Hartree-Fock orbitals). Creation and annihilation operators in the new basis $c_{\alpha\sigma}^\dagger$ and $c_{\alpha\sigma}$ are given by the transformation $c_{\alpha,\sigma}^\dagger = \sum_i \phi_\alpha^\sigma(i) c_{i,\sigma}^\dagger$ and $c_{\alpha,\sigma} = \sum_i \phi_\alpha^{\sigma*}(i) c_{i,\sigma}$. Employing the variational principle, we look for the self-consistent set of eigenvectors $\phi_\alpha^\sigma(i)$ that minimize the ground state energy E_G for a given number of electrons n and a definite component of spin along an arbitrary z axis, S_z . The ground state will be a Slater determinant $|\Psi_G\rangle$ that correspond to the n_σ electrons in the states $\phi_\alpha^\sigma(i)$ for $\alpha = 1, \dots, n_\sigma$ and $\sigma = \uparrow, \downarrow$ ($n_\uparrow + n_\downarrow = n$):

$$|\Psi_G\rangle = \prod_{\alpha=1}^{n_\uparrow} c_{\alpha,\uparrow}^\dagger \prod_{\alpha=1}^{n_\downarrow} c_{\alpha,\downarrow}^\dagger |\Psi_0\rangle \quad (2)$$

where $|\Psi_0\rangle$ is the vacuum [29]. The eigenvectors $\phi_\alpha^\sigma(i)$ and the corresponding Lagrange multipliers ϵ_α^σ that give the lowest energy solution for the ground state energy $E_G = \langle \Psi_G | H | \Psi_G \rangle$ will be calculated by the variational principle. After a straightforward calculation one obtains the following spin-separable Hamiltonian $H^{eff} = \sum_\sigma H_\sigma$ for $\sigma = \uparrow, \downarrow$:

$$H_\sigma = \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i [\omega_i + V_D(i) + V_{Hub}^\sigma(i)] n_{i,\sigma} - \sum_{i \neq j} V_{Ex}^\sigma(i,j) c_{i\sigma}^\dagger c_{j\sigma} \quad (3)$$

with $\phi_\alpha^\sigma(i)$ and ϵ_α^σ eigenvectors and eigenvalues of Eq. (3): $H_\sigma |\phi_\alpha^\sigma\rangle = \epsilon_\alpha^\sigma |\phi_\alpha^\sigma\rangle$. The time reversal symmetry of H ensures the possibility of choosing a real system of eigenvectors.

The matrix elements $V_D(i)$, $V_{Ex}^\sigma(i,j)$ and $V_{Hub}^\sigma(i)$ (direct, exchange and Hubbard interactions, respectively) are related to the single particle eigenvectors by the following formulae (we stress that in the following $\bar{\sigma}$ means the opposite spin of σ):

$$V_D(i) = 2U \sum_{j \neq i} \frac{\sum_\sigma \sum_{\alpha=1}^{n_\sigma} |\phi_\alpha^\sigma(j)|^2}{|i-j|} \quad (4)$$

$$V_{Ex}^\sigma(i,j) = 2U \frac{\sum_{\alpha=1}^{n_\sigma} \phi_\alpha^{\sigma*}(j) \phi_\alpha^\sigma(i)}{|i-j|} \quad (5)$$

$$V_{Hub}^\sigma(i) = U_{Hub} \sum_{\alpha=1}^{n_{\bar{\sigma}}} |\phi_\alpha^{\bar{\sigma}}(i)|^2 \quad (6)$$

The ground state energy is given by:

$$E_G = \sum_{\alpha\sigma} \epsilon_\alpha^\sigma + U \sum_{\alpha\sigma, \beta\sigma'} V_{\alpha\sigma, \beta\sigma'}^{\alpha\sigma, \beta\sigma'} - U \sum_{\alpha\sigma, \beta\sigma} V_{\alpha\sigma, \beta\sigma}^{\beta\sigma, \alpha\sigma} + U_{Hub} \sum_{\alpha\sigma, \beta\bar{\sigma}} C_{\alpha\sigma, \beta\bar{\sigma}}^{\alpha\sigma, \beta\bar{\sigma}} \quad (7)$$

where the second and the third terms are the contributions of direct and exchange interaction, respectively, to the ground state energy, and the last term is the Hubbard interaction. The summations in Eq. (7) are over the occupied states $|\alpha\sigma\rangle$ from Eq. (2). The Coulomb and Hubbard interaction matrix elements are given as

$$V_{\alpha\sigma,\beta\sigma'}^{\gamma,\delta\sigma'} = \sum_{i \neq j} \frac{\phi_{\alpha}^{\sigma*}(i)\phi_{\gamma}^{\sigma}(i)\phi_{\beta}^{\sigma'*}(j)\phi_{\delta}^{\sigma'}(j)}{|i-j|}, \quad (8)$$

$$C_{\alpha\sigma,\beta\sigma'}^{\gamma,\delta\sigma'} = \sum_i \phi_{\alpha}^{\sigma*}(i)\phi_{\gamma}^{\sigma}(i)\phi_{\beta}^{\sigma'*}(i)\phi_{\delta}^{\sigma'}(i). \quad (9)$$

Omitting the off-diagonal matrix elements ($(\alpha,\beta) \neq (\gamma,\delta)$) in Eq. (7) yields the Hartree-Fock approximation. The reason for doing this will be discussed subsequently.

The basic parameters of our theoretical framework are the electron number n , the long-range Coulomb interaction U , the Hubbard interaction strength U_{Hub} , and the disorder amplitude W . Equations (3-7) constitute a set of self-consistent equations to yield the eigenstates $\phi_{\alpha}^{\sigma}, \epsilon_{\alpha}^{\sigma}$ and the energy E_G for a given set of spin occupation numbers $(n_{\uparrow}, n_{\downarrow})$ with $n_{\uparrow} + n_{\downarrow} = n$. At every step of the numerical calculation, the matrix elements [described by Eqs. (4-6)] of H^{eff} will be calculated for the spin occupation numbers that give the minimum energy in the previous step. The first Slater determinant of Eq. (3) will be formed by noninteracting eigenfunctions of Hamiltonian [Eq. (1)] with $U = U_{Hub} = 0$. Varying the spin occupation numbers so that $M_z \in [0, 1]$ we calculate $E_G(M_z)$ whose minimum value gives the spin magnetization M_z of the system. The stability of the self-consistent solutions is very sensitive at larger Coulomb interaction strengths, forcing us to keep a relatively small values of the interaction parameter U . Because of the spin rotational symmetry of the Hamiltonian, one limits the numerical calculations only to positive spin magnetization ($n_{\uparrow} \geq n_{\downarrow}$).

Increasing the amplitude of disorder the spectrum of noninteracting Hamiltonian $H_0 = t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} \omega_i n_{i,\sigma}$ evolves from weakly to strongly localized regime while the eigenvalue statistics exhibits a crossover between Wigner and Poisson distributions [30]. As a consequence the distribution function of neighboring level spacing undergoes a continuous crossover from Wigner surmise $P_W(s) = \pi s/2 \cdot \exp(-\pi s^2/4)$ with the variance $\delta(s) = \sqrt{4/\pi - 1} \simeq 0.52$ toward Poisson $P_P(s) = \exp(-s)$ with $\delta(s) = 1$. (s is the dimensionless level spacing measured in the unit of the mean level spacing $\Delta = \langle S \rangle$). This scenario is also available when the Hubbard interaction is taken into account. For nonzero spin magnetization, the whole spectrum of H^{eff} consists of two distinct sequences of the two spectra of the H_{\uparrow} and H_{\downarrow} . The spectrum of H_{\uparrow} depends on the site occupation number $n_{\uparrow}(i)$ [c.f. Eq. (6)] that will become zero at large U_H (when $M_z = 1$ and $n_{\uparrow} = n$), conserving the eigenstates degree of localization as in the noninteracting case. Meanwhile, the spectrum of H_{\downarrow} depends on

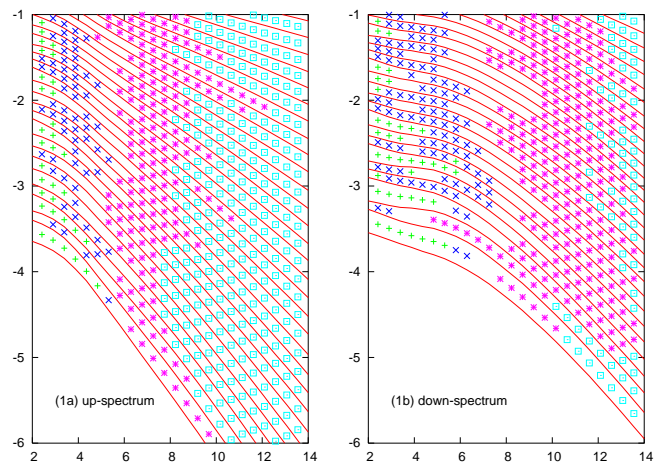


FIG. 1: The eigenspectrum of H_{\uparrow} (a) and H_{\downarrow} (b) versus the disorder amplitude W for a system $L^2 = 8 \cdot 9$, $U_H = 4$, $U = 0$ and the electron number $n = 8$. The mark symbols between the eigenvalue lines show different values of the variance of the neighboring level spacing $\delta(s)$. From left to right they indicate: $\delta(s) < 0.5$ (crosses), $\delta(s) \in [0.5, 0.54]$ (times), $\delta(s) \in [0.6, 0.7]$ (stars) and $\delta(s) > 0.7$ (boxes). The averages are made over an ensemble of 500 configurations.

the site occupation number $n_{\uparrow}(i)$ (whose average over disorder configurations will become equal to n/L^2) and moves up at a rate of $\langle V_{Hub}^{\downarrow} \rangle_{disorder} = U_{Hub} \cdot n/L^2$. The spectrum of H_{\downarrow} becomes delocalized as a counterpart of $V_{Hub}^{\downarrow}(i)$ against the disorder potentials $\omega(i)$. In Fig. 1 we show the differences in the two sequences of spectrum, H_{\downarrow} states being more delocalized compared to H_{\uparrow} states at the same W . The variance $\delta(s) \simeq 0.7$ in Fig. 1(a) for $W = 10$ as for the noninteracting spectrum in the inset of Fig. 2(c). In Fig. 2(c) the variance $\delta(s) \geq 0.8$ for a system size $L^2 = 8 \cdot 9$ with disorder amplitude $W = 20$. One notes that for a finite system the discreteness of the energy spectrum does not allow for a real Poisson distribution and the level repulsion characteristic to Wigner surmise is present even at the critical point of Anderson transition [36]. The effect of the Coulomb interaction ($U \neq 0, U_{Hub} = 0$) over the spectrum properties concerns the localization effect of long range interaction for $\xi \geq L$ [23], the edge localization of the occupied Hartree levels [31] suggested also in [34] and increasing gap near ϵ_F [34]. In the large lattice size limit the Coulomb interaction induces a delocalization process by the meaning of Poisson-Wigner transition of level spacing distributions [35].

III. INTERACTION MATRIX FLUCTUATIONS

The Coulomb interaction matrix elements (CME) $V_{\alpha,\beta}^{\gamma,\delta}$ from Eq. (8) and the Hubbard matrix elements (HME) $C_{\alpha,\beta}^{\gamma,\delta}$ from Eq. (9) are calculated for disorder functions in different localization regimes. To this purpose, we

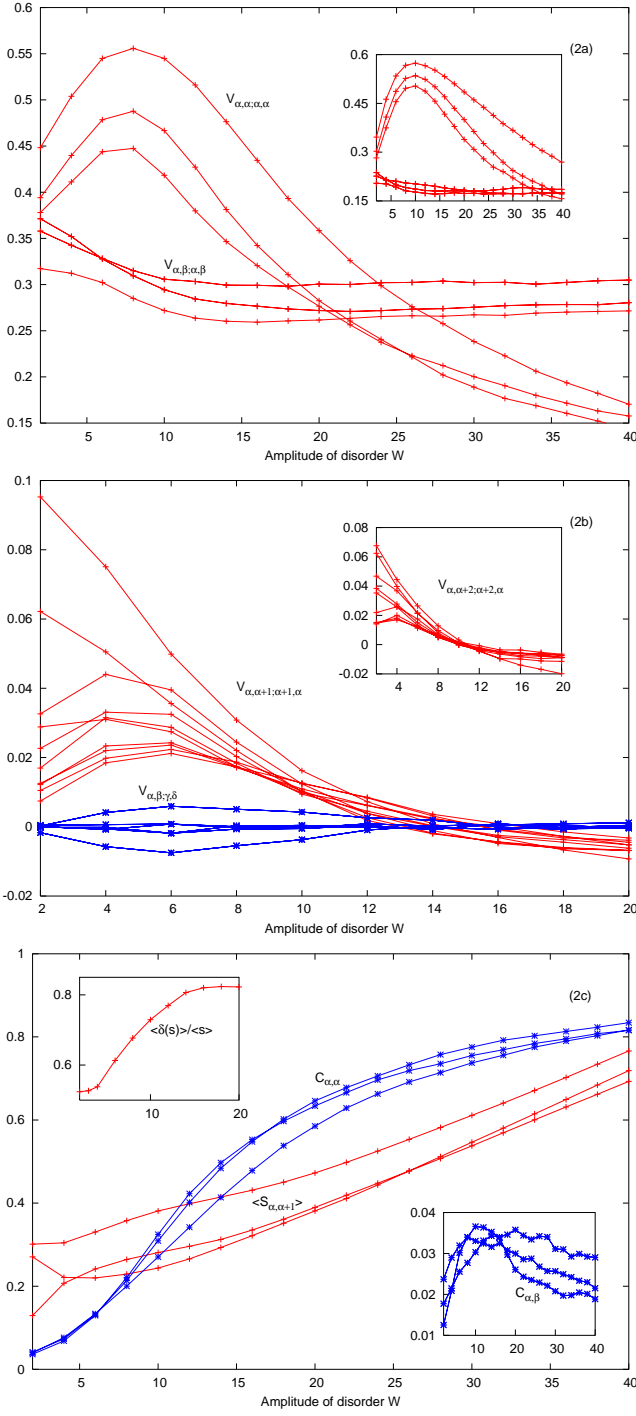


FIG. 2: The mean values of the interaction matrix elements versus amplitude of disorder W . $L^2 = 8 \cdot 8$. (a) Direct matrix elements $V_{\alpha\alpha}^{\alpha}$ with $\alpha = 1, 2, 3$ and $V_{\alpha\beta}^{\alpha\beta}$ with $\alpha, \beta = 1, 2, 3$; (in the inset are represented the same matrix elements for $L^2 = 14 \cdot 14$). (b) Exchange matrix elements $V_{\alpha,\alpha+1,\alpha}^{\alpha+1,\alpha}$ with $\alpha = 1 \dots 10$ and the off diagonal matrix elements $V_{\alpha\beta}^{\gamma\delta}$ with $\alpha, \beta, \gamma, \delta = 1, 2, 3$. In the inset $V_{\alpha,\alpha+2,\alpha}^{\alpha+2,\alpha}$ for the same system. (c) Hubbard matrix elements $C_{\alpha\alpha}$ and level spacing $S_{\alpha\alpha+1} = \epsilon_{\alpha+1} - \epsilon_{\alpha}$. In the bottom inset the off diagonal Hubbard elements $C_{\alpha\beta}$ with $\alpha \neq \beta$. $\alpha, \beta = 1, 2, 3$. In the top inset the variance of neighboring level spacing shows the transition from extended regime ($\delta(s) = 0.52$) to localized one ($\delta(s) \rightarrow 1$). The averages are made over 1500 configurations.

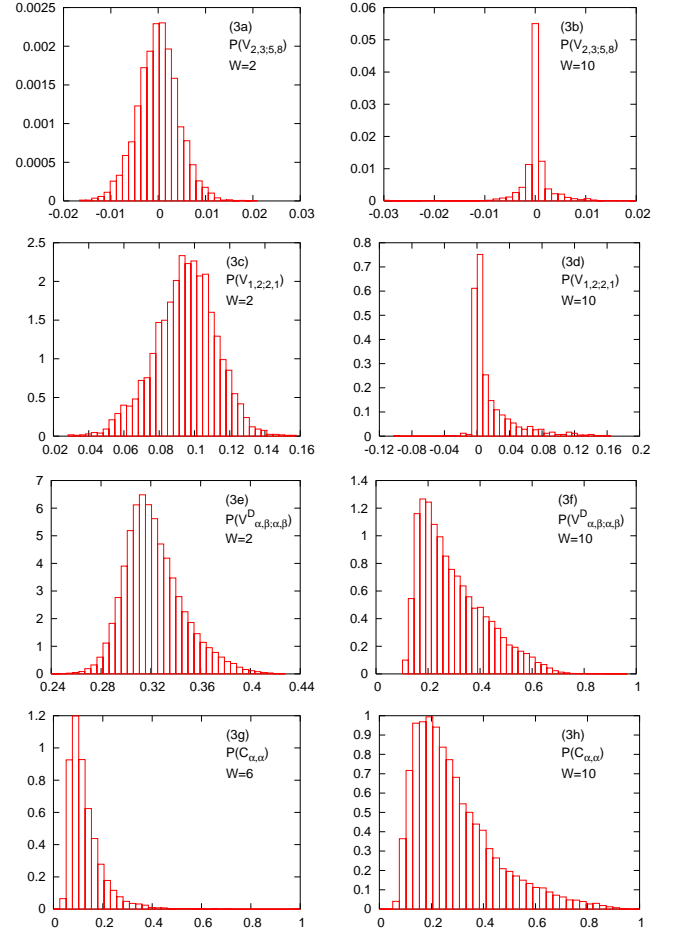


FIG. 3: The probability density distributions of the interaction matrix elements. The system dimension $L^2 = 8 \cdot 8$. The elements involved and the disorder amplitude are marked in every figure. In (e ... h) we represented the distributions of direct and Hubbard interaction matrix elements with any $\alpha, \beta \in [1, 11]$. For $W = 10$ all distributions (except for the off-diagonal element) are asymmetric with the long tails toward the values larger than the disorder averages. The histograms are represented so that the calculated integral be equal to the mean value of the corresponding element.

use the eigenvectors ϕ_{α} ($\alpha = 1 \dots L^2$) generated by the noninteracting Hamiltonian H_0 for different degrees of disorder characterized by W . For a 2D lattice with $L^2 = L_x \cdot L_y = 8 \cdot 9$ we have identified three disordered regimes: (i) extended, when $\delta(s) \simeq 0.52 \pm 0.01$ for $W \in [1, 4]$ (Fig. 2(c)); (ii) strongly localized regime with $\xi < L$ and Poisson like repulsion eigenvalues ($\delta(s) > 0.8$ and $W > 15$); (iii) weak localization as intermediate for $W \in [4, 15]$ when the localization length ξ crosses the system length L . The identification of these three regimes of localization is made for the purpose of analyzing numerical results presented in this work and to help in discussing the features of the interaction matrix elements values. When transport properties are involved, extended and weakly localized regimes have a common

meaning, usually addressed as a metallic regime with $\xi > L$ and $g \geq 0.5$ (where g is dimensionless conductance). In the following we discuss the main properties of the interaction matrix elements in various disordered regimes.

A. The disorder average of the CME with equal indexes $\langle V_{\alpha,\alpha}^{\alpha,\alpha} \rangle$ depends on the eigenvectors correlations $\langle |\phi_\alpha^2(i)| * |\phi_\alpha^2(j)| \rangle$ with $i \neq j$. It has large values in the extended and weak localization regimes where the correlations of the same eigenvectors are proportional to $1/g$ for large distances [33] and decreasing to zero when the states became strongly localized on singular lattice points $\phi_\alpha(i) = \delta_{i,i_\alpha}$ (Fig. 2(a)). We note that these matrix elements together with the Hubbard term $C_{\alpha,\alpha}^{\alpha,\alpha}$ give the whole interaction energy of the two electrons (with opposite spin) in the state α (c.f. Eq. (7)). In contrast, the direct matrix elements $\langle V_{\alpha,\beta}^{\alpha,\beta} \rangle$ with $\alpha \neq \beta$ are decreasing when the disorder is increased, keeping constant values for strong disorder (Fig. 2(a)). In this case, assuming that the two states ϕ_α, ϕ_β are strongly localized in the two random points i_α, i_β we obtain $\langle V_{\alpha,\beta}^{\alpha,\beta} \rangle_{config} = \langle \sum_{i_\alpha \neq j_\beta} \frac{1}{|i_\alpha - j_\beta|} \rangle_{r.p.}$, where the last average is made over all possible random pairs of points (i_α, i_β) . For a 2D system with $L^2 = 8 \cdot 8$ and vanishing boundary conditions $\langle \sum_{i_\alpha \neq j_\beta} \frac{1}{|i_\alpha - j_\beta|} \rangle_{r.p.} = 0.319$ and for $L^2 = 14 \cdot 14$ it is equal to 0.194 and these values are close to the averages reached by $\langle V_{\alpha,\beta}^{\alpha,\beta} \rangle_{config}$ in Fig. 2(b).

B. The exchange matrix elements $\langle V_{\alpha,\beta}^{\beta,\alpha} \rangle$ and the off-diagonal matrix elements $\langle V_{\alpha,\beta}^{\gamma,\delta} \rangle$ (with $(\alpha, \beta) \neq (\gamma, \delta)$) in Fig. 2(b) have maximum values in the weak localization regime for $W \simeq 5.5 \pm 0.5$ when $\xi > L$. This is the region where the eigenvector correlations are large. For uncorrelated states in the strongly localized regime, the off-diagonal matrix elements are decreasing to zero faster than the exchange matrix elements. This is also possible for weakly localized regime when the exchange elements are calculated between the uncorrelated states whose eigenvalues are well separated. In the inset of Fig. 2(b) the exchange matrix elements $V_{\alpha,\beta}^{\beta,\alpha}$ are lower when eigenvalue differences $S_{\alpha\beta}$ are increased. The negative values in Fig. 2(b) for $V_{\alpha,\beta}^{\beta,\alpha}$ when $1 \leq \xi \ll L$ are a property of the finiteness of the system and the orthogonality of the eigenvectors ϕ_α, ϕ_β .

C. The Hubbard matrix elements are given by the inverse participation ratio of a state ϕ_α , $C_{\alpha,\alpha} = \sum_i \phi_\alpha^4(i)$ that evolves from $1/L^2$ for extended states to 1 for strongly localized ones (Fig. 2(c)). The off-diagonal terms $C_{\alpha,\beta} = \sum_i \phi_\alpha^2(i) \phi_\beta^2(i)$ decay to zero for strongly localized states and have maximum values in the weakly localized regime where the correlations of two different eigenfunctions are proportional to $1/g$ [33]. This suggests that the spin polarization transition when $U_H \neq 0$ is larger in the strongly disordered regime. As a characteristic of a finite system, the saturation of the inverse participation ratio ($C_{\alpha,\alpha} = 1$) corroborated with the linear increase of the mean level spacing makes impossible

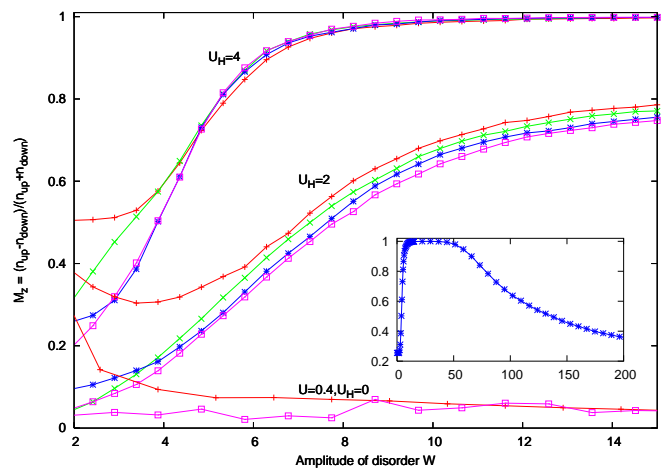


FIG. 4: The spin magnetization $\langle M_z \rangle$ vs. disorder amplitude W for the filling factor $n/L^2 = 1/9$ and for different interaction strengths ($U_H = 4, U = 0$), ($U_H = 2, U = 0$) and ($U_H = 0, U = 0.4$). The electron number and the system size are $n = 4$ and $L^2 = 6 \cdot 6$ (crosses), $n = 6$ and $L^2 = 6 \cdot 9$ (stars), $n = 8$ and $L^2 = 8 \cdot 9$ and $n = 10$ and $L^2 = 9 \cdot 10$ (boxes). In the inset for $U_H = 4$ and $L^2 = 8 \cdot 9$ the effect of disorder induced spin magnetization disappears when $W > 50$. The averages are made over 200 ~ 1000 configurations. The large values of $\langle M_z \rangle$ for $L^2 = 6 \cdot 6$ when $W < 4$ are due to the degeneracies of the spectrum and have no significance for the disorder induced transition.

a spin polarization transition for very large disorder. It does not take place in the thermodynamic limit ($L \rightarrow \infty$ and lattice parameter $a = const.$) when the neighboring level separation $S \rightarrow 0$.

The fluctuations of the interaction matrix elements for different disorder ranges are presented in Fig. 3. For small disorder, the probability density distributions of the IME are large and they typically have a Gaussian shape. The exchange (and off-diagonal) matrix element fluctuations become sharper when their mean values become zero and the inverse participation ratio has larger fluctuations when disorder is increased, with a shape evolution similar to increasing the Coulomb interaction strength (compare with Fig. 5 in Levit and Orgad[34]). We notice the asymmetric long tail fluctuations of direct, exchange and Hubbard matrix elements (Fig. 3 for $W = 10$), the last two permitting an increased probability of the spin polarization transition even when the Stoner criterion does not allow it.

IV. DISORDER ENHANCED SPIN POLARIZATION

The formula of E_G given in Eq. (7) for the ground state energy written as an unrestricted Slater determinant [Eq. (2)] means that we omit the off-diagonal matrix elements from expansion of E_G . In Fig. 2(b) the largest values of the off-diagonal elements in the weak localiza-

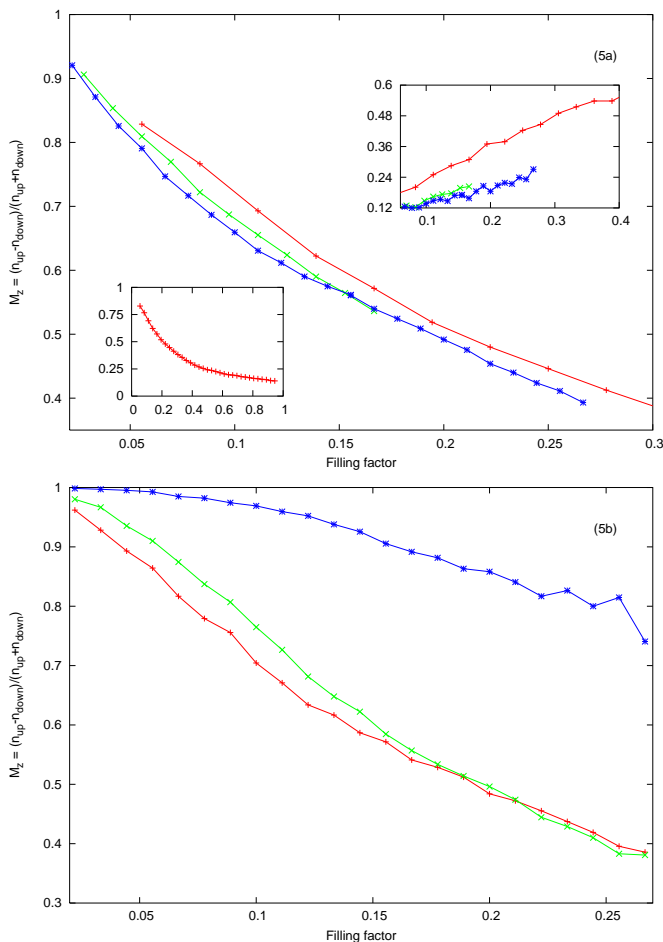


FIG. 5: The spin magnetization $\langle M_z \rangle$ vs. the filling factor n/L^2 . (a) The interaction is $U_H = 2, U = 0$ and disorder $W = 10$. In upper inset the transmittance of the last occupied level. The three set of lines are calculated for $L^2 = 6 \cdot 6$ (crosses), $L^2 = 9 \cdot 10$ (times) and $L^2 = 9 \cdot 10$ (stars). In down inset $\langle M_z \rangle$ is decreasing to zero at $n/L^2 \propto 1$. (b) For $W = 10$ and $L^2 = 9 \cdot 10$ the interaction strengths are $U_H = 2, U = 0.1$ (crosses), $U_H = 2, U = 0.2$ (times) and $U_H = 3, U = 0.3$ (stars). The averages are made over 200 ~ 1000 configurations.

tion regime ($V^{off} \simeq 0.008 \pm 0.01$) are much lower than the mean level spacing ($\delta(S) \simeq 0.2 \pm 0.1$ in Fig. 2(c)) providing us a good approximation in neglecting them when the Coulomb interaction strength $U \ll 5$. The Stoner criterion for itinerant magnetism is related to the exchange energy gain by an antisymmetric spin polarized two-body wave function that compensates the reduction of the kinetic energy. With our ansatz, in the regime of extended metallic waves it is expected that the large exchange matrix elements (especially the elements $V_{\alpha\alpha+1}^{\alpha+1\alpha}$) can favor a singlet-triplet transition when $U \cdot V^{ex} \simeq S$. For a 2D system with $L^2 = 8 \cdot 9$, $\langle S \rangle \simeq 0.2$ and $\langle V^{ex} \rangle \simeq 0.05$ (in the weak localization regime for $W = 6$) the interaction strength U must be at least 4. Besides, the enhanced interaction due to the increased return probability exhibits a finite temperature partial spin polarization [20].

By increasing the disorder, the exchange matrix elements have positive long tail fluctuations at values larger than the disorder averages (Fig. 3(a)) compensating the level repulsion of neighboring levels (and favoring also a less probable singlet-triplet transition). This will not be possible for strongly localized states when any overlap integral is equal to 0. In Fig. 4 we can see this scenario for a small value of the Coulomb interaction $U = 0.4$. Difficulties in solving the self-consistent equations [Eqs. (3-7)] for larger values of the interaction strength U prevent us from obtaining reasonable polarization transition when $U_H = 0$. The small values of M_z in this case represent the rare events in the disorder configuration space when the fluctuations of V^{ex} are larger than level repulsion.

The disorder induced spin polarization was previously obtained [22] for the periodic boundary conditions with $U = U_H$ and for a truncated many-body Hilbert space. This is possible for nonzero Hubbard interaction strength U_H when the evolution of S_z is increased by disorder (different curves in Fig. 4). The full polarization regime ($M_z = 1$) for a large value of W seems to be stable for the constant filling factor n/L^2 when the system size is increased. As it was stressed before, for linearly increasing level spacing at larger disorder values, the spin alignment will be turned off when $U_H \cdot C_{\alpha,\alpha} = U_H < S_{\alpha,\alpha+1} \simeq W/L^2$ (see inset of Fig. 4). In Fig. 5 we calculate the evolution of M_z varying the 2D electron density (n/L^2) for $W = 10$. When the electron number is increased the system shows a smooth decrease in M_z . At the same time, the transmittances calculated with Landauer formula for electrons at Fermi level show the features of 'insulator-metal' transition (in the inset of Fig. 5(a) the transmittances are enhanced by a factor of about 4). As a function of system properties (W and U_H) the spin magnetization can decrease from full or partially spin alignments. Our data show a possible transition toward a fully polarized state when the electron number n is decreased, suggestive of and similar to experimental results of Vitkalov *et al.* [3] and Shashkin *et al.*[4]. This takes place only for the values of interaction/disorder parameters that allow for a total spin alignment at low electron density (see Fig. 5(b)).

V. CONCLUSION

In this work we have studied the interplay between the disorder and interaction effects with regard to the spin magnetization of correlated electrons on a finite 2D lattice. Our numerical calculations suggest that spin polarization occurs for a finite 2D system with a model of disorder both for extended and localized regimes. The main results we derive are listed below.

(i). The level repulsion of neighboring states in the extended (and weak localization) regime is balanced by the large values of exchange energy or by their long tail asymmetric fluctuations when the system is gradually localized and the eigenfunctions become (extremely) sparse.

When the exchange elements decrease towards zero (increasing W) the spin polarization is not allowed unless strong Hubbard repulsion is turned on $U_H \neq 0$.

(ii). The disorder induced spin polarization is calculated for a finite 2D strongly correlated system and the data are self scaled in the limit of $n/L^2 = \text{constant}$. In the framework of unrestricted HF orbitals this is due to the increased separation of up and down sequences of the spectrum. When the full polarization is assigned, the short range Hubbard interaction will have no localization effect over the occupied orbitals while the opposite spin orbitals become increasingly delocalized. For a finite system the disorder induced spin polarization will be cut off when the linearly increasing level spacing exceeds the saturation value of inverse participation ratio.

(iii). When the number of electrons n decreases the 2D system can show a transition to a fully spin-polarized state. This, however, takes place only when the disorder (W) and interaction (U_H) strengths are properly tuned to allow for a ferromagnetic spin alignment in the system at low densities.

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