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LETTER TO THE EDITOR

Spin exchange in quantum rings and wires in the Wigner-crystal limit

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Abstract

We present a controlled method for computing the exchange coupling in strongly correlated one-dimensional electron systems. It is based on the asymptotically exact relation between the exchange constant and the pair-correlation function of spinless electrons. Explicit results are obtained for thin quantum rings with realistic Coulomb interactions, by calculating this function via a many-body instanton approach.

1. Introduction

Much attention has been devoted to the spin degree of freedom in one-dimensional (1D) conductors, both of a linear shape (quantum wires [1], carbon nanotubes [2]) and of a circular one (quantum rings [3–5]). Physical parameters of such systems, e.g., average distance between the electrons a, their total number N, effective mass m, dielectric constant ϵ, etc, can vary over a broad range or can be tuned experimentally. This creates unique opportunities for studying the effect of reduced dimensionality and strong Coulomb interactions on quantum magnetism. A number of new developments have generated a particular interest in the physics of a 1D Wigner crystal (WC). Unlike the case in higher dimensions, in 1D the crossover to this strongly correlated regime occurs at easily achievable electron densities [6], $r_s \equiv a/2a_B > 4$, where $a_B = \hbar^2\epsilon/me^2$ is the effective Bohr radius. Disorder has been the only major obstacle to realizing the 1D WC experimentally [1]. A promising solution to this problem has been apparently found, at least, for the case of carbon nanotubes. Very large r_s values have been recently demonstrated in suspended nanotube devices without appreciable intervention of disorder effects [2]. Because of their finite length, in the desired range $r_s > 4$ these devices contained only a few electrons, $N < 25$. Such finite-size systems are traditionally referred to as Wigner molecules [7]. The progress towards realizing Wigner-crystal (molecule) states in GaAs quantum wires has also been very encouraging [1]; therefore, one may hope that they will soon follow suit.

On the theoretical side, the 1D WC is interesting because of a dramatic difference between the characteristic energy scales for orbital and spin dynamics. This *strong* spin-charge

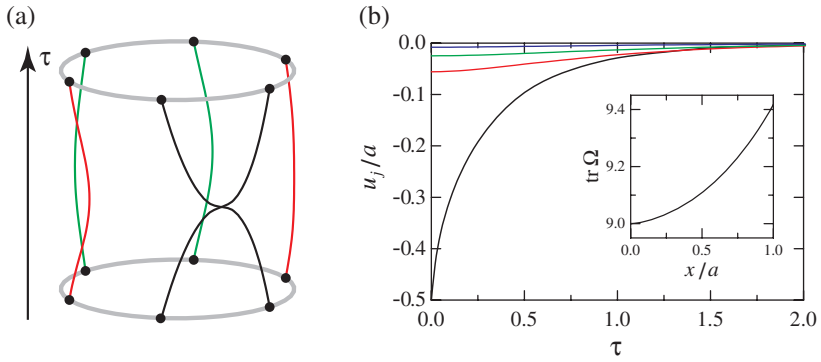

Figure 1. The instanton trajectories. (a) Schematic representation for an $N = 6$ Wigner molecule on a ring. (b) The trajectories of $1 \leqslant j \leqslant 4$ electrons for $N = 8$ (for notations used see the main text). Inset: function tr $\mathbf{\Omega}(x)$. The units of τ and $\mathbf{\Omega}$ are $\sqrt{2}a/s_0$ and its inverse.

(This figure is in colour only in the electronic version)

separation has been recently predicted to cause anomalies in many essential electron properties, e.g., ballistic conductance [8] of quantum wires and persistent current of quantum rings [7]. In view of the above, obtaining a reliable estimate of the spin-related energy scales, notably the exchange coupling J of the nearest-neighbour electrons, is desirable. It has been an outstanding challenge, though. As depicted in figure 1(a), J is determined by the acts of quantum tunnelling in which any two such electrons interchange. At $r_s \gg 1$ the corresponding potential barrier greatly exceeds the kinetic energy of the electron pair, which makes J exponentially small and difficult to compute numerically [7]. Attempts to derive J analytically (for the nontrivial case $N > 2$) were based on the approximation that neglects all degrees of freedom in the problem except the distance between the two interchanging electrons [8, 9]. We call this the frozen lattice approximation (FLA). The accuracy of the FLA is unclear because it is not justified by any small parameter. When a given pair does its exchange, it sets all other electrons in motion, too (figure 1). To obtain the much needed reliable estimate of J one has to treat the spin exchange in a Wigner molecule (or a WC) as a truly many-body process. This is done below in this letter, where we compute J to the leading order in the large parameter r_s.

2. Model and results

We assume that electrons are tightly confined in the transverse dimensions on a characteristic length scale $R \ll a_B$. This allows us to treat the problem as strictly 1D, provided we replace the Coulomb law by the appropriate effective interaction that goes to a finite value at distances $r \ll R$. We adopt a simple model form [10, 11] $U(r) = e^2/\epsilon(r + R)$, which is the simplest expression that correctly captures both short- and long-range behaviour of the (unscreened) Coulomb interaction for *any* realistic confining potential and is similar to other forms used in the literature [12, 13]. For convenience, we focus on the quantum ring geometry where $r = (Na/\pi)|\sin(\pi x/Na)|$ is the chord distance and x is the coordinate along the circumference.

In the Wigner molecule configuration electrons reside at the corners of a regular polygon. The effective low-energy Hamiltonian of such a state is given by [7]

$$H = \frac{\hbar^2}{2I}L^2 + J\sum_j \mathbf{S}_j\mathbf{S}_{j+1} + \sum_\alpha n_\alpha \hbar\omega_\alpha, \tag{1}$$

Table 1. Results for Wigner molecules on a ring (finite N) and for wires ($N = \infty$).

N	3	4	6	8	∞	∞-FLA
η	2.8009	2.7988(2)	2.7979(2)	2.7978(2)	2.7978(2)	2.8168
κ	3.0448	3.18(6)	3.26(6)	3.32(7)	3.36(7)	2.20

where L is the centre-of-mass angular momentum, $\mathbf{S}_j$ are electron spins and n_α are the occupation numbers of 'molecular vibrations'. At large r_s, the total moment of inertia I and the vibrational frequencies ω_α are easy to compute because they are close to their classical values. In order to calculate J, which is more difficult, we first show that the asymptotically exact relation exists between J and the pair-correlation function (PCF) $g(x)$ of a *spin polarized* 1D system. For an ultrathin wire, $\mathcal{L} \equiv \ln(a_B/R) \gg 1$, it is particularly compact:

$$J = (e^2 a_B^2/2\mathcal{L}\epsilon) g''(0), \qquad r_s \gg 1/\mathcal{L}. \tag{2}$$

By virtue of (2), the calculation of J reduces to an easier task of computing $g(x)$. Using the instanton method described below we arrive at the final result

$$J = \frac{\kappa}{(2r_s)^{5/4}} \frac{\pi}{\mathcal{L}} \frac{e^2}{\epsilon a_B} \exp(-\eta\sqrt{2r_s}), \qquad r_s \gg 1. \tag{3}$$

The values of η and κ are given in table 1. They demonstrate that the FLA [8, 9] errs significantly in κ, by about 50%, but surprisingly little in η, only by 0.7%.

3. Three electrons on a ring

We start with the simplest nontrivial case: $N = 3$. Let $0 \leqslant x_j < 3a$, $j = 0, 1, 2$, be the electron angular coordinates. We will compute the exchange coupling J between the $j = 0$ and the $j = 1$ electrons. It is convenient to go to new variables: the relative distance of the pair, $x \equiv x_1 - x_0$, and the location of the $j = 2$ electron with respect to the centre of mass, $X_2 \equiv x_2 - x_{cm} - a$. The motion of the centre of mass x_{cm} can be ignored. We arrive at the problem with one fast (x) and one slow (X_2) degree of freedom. (Classically, $X_2 = 0$.) The total potential energy $U_{tot}(x, X_2) = U(x) + U[(3/2)(X_2 + a) - x/2] + U[(3/2)(X_2 + a) + x/2]$ has two global minima in the fundamental domain $|x| < 3/2a$, at $x = \pm a$, $X_2 = 0$. They give rise to the two lowest-energy multiplets: the spin-singlet ground state $\mathbf{S}_0 + \mathbf{S}_1 = 0$ with an orbital wavefunction $\Phi_s(x, X_2)$ and the triplet with a wavefunction Φ_t. Their energy splitting is the desired exchange coupling J. It is given by the formula [14, 15]

$$J = (2\hbar^2/\mu) \int dX_2 \Phi_1 \partial_x \Phi_1|_{x=0}, \tag{4}$$

where the (normalized to unity) 'single-well' wavefunction $\Phi_1(x, X_2)$ is the ground state of the Hamiltonian with a modified potential $U_{tot} \to U_1 \equiv U_{tot}(\max\{x, 0\}, X_2)$ and $\mu = m/2$. Equation (4) is valid to order $O(J^2)$ [14]; with the same accuracy, the singlet and triplet wavefunctions are symmetric and antisymmetric combinations of the single-well wavefunctions, $\Phi_{s,t} = [\Phi_1(x, X_2) \pm \Phi_1(-x, X_2)]/\sqrt{2}$.

Let us discuss the form of $\Phi_1(x, X_2)$. Near its maximum at $x = a$, $X_2 = 0$, it is a simple Gaussian in both variables, characterized by an amplitude l of the zero-point motion in x and a frequency $\Omega(a)$ of the zero-point oscillations in X_2. Away from its maximum Φ_1 rapidly decays at $|X_2| \gtrsim l \gg a$. This justifies the following Gaussian approximation[1] in the *entire* fundamental domain of x:

$$\Phi_1 = \phi(x) \exp[-(M/2\hbar)\Omega(x) X_2^2], \tag{5}$$

[1] The Gaussian ansatz has been used previously for computing spin exchange in ^{3}He crystals [16].

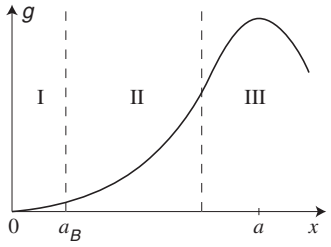

Figure 2. The PCF of a spin-polarized system (schematically). Regions I, II and III are described in the main text.

where $M = 3\mu$. It is important that at $x \ll a$, where the tunnelling barrier is large, Ω is a slow function of x. Hence, if $g(x)$ denotes the PCF of a spin-polarized molecule,

$$g(x) \equiv 2 \int \prod_{j=2}^{N-1} \mathrm{d}X_j \Phi_{\mathrm{t}}^2(x, X_2, \ldots, X_{N-1}), \qquad |x| < 3a/2, \tag{6}$$

then (4) immediately entails $J = (\hbar^2/4\mu)[\phi(0)/\phi'(0)]g''(0)$. Anticipating the discussion below, (6) is written for an arbitrary $N > 2$, with the notation $X_j \equiv x_j - x_{\mathrm{cm}} + (N-1-2j)(a/2)$ being used; the PCF is normalized as appropriate in the WC limit, $\int_0^{3a/2} g(x)\,\mathrm{d}x = 1$.

The equations on $\phi(x)$ and $\Omega(x)$ are obtained by substituting (5) into the Schrödinger equation and neglecting terms small in l/a. This results in the dependence of $g(x)$ on x sketched in figure 2. Near its $x = a$ maximum (region III) $g(x)$ is a Gaussian of width l. In region II the quasiclassical approximation applies. Finally, in an ultrathin wire, $\mathcal{L} \gg 1$, there is also region I, $x \lesssim a_{\mathrm{B}}$, where the quasiclassical approximation breaks down. Fortunately, the equations on $\phi(x)$ and $\Omega(x)$ can be simplified there, as $\Omega(x) \simeq \Omega(0)$ and $U_{\mathrm{tot}}(x) \simeq U(x) + 2U(3a/2)$. Similar to [10], this leads to $\phi(0)/\phi'(0) \simeq a_{\mathrm{B}}/\mathcal{L}$, which, combined with the expression for J, yields equations (2) and (3), with η and κ given by

$$\eta = 2 \int_0^a \frac{\mathrm{d}x}{a} \left[\frac{\epsilon a}{e^2} \Delta U_{\mathrm{tot}}(x) \right]^{1/2}, \tag{7}$$

$$\kappa = \frac{2^{5/4}}{\sqrt{\pi}} \mathrm{e}^{\xi(0)} \sqrt{\frac{\Omega(a)}{\Omega(0)}} \left[\frac{\epsilon a^3}{e^2} U''_{\mathrm{tot}}(a) \right]^{3/4}. \tag{8}$$

Thus, for the $N = 3$ case we were able to reduce the original complicated three-body eigenvalue problem to routine operations of solving an ordinary differential equation on $\Omega(x)$ and taking two quadratures. The resultant η and κ are listed in table 1. In comparison [8], the FLA underestimates κ by about 50%. It gets η correctly but only for $N = 3$; see more below.

One important comment is in order. The antisymmetry of the total fermion wavefunction imposes certain selection rules [17] for the allowed values of L (see (1)) at a given total spin S. The lowest-energy L eigenstates for the two possible S values in the $N = 3$ system, $S = 1/2$ and $3/2$, are $|L| = 1$ and 0, respectively. Since $J \ll \hbar^2/I$ at large r_{s}, the ground state of the system is the $L = 0$ spin quartet [7, 11].

4. $N > 3$ electrons on a ring

In a system of more than three electrons, the single-well function $\Phi_1(x, \mathbf{X})$ can be sought in the form similar to (5), but with the argument of the exponential replaced by

$(-1/2\hbar)(\Delta\mathbf{X}^{\dagger}\mathbf{M}^{1/2})\mathbf{\Omega}(x)(\mathbf{M}^{1/2}\Delta\mathbf{X})$, where $M_{ij}^{-1/2} = m^{-1/2}[\delta_{ij} - (1-\sqrt{2/N})/(N-2)]$. In the language of quantum tunnelling theory, $\mathbf{\Omega}(x)$ is a matrix that controls Gaussian fluctuations $\Delta\mathbf{X} = \mathbf{X} - \mathbf{X}^*$ around the instanton trajectory $\mathbf{X}^*(x)$, where $\mathbf{X} = (X_2, \ldots, X_{N-1})^{\mathrm{T}}$. Switching to the usual parametrization of the instanton by an 'imaginary time' τ, we seek $x(\tau)$ and $\mathbf{X}^*(\tau)$ that minimize the action

$$S_N = \int_0^\infty \frac{\mathrm{d}\tau}{\hbar}\left[\frac{\mu}{2}(\partial_\tau x)^2 + \frac{1}{2}(\partial_\tau \mathbf{X})^{\dagger}\mathbf{M}\partial_\tau\mathbf{X} + \Delta U_{\mathrm{tot}}\right], \tag{9}$$

subject to the boundary conditions $x(0) = 0$, $x(\infty) = a$ and $\mathbf{X}(\infty) = 0$. Henceforth U_{tot} is always meant to be evaluated on the instanton trajectory and ΔU_{tot} stands for the difference of its values at a given τ and at $\tau = \infty$. Repeating the steps of the derivation for the $N = 3$ case, we derive the following equations on $\phi(x)$ and $\mathbf{\Omega}(x)$:

$$\begin{aligned} &\partial_\tau \mathbf{\Omega} = \mathbf{\Omega}^2(\tau) - \boldsymbol{\omega}^2(\tau), \\ &\{(\hbar^2/2\mu)\partial_x^2 - U_{\mathrm{tot}}(x) - (\hbar/2)\,\mathrm{tr}\,\mathbf{\Omega}(x) + E\}\phi(x) = 0, \end{aligned} \tag{10}$$

where $\boldsymbol{\omega}$ is a positive-definite matrix such that $\boldsymbol{\omega}^2 = \mathbf{M}^{-1/2}\mathbf{\Xi}\mathbf{M}^{-1/2}$ and $\mathbf{\Xi}$ is the matrix of the second derivatives $\Xi_{ij} = \partial_{X_i}\partial_{X_j}U_{\mathrm{tot}}$. The equations are mutually consistent if $E = U_{\mathrm{tot}}(a) + (\hbar/2)[\mathrm{tr}\,\boldsymbol{\omega}(a) + \omega_0]$, $\omega_0 \equiv \hbar/\mu l^2$ and $\mathbf{\Omega}(a) = \boldsymbol{\omega}(a)$.

The PCF $g(x)$ in the quasiclassical region can be written in terms of the tunnelling action (9) and the appropriate prefactor as follows:

$$g(x) = \frac{a}{l^2}\left[\frac{1}{2\pi}\frac{\Omega(a)}{\Omega(x)}\frac{\hbar\omega_0}{U(x)}\right]^{1/2} \mathrm{e}^{\xi(x)-2S_N(x)}, \tag{11}$$

$$\xi(x) = \int_x^a \mathrm{d}y\left\{\frac{\omega_0 + \mathrm{tr}\,\mathbf{\Omega}(a) - \mathrm{tr}\,\mathbf{\Omega}(y)}{[(2/\mu)\Delta U_{\mathrm{tot}}(y)]^{1/2}} - \frac{1}{a-y}\right\}. \tag{12}$$

Here the action S_N is defined to be the value of the integral in (9) when its lower limit is replaced by $\tau = \tau(x)$. For η we find $\eta = 2S_N/\sqrt{2r_{\mathrm{s}}}$, while κ is given by equation (8) after the replacement $\Omega \to \det\mathbf{\Omega}$.

5. Calculation of the instanton

A few properties of the instanton follow from general considerations. The dimensional analysis of action (9) yields $S_N \propto \sqrt{r_{\mathrm{s}}}$, so that η is indeed just a constant. Also, from the symmetry of the problem, $X_{N+1-j}(\tau) = -X_j(\tau)$. Thus, in the special case of $N = 3$, the instanton trajectory is trivial: $X_2 \equiv 0$, i.e., the $j = 2$ electron does not move. This is why we were able to compute S_3 in a closed form. For $N > 3$ the situation is quite different: all electrons (except $j = (N+1)/2$ for odd N) *do* move. In order to investigate how important is the motion of electrons distant from the $j = 0, 1$ pair, let us consider the $N = \infty$ (*quantum wire*) case, where the far-field effects are the largest. If the X_j were small, we could expand ΔU_{tot} in (9) to the second order in X_j to obtain the harmonic action

$$S_{\mathrm{h}} = \frac{1}{2}\frac{m}{\hbar}\int\frac{\mathrm{d}k}{2\pi}\int\frac{\mathrm{d}\omega}{2\pi}|u_{k\omega}|^2[\omega^2 + \omega_p^2(k)], \tag{13}$$

where $u_{k\omega}$ is the Fourier transform of electron displacement $u_j(\tau) \equiv x_j - x_j^0$ from the classical equilibrium position $x_j^0 \equiv (j - 1/2)a$, $j \in \mathbb{Z}$, $\omega_p(k) \simeq s_0 k \ln^{1/2}(4.15/ka)$ is the plasmon dispersion in the 1D WC and $s_0 \equiv (e^2/\epsilon\mu a)^{1/2}$. Minimization of S_{h} with the specified boundary conditions yields $u_j(\tau) \propto vx_j^0/[(x_j^0)^2 + v^2\tau^2]$, where $v \simeq (s_0/2)\ln\{[(x_j^0)^2 + s_0^2\tau^2]/a^2\}$. Substituting this formula into harmonic action (13), we find that the contributions of distant electrons to S_{h} rapidly decay with $|j|$. Thus, a fast convergence of

η to its thermodynamic limit is expected as N increases. Encouraged by this conclusion, we undertook a direct numerical minimization of S for the set of N listed in table 1 using standard algorithms of the popular software package MATLAB. The optimal trajectories that we found for the case of $N = 8$ are shown in figure 1(b). As one can see, electron displacements reach some finite fractions of a at $\tau = 0$. This collective electron motion lowers the effective tunnelling barrier and causes η to drop below its FLA value, although only by 0.7%; see table 1.

Let us now discuss the prefactor κ. In the inset of figure 1(b) we plot $\mathrm{tr}\,\boldsymbol{\Omega}(x)$ computed by solving (10) numerically. To reduce the calculational burden, the matrix $\boldsymbol{\omega}$ and the potential energy U_{tot} in this equation were evaluated on the FLA trajectory $\mathbf{X}(\tau) = 0$ instead of the true instanton trajectory shown in figure 1(b). The error in κ incurred thereby is $\sim$2% [19]. In comparison, the FLA, where $\mathrm{tr}\,\boldsymbol{\Omega}(x) = \mathrm{const}$, yields κ about 50% smaller than the correct result, similar to $N = 3$.

A straightforward interpolation of our finite-N results from table 1 to larger number of electrons indicates that the changes in η and κ from $N = 8$ to $N = \infty$ are smaller than the accuracy of our numerical procedure.

6. Relation to current experiments

For carbon nanotube quantum dots [2], where the WC limit has apparently been realized, our formula (3) gives $J \sim 1$ K at $r_s = 4$, which should be verifiable experimentally. Unfortunately, the lowest measurement temperature was 0.3 K; therefore, the exchange correlations may have been washed out. We hope that our predictions can be checked in the next round of experiments. Energy-level spectroscopy of quantum rings [3–5] is another promising area where our results may apply. In longer 1D wires, J determines the velocity $v_\sigma = (\pi/2)Ja/\hbar$ of spin excitations, which can be measured by tunnelling [1], photoemission [18], or deduced from the enhancement of the spin susceptibility and electron specific heat [10]. Our result for v_σ reads (cf table 1)

$$v_\sigma/v_F = 5.67(\pi/\mathcal{L})r_s^{3/4}\mathrm{e}^{-\eta\sqrt{2r_s}}, \qquad \eta = 2.7978(2), \tag{14}$$

where $v_F = (\pi/2)(\hbar/ma)$ is the Fermi velocity.

Being asymptotically exact in the $r_s \to \infty$ limit, equations (3) and (14) are most accurate at large r_s. Additional arguments [19] suggest that at $r_s = 3$–4, where the Wigner molecule just forms, the accuracy of these equations is better than 50%. In principle, even higher accuracy at such r_s can be achieved if g in equation (2) is computed by the quantum Monte Carlo technique [20]. This is worth a separate investigation.

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Note added. After the completion of this work, we learned that Klironomos *et al* [21] independently computed $\eta = 2.798\,05(5)$, but not the prefactor κ. These authors also considered a correction to η due to a finite radius of the wire R. We can show that as R increases the ratio $\pi/\mathcal{L}$ in (14) is replaced by a more complicated expression that tends to unity at $R > a_B$.

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