ELECTRON SPIN AND LOW ENERGY EXCITATIONS IN QUANTUM DOTS AND SMALL RINGS

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Abstract. The lowest excitation energies of confined and strongly interacting electrons with spin are calculated in terms of localized few particle 'pocket states'. The method, which becomes exact in the low density limit, is briefly explained. It is applied to quantum dots in one and two dimensions, and to a one–dimensional ring with an impurity and subject to an Aharonov–Bohm flux. The electron spin influences qualitatively observable quantities like the transport properties and the persistent current.

1. Introduction

Improved techniques for designing extremely small metal gates on top of the very mobile two dimensional (2D) electron systems in semiconductor hetero–structures created the new field of artificial, strongly interacting few electron systems [1]. Various interesting properties were discovered.

Quantum dots containing only small numbers of charge carriers ($N \lesssim 20$) [2, 3] were investigated. Coulomb interactions are important and result in well known single electron effects like the Coulomb blockade in small metallic islands connected to leads by tunnel barriers [6] and the conductance oscillations in quantum dots [4, 5]. Other properties of the latter are more specific for semiconductors. Small steps of the current with changing transport or gate voltages [7, 3] are due to the discreteness of the excitation energies of these 'artificial atoms'. Negative differential conductances were observed [7, 3] in non–linear transport. Electron correlations and spin play a crucial role for their understanding [8].

Other experiments are related to quantum coherence phenomena in *small rings* [9, 10]. A magnetic flux penetrating the ring gives rise to a persistent current [11]. In metallic rings the currents observed so far are much larger than expected. The reason for this is presently unclear, although it is believed that interactions should be of importance besides disorder. We will show that in addition to the Coulomb interaction the electron spin can strongly influence the persistent current.

At low dimensionality, electron density and temperature the formation of ordered structures in the charge density distribution is possible. The system reduces its kinetic energy [14], and the electrons stay close to sites of minimum electrostatic energy. For mean electron distances $a \gtrsim a_B$ (a_B Bohr radius) a charge density wave like state was predicted [15, 16] in one dimension (1D). Wigner crystallization takes place only for $a \gtrsim 100\, a_B$. Our calculations in terms of localized many body states which include electron correlations right from the beginning are designed for the intermediate regime $a_B \lesssim a \lesssim 100\, a_B$. We use 'pocket state' basis functions that reflect the tendency of the charge to localize. Electron spin can be incorporated.

The ratios between the lowest excitation energies were found to be independent of the electron density and of the precise form of the interaction. The eigenstates differ in their total spins. This can influence the transport properties of quantum dots [8] and also the magnitude and sign of the persistent current in small rings, when penetrated by an Aharonov–Bohm flux. Odd electron numbers respond diamagnetically to a magnetic flux for strong interaction, in contrast to the electron gas. In the presence of disorder levels of different spins can intersect when changing the flux. This causes, at $T = 0$, discontinuities in the persistent current. The current is periodic in the flux quantum and its magnitude increases with increasing electron–electron repulsion but cannot become as large as in clean rings.

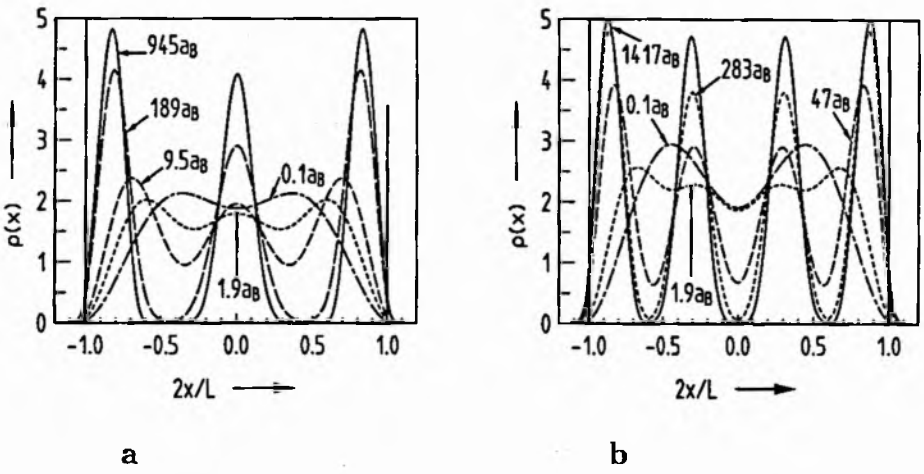
2. Pocket States

The Hamiltonian for electrons confined by a potential $v(x)$, is

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + v(x_i) \right) + \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} w(|x_i - x_j|) \quad , \tag{1}$$

where x_i and p_i are the (continuous) position and momentum of the i–th electron with effective mass m . The spin σ has to be taken into account via the Pauli principle, $w(|x|) = e^2/\varepsilon|x|$.

For a square well $v(x) = V_0\Theta(|x| - L/2)$ in one dimension (1D) the ground state charge density distribution $\varrho(x) = \sum_\sigma \langle \Psi_\sigma^+(x)\Psi_\sigma(x) \rangle$ was



a b

Figure 1. Charge density $\varrho(x)$ of (a) $N = 3$ and (b) $N = 4$ electrons in the ground state of a 1D square well potential of depth V_0 for different L [16] ($\varrho(x)$ in units of $2N/L$).

calculated numerically [16] (Figure 1). With increasing inter particle spacing $a \equiv L/(N-1)$ pronounced maxima and minima of $\varrho(x)$ appear. Two different density regimes $a_B < a < 100\, a_B$ (charge density wave) and $100 a_B \lesssim a$ (Wigner molecule) can be distinguished according to the amount of charge between the peaks. In the latter regime the electrons are completely separated like classical charged particles. Their spin leads to degeneracies of the vibrational energy levels determined from the inter–particle forces $-\partial w/\partial x$. A power law interaction, like the Coulomb potential, yields an algebraic decay of the typical excitation energies Ω with a.

For smaller a the spin–degenerate levels split (Figure 2). The individual levels have well defined total spins S and are, in the absence of spatial symmetries of the quantum dot, $(2S+1)$–fold degenerate. The number of levels for a given spin $S \leq N/2$ in the lowest multiplet is

$$n_s = \nu \frac{(2S+1)N!}{(N/2+S+1)!(N/2-S)!} \quad . \tag{2}$$

Here, ν is the number of configurations to minimum electrostatic energy that can be realized with classical electrons in a dot of given geometrical shape. For instance $\nu = 2(4)$ for two (three) electrons in a square. In 1D always $\nu = 1$. For this density, $a_B < a < 100\, a_B$, the pocket state approximation (PSA) applies.

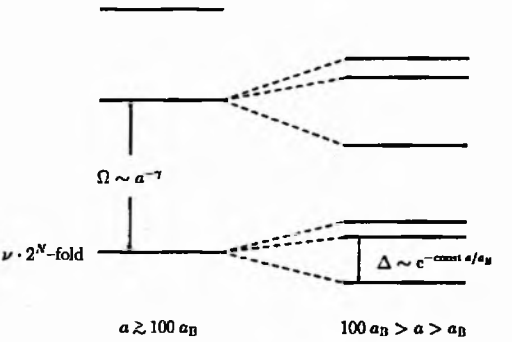


Figure 2. Scheme of the energy levels of a few strongly interacting electrons. The phonon like excitation energies Ω of the Wigner crystal at large electron distances a ($a \gtrsim 100\, a_B$) do not depend on spin. The levels are $\nu \cdot 2^N$–fold degenerate (left). With decreasing a they split because of tunneling between equivalent electron configurations (right). In the absence of spatial symmetries, the sublevels are associated uniquely with values of total spins S.

The splitting Δ of the vibrational levels is caused by tunneling between the $\nu \cdot N!$ different possibilities to distribute N localized electrons onto their equilibrium sites. Being interested only in the low energy excitations we can restrict the Hilbert space to 'pocket' states $|p\rangle$ ($1 \leq p \leq \nu \cdot N!$) corresponding to points of minimum Coulomb energy in configuration space [18]. They represent correlated N–particle states. The locations of the maxima of $|\langle x_1, \ldots, x_N | p\rangle|$ and of $|\langle x_1, \ldots, x_N | p'\rangle|$ differ in the permutations of their coordinates. The energetically lowest eigenstates of (1) are approximated by the eigenvectors of the matrix $H_{pp'} \equiv \langle p|H|p'\rangle$. Their behaviour under permutations of the particles determines uniquely the total spin S required to make this a Fermion state. In general this is not possible for all eigenvectors of $H_{pp'}$. The off–diagonal elements of $H_{pp'}$ for $p \neq p'$ determine the tunnel splittings Δ.

The matrix $H_{pp'}$ is block diagonal in the symmetrized basis of linear combinations $\mathcal{O}_\Gamma\{|p\rangle\}$ of the pocket states. $\mathcal{O}_\Gamma$ is the projector to the subspace which corresponds to the irreducible representation Γ of the group of permutations of N elements. Only blocks belonging to Fermion states are needed and must be diagonalized. For a 1D quantum dot this can be done analytically up to $N = 4$, while numerical results [16, 17, 18] require to handle up to 15000×15000 matrices.

The PSA is valid if Δ is small as compared to other excitation energies, for instance the vibrational excitations. Numerical calculations showed [18] that Δ decreases exponentially with increasing a as expected for tunneling

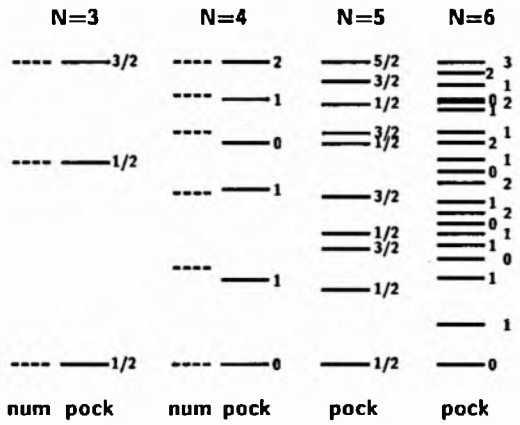


Figure 3. Fine structure multiplets for $N = 3, \ldots, 6$ as obtained within PSA (pock). Numerical results (num) (dashed) have been obtained [18] for systems of length $L = 11.3\, a_B$, $N = 3$ and $L = 13.2\, a_B$, $N = 4$. The energy scale t_N has been adjusted to normalize the overall width of the multiplets. No numerically calculated spectra are available for $N = 5, 6$.

integrals. Thus the PSA becomes exact for dilute systems, as $a \to \infty$. In the following, two applications will be discussed.

3. Quantum Dots

For quantum dots the electrons are confined by $v(x)$ (1). One type of off-diagonal matrix elements $H_{pp'}$ $(p \neq p')$, say t_N, dominates exponentially all others for large a. Retaining only the former leads to eigenvalues that are proportional to t_N [18]. The ratios between the low energy excitations are independent of a and of the precise form of the interaction $w(|x|)$.

In Figure 3 low energy spectra for the 1D square well model $v(x) = V_0\Theta(|x| - L/2)$ are shown for $N \leq 6$. Their ratios agree very well with the numerical values (dashed). The spectra obey $E(S) > E(S')$ if $S > S'$ as was proven by Lieb and Mattis [19] for interacting electrons in 1D. The energy $E(S)$ denotes the lowest energy eigenvalue of the system for a given spin S. The proof only requires $w(|x|)$ to be bounded and independent of spin. In particular, the ground state has always $S = 0$ or $S = 1/2$ depending on the parity of N. Furthermore, as can be proven via the corresponding spectra for Bosons [28], the energetically highest state is spin polarized, $S = N/2$. These "ferromagnetic" states play a particular role in non-linear transport through the quantum dot [8]. They are the ground states when considering spinless electrons. The spin degree of freedom allows the

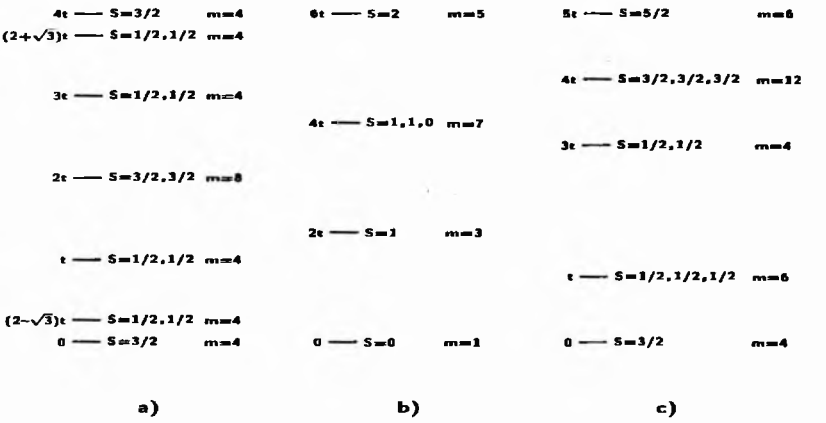


Figure 4. Multiplets for a) $N = 3$, b) $N = 4$, c) $N = 5$ electrons in a 2D square as obtained using the PSA (S total spin, m degeneracy of the levels).

interacting electrons to lower their ground state energy. A similar result was found recently also for the Wigner crystal in 3D [20].

In 2D the validity of the PSA requires $w(|x|)$ to decay slower than $w(|x|) \sim |x|^{-2}$. Furthermore no continuous symmetry should destroy the peaks in the charge density distribution. We consider therefore a square with hard walls and $N = 2, \ldots, 5$. Now $\nu > 1$ different classical electron arrangements to equal electrostatic energies exist. For instance two electrons like to stay in diagonally opposite corners. There are $\nu = 2$ possibilities for such configurations. The corner that $N = 3$ electrons leave empty can have $\nu = 4$ different positions. The number of states in the lowest multiplet is $\nu \cdot 2^N$. In contrast to 1D, where the dominant tunneling process always exchanges two adjacent electrons, the dominant processes in 2D are more complicated. For small N they can be approximated within the WKB approximation [28]. For $N = 2$ the transition between the two classical ground state configurations, and for $N = 3$ the jump of the hole between nearest corners dominate. For $N = 4$ the exchange of adjacent electrons is slightly favourable compared to the ring exchange involving all 4 electrons simultaneously. For $N = 5$ the exchange with the electron sitting in the middle of the square dominates.

Analytical results are shown in Figure 4. Most importantly, and in contrast to 1D, the spin of the ground state is not minimal in 2D. The $N = 3$ ground state is spin polarized and equals the five electron ground state with spin $S = 3/2$. This shows explicitly that the Lieb and Mattis–theorem [19]

is not valid in higher dimensions if $N > 2$. This has important consequences for the non-linear transport properties of quantum dots [29]. Spin selection rules can prohibit direct ground state to ground state transitions in some cases.

4. Persistent Currents

The method described in Section 2 can also be used to obtain the persistent currents circulating in small, normally conducting rings in the presence of an Aharonov–Bohm flux. The origin of the discrepancy of at least one order of magnitude between experimental results [9] and theoretical estimates is still not understood. It is now common belief that proper inclusion of the electron–electron interaction would improve the theoretical result but that the Hartree–Fock approximation is not sufficient [13, 21].

The influence of the Coulomb interaction in the presence of disorder is also not understood. Within a continuum model the Coulomb interaction is claimed to enhance strongly the current as compared to its (low) value caused by the disorder [22]. On the other hand, for a discrete Hubbard-type model including long range interactions [23] a reduction of the current even below the value for vanishing interaction is obtained.

An interesting question is the importance of the electron spin which has been investigated only for the one-dimensional Hubbard model in the absence of disorder [24]. Neither spinless impurities nor the Aharonov–Bohm flux destroy the total electron spin as a good quantum number. Only levels of equal spin repel each other when the flux is changed; levels corresponding to different spins can intersect.

We consider N electrons in a quasi 1D ring penetrated by a flux $\Phi \frac{h}{e}$ (Φ denotes the number of flux quanta). In polar coordinates,

$$H = B \sum_{j=1}^{N} (-i \frac{\partial}{\partial \vartheta_j} - \Phi)^2 + \frac{1}{2} \sum_{j,j'} w(|\vartheta_j - \vartheta_{j'}|) + \sum_j v(\vartheta_j) \,, \qquad (3)$$

$B = h^2/2mL^2$ is the rotational constant of a mass m on a ring of circumference L.

For simplicity we assume that only one impurity is present, described by the potential $v(\vartheta)$. Its range is shorter than $a = L/N$.

The pocket state approximation requires that vibrational excitation energies even of long wave lengths should be large,

$$2\pi \frac{e^2}{a_B} \frac{a_B}{L} \sqrt{\frac{a_B}{a}} \gg \frac{B}{N} \quad \Longleftrightarrow \quad \varepsilon \sqrt{\frac{a}{a_B}} N^2 \gg \pi \qquad (4)$$

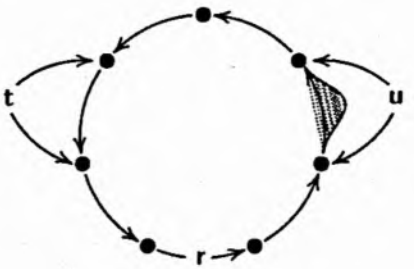


Figure 5. Illustration of the exchange processes associated with the tunneling integrals r, t and u (see text).

compared to the maximum possible value of Δ which is given by the rotational constant of the whole, rigid Wigner molecule. Here we assumed a transversal width $b2\pi L$ of the ring and Coulomb interactions $w(|\vartheta|) = 2\pi e^2/\varepsilon L\sqrt{\vartheta^2 + b^2}$ between the electrons. An additional impurity barrier leaves Ω almost unchanged while Δ is reduced. So the condition (4) is on the safe side for the applicability of the PSA.

Three different off-diagonal matrix elements $H_{pp'}$, $p \neq p'$, are important (Figure 5). The amplitude t for the pair exchange of two adjacent electrons on the ring causes a splitting of the 2^N-fold lowest vibrational multiplet into levels of different total spins. The stronger the electron–electron interaction is, the smaller is $|t|$. We assume all of the t to be equal, except one. The amplitude u for the exchange of the two electrons located on either side of the impurity is reduced, $|u| < |t|$. In addition to the Coulomb repulsion the particles have to tunnel through a barrier. When $u = t$ there is no impurity. Neither u nor t depend on the flux. The amplitude r for the (collective) ring exchange transferring the electrons cyclically by a around the ring contains a phase factor $e^{2\pi i\Phi}$. The phase is independent of N and equal to the phase that a one electron wave function acquires by turning its coordinate $\vartheta \longrightarrow \vartheta + 2\pi$ once around the loop.

The energy splitting caused by r cannot exceed the rotational constant for a circulating mass Nm. This gives an upper limit

$$|r| < \left\{\begin{matrix}2\\1\end{matrix}\right\} \frac{N\hbar^2}{4mL^2} \quad \text{for} \quad N \quad \left\{\begin{matrix}\text{even}\\\text{odd}\end{matrix}\right. .$$

One of the electrons has to pass the impurity barrier simultaneously with the cyclic ring exchange. This, apart from the large mass which is involved in such a process, is the main factor limiting $|r|$. It determines the magnitude of the persistent current. The calculation of $|r|$ is connected with

the transport and the pinning of a 1D Wigner crystal [15, 25]. The resulting non-trivial renormalizations of the impurity barrier at zero and at finite temperatures are basically the consequences of phonon like excitations. For spinless electrons they are the leading low energy contributions. In the PSA, we ignore vibrational excitations and thus, for consistency, neglect the influence of the strength of the $e-e$ interaction on r. Therefore our results are not valid at temperatures of the order of the vibrational energies. For $\Phi = 0$ t, u and r are negative. Their magnitudes and ranges are

parameter	depends on the	is small for	maximum value
$\|r\|$	impurity	strong impurity	$NB/(2\pi)^2$
t	interaction	strong interaction	$\|t\| \gg \|r\|$
u	impurity	strong impurity	$u = t$

TABLE 1. Magnitudes of the dominant tunneling integrals within the pocket state description.

summarized in Table 1. Diagonalization of the Hamiltonian matrix in the basis of pocket states, yields the desired eigenenergies, now as a function of Φ. For the spin polarized states $S = N/2$ they are

$$E_{S=N/2}(\Phi) = (-1)^N 2|r| \cos 2\pi\Phi \; - \; ((N-1)t \; + \; u) \quad . \tag{5}$$

The (negative) derivatives of the (lowest) energies with respect to Φ determine the persistent current.

Figures 6 and 7 show the lowest energy levels for $N = 4$ and $N = 5$ electrons. In both Figures 6 a and 7 a the strength of the $e-e$ interaction is increased compared to Figures 6 b and 7 b leaving the impurity unchanged. Figure 6 c shows the case of strong impurity scattering but weak interaction. In the latter case, the Φ-dispersion of the eigenvalues and thus the magnitude of the persistent current becomes small. The spin of the ground state is $S = 0$ or $S = 1/2$.

Various other features can be observed. In contrast to the case of spinless electrons, an impurity does not remove the discontinuities in the persistent current at zero temperature. This is because levels of different spins may intersect yielding jumps in the magnitude (mostly also in the sign) of the current at certain fluxes. Only at very weak $e-e$ interaction $|t| \gg |r|$

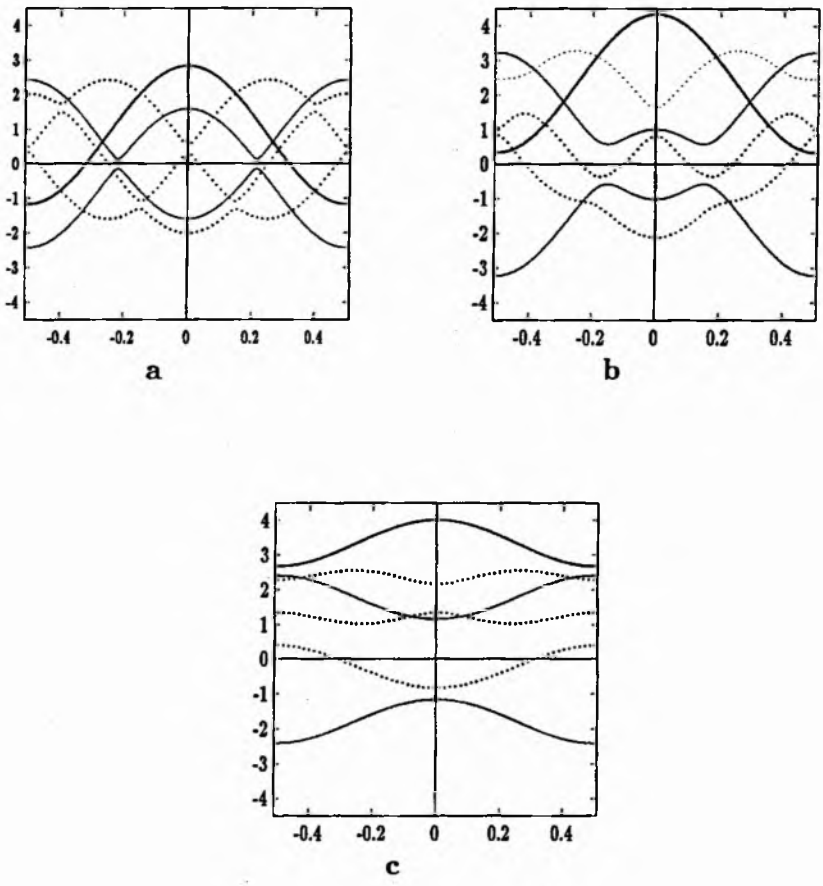


Figure 6. Energy levels versus the magnetic flux $\Phi \frac{h}{e}$ for $N = 4$ electrons. Thick solid lines : $S = 2$, dotted lines : $S = 1$, thin solid lines : $S = 0$. The parameters are (a) $r = -1$, $t = -1/4$, $u = -1/12$; (b) $r = -1$, $t = -3/4$, $u = -1/12$; (c) $r = -1/3$, $t = -1$, $u = -1/3$ (see text and Figure 5). (b) corresponds to increased strength of the interaction, (c) to increased height of the barrier and reduced strength of the interaction.

the spin of the ground state is fixed and the disorder smoothes the current, Figure 6 c.

The current is periodic in the flux quantum though weak interactions cause pronounced $h/2e$ contributions, visible in Figures 6 b and 7 b,c [26]. For very strong interaction $|t| \ll |r|$, the spin polarized state $S = N/2$ reaches almost the ground state for flux values $\Phi = 0$ or $\Phi = 1/2$ (depending on the parity of N). Its h/e periodicity (5) is not affected by impurities.

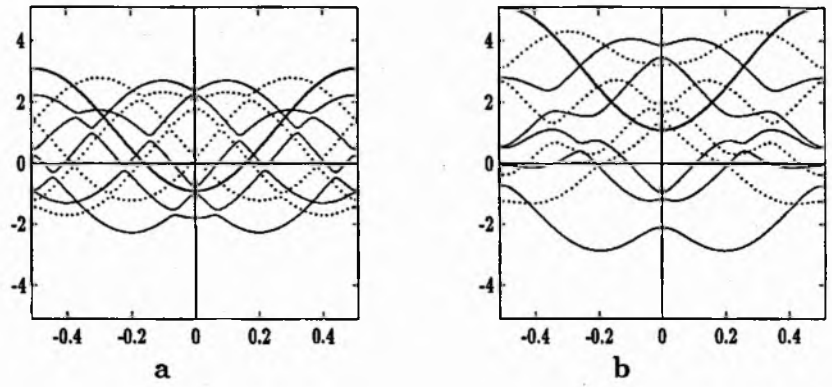


Figure 7. Same as Figures 6 a and 6 b but for $N = 5$. Thick solid lines : $S = 5/2$, dotted lines : $S = 3/2$, thin solid lines : $S = 1/2$.

The barrier reduces the current in two ways. Firstly, the magnitude of $|r|$ is reduced by the impurity potential, and secondly, the increasing repulsion between levels of the same spin causes a flattening of their dispersion in Φ. Increasing interaction does not alter the former but reduces significantly the level repulsion (compare Figures 6 b and 7 b with 6 a and 7 a). The level repulsion is reduced because $t \to 0$ means that also u vanishes. We find, in qualitative agreement with [21, 22], that (within the continuum model (3) in 1D) strong $e - e$ correlations can increase the persistent current compared to its value for weak interaction though the value for the clean ring should not be recovered.

The $e - e$ interaction influences the persistent current in magnitude and sign even in absence of the impurity. From Figures 6 a and 7 a can be deduced that the ground state energy oscillates with flux even when $t = u$ so that the levels do not repel. This is in contrast to previous claims [21]. Increasing $t = u$ moves the lines of different spins up or down in energy leaving their Φ–dispersion unchanged. Therefore the ground state may or may not change spin with Φ.

The sign of the susceptibility at small fluxes, dia– or paramagnetic, depends on N, and in general on both, interaction and impurity strengths. The following limiting behaviours are found. Weak interaction and impurity cannot alter the sign of the response compared to non–interacting electrons on a clean ring. The latter is diamagnetic only if $N - 2$ divided by 4 is an integer (including the case $N = 2$), otherwise paramagnetic [27], in

agreement with our results for $|t| \gg |r|$.

Very strong interaction $|t| \ll |r|$ causes the $S = N/2$ state to become (almost) the ground state at $\Phi = 0$ if N is odd. Its energy, in contrast to the non–interacting case, increases with Φ (5) which means that the response is diamagnetic.

5. Summary and Conclusions

We have discussed the low excitation energies of strongly interacting few electron systems. At small electron densities the Hilbert space can be restricted to localized many body 'pocket states'. They reflect correlations and the inhomogeneity of the charge density distribution. The latter is enhanced around the electrostatically favourable places. Spin can be included. The "permutational" tunneling between different arrangements of the electrons, preferrably located on equilibrium sites, determines the lowest energies.

One– and two dimensional quantum dots were investigated. At sufficiently large mean electron distance a the *ratios* between the excitation energies are independent of the precise form of the electron–electron potential (in 2D it should not decay faster than $\sim |x|^{-2}$) and of a.

The pocket state approximation is also applied to the persistent current in a one–dimensional ring with an impurity, threaded by an Aharonov–Bohm flux $\Phi \frac{h}{e}$. The different permutational tunneling processes are discussed. Results for the energy levels $E(\Phi)$ are presented for $N = 4$ and $N = 5$ electrons. Spin influences the persistent current qualitatively. Energy levels of different total spins can intersect and therefore limit the direct applicability of random matrix theory to this model. Disorder does not smooth the persistent current at zero temperature. It is periodic in the flux quantum h/e and increases with increasing interaction strength. The value for a clean ring, which itself depends on the electron–electron interaction, is not reached in presence of an impurity. Strong interaction leads to diamagnetic response at small fluxes when the electron number is odd, in contrast to the case of non–interacting electrons.

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