Exchange coupling in quantum rings and wires in the Wigner-crystal limit

M.M. Fogler\textsuperscript{1} and E. Pivovarov\textsuperscript{1}

\textsuperscript{1}University of California San Diego, Department of Physics, 9500 Gilman Drive, La Jolla, CA 92039, USA

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

1. INTRODUCTION

Quantum magnetism of nanostructures has become the latest avenue for exploring a perennial question of the condensed-matter physics, the effect of Coulomb interaction on the electron spin degree of freedom. Much interest has been devoted to one-dimensional (1D) conductors, both of linear shape (quantum wires, carbon nanotubes) and recently, of a circular one (quantum rings) \cite{1–3}. Parameters of these systems, e.g., average distance between the electrons $a$, their total number $N$, their effective mass $m$, dielectric constant $\varepsilon$, effective Bohr radius $a_B = \hbar^2/\varepsilon m^2$, etc., can vary over a broad range or can be tuned experimentally, creating an intriguing opportunity of reaching the Wigner-crystal (WC) limit, $r_s \equiv a/2a_B \gg 1$, where the energy scales for orbital and spin dynamics are drastically different. This strong spin-charge separation is expected to cause anomalies in many essential electron properties, e.g., ballistic conductance \cite{4} of quantum wires and persistent current of quantum rings \cite{5}. In the latter geometry electrons reside at the corners of a regular polygon forming a configuration known as a “Wigner molecule.” The effective low-energy Hamiltonian of such a state is given by \cite{5}

$$H = \frac{\hbar^2}{2l} L^2 + J \sum_j S_j S_{j+1} + \sum_s n_s \hbar \omega_s,$$ (1.1)

where $L$ is the center-of-mass angular momentum, $S_j$ are electron spins, and $n_s$ are the occupation numbers of “molecular vibrations”. (The same Hamiltonian applies to small-$N$ quantum dots). At large $r_s$, the total moment of inertia $I$ and the vibrational frequencies $\omega_s$ are easy to compute because they are close to their classical values.

In contrast, the calculation of the exchange coupling $J$, which governs the spin-related quantities, is an important open question. Physically, $J$ is determined by the acts of quantum tunneling in which two adjacent electrons interchange. At $r_s \gg 1$ the corresponding potential barrier greatly exceeds the kinetic energy of the electron pair, which makes $J$ exponential small and difficult to compute numerically \cite{5}. Attempts to estimate $J$ 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 \cite{4, 6}. We call this a 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. In view of the recent intriguing experimental \cite{7, 8} and theoretical \cite{4} work on spin-related effects in 1D conductors a reliable estimate of $J$ is desirable. It is obtained in this paper, where we treat the spin exchange in a Wigner molecule (or a WC) as a many-body process and 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 lengthscale $R \ll a_B$. This allows us to treat the problem as strictly 1D, provided we replace the Coulomb law by the proper effective interaction [9]. We adopt a simple model form [10] $U(r) = \epsilon^2/(r + R)$, which nevertheless captures correctly both the short- and the long-range behavior of the interaction for any realistic confinement and is similar to other expressions used in the literature [9, 11].

On a ring, $r$ stands for the chord distance, $r = (Na/\pi)|\sin(\pi x/Na)|$, where $x$ is the coordinate along the circumference.

We find 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, $L \equiv \ln(a_B/R) \gg 1$, it is particularly simple:

$$J = \left(\frac{\epsilon^2 a_B^2}{2Le}\right) g'(0), \quad r_s \gg 1/L. \quad (2.1)$$

By virtue of Eq. (2.1), the calculation of $J$ reduces to an easier task of computing $g(x)$. Our final result is

$$J = \frac{\kappa}{(2\pi)^{5/4} L\epsilon a_B} \frac{\pi \epsilon}{e} \exp \left(-\eta \sqrt{2r_s}\right), \quad r_s \gg 1, \quad (2.2)$$

where the values of $\eta$ and $\kappa$ are given in Table 1, alongside the predictions of the FLA [4, 6]. The latter errs by about 50% in $\kappa$ but surprisingly little in $\eta$, only by 0.7%.

3. CALCULATIONAL METHOD

For $N \geq 3$ electrons on a ring, consider the exchange of two adjacent electrons with (angular) coordinates $x_0$ and $x_1$. Introduce notation $x = x_1 - x_0$. Let $X$ be a column vector with components $X_j \equiv x_j - x_{cm} + (N - 1 - 2j)(a/2)$, where $2 \leq j \leq N - 1$ and $x_{cm}$ is the center of mass of the system. Let $\Phi_i = (x, X)$ be the orbital wavefunction of the lowest-energy fully spin-polarized state (neglecting the irrelevant center-of-mass motion). As shown long ago by Herring [12], it is possible to define a (normalized and real) “single-well” wavefunction $\Phi_1$ such that at $0 < x < 3a/2$ (1) it satisfies the many-body Schrödinger equation (2) it is related to $\Phi_0$ according to $\Phi_i = [\Phi_1(x, X_2) - \Phi_1(-x, X_2)]/\sqrt{2} + O(J^2)$, and (3) it determines $J$ to order $O(J^2)$ through the formula

$$J = \frac{(2\hbar^2/\mu)}{E} \left| \prod_{j=2}^{N-1} dX_j \Phi_1 \phi|_{x=0} \right|. \quad (3.1)$$

In comparison, the PCF of a spin-polarized molecule is given by

$$g(x) = 2\sqrt{\prod_{j=2}^{N-1} dX_j/\Phi_1^2(x, X)}, \quad |x| < 3a/2. \quad (3.2)$$

For a given small $x$, the PCF is exponentially small and is dominated by a certain saddle-point (instanton) $X = X^*(x)$. Similarly, $J$ is determined by the neighborhood of $X^*(0)$. Switching to the usual parametrization of the instanton by an “imaginary-time” $\tau$, one can show that $x(\tau)$ and $X^*(\tau)$ must minimize the action

$$S = \int_0^\infty d\tau \left[ \frac{\mu}{2} \left(\frac{\partial \phi}{\partial \tau}\right)^2 + \frac{1}{2} \langle \hat{\phi}, \hat{X} \rangle M \hat{\phi}, \hat{X} + \Delta U_{\text{tot}} \right], \quad x(0) = 0, x(\infty) = a, X(\infty) = 0. \quad (3.3)$$

Here $\mu = m/2$ and the matrix elements of $M^{-1/2}$ are given by $M_{ij}^{-1/2} = m^{-1/2} [\Delta_{ij} - (1 - \sqrt{2}/N)/(N - 2)]$. Furthermore, it is legitimate to seek $\Phi_1$ in the form [13]

$$\Phi_1 = \phi(x) \exp \left[-(1/2\hbar)\Delta X^\dagger M_{ij}^{1/2} \Omega(x) M_{ij}^{1/2} \Delta X \right], \quad \Delta X(x) \equiv X(x) - X^*(x), \quad (3.4)$$
where matrix $\Omega$ determines the Gaussian fluctuations around the instanton. Substituting the last ansatz into the Schrödinger equation we obtain, after some algebra:

$$\hat{\epsilon}_x \Omega = \Omega^2(\tau) - \omega^2(\tau), \quad \{ (h^2/2\mu)\dot{\epsilon}_x^2 - U_{\text{tot}}(x) - (h/2) \text{tr} \Omega(x) + E \} \phi(x) = 0. \quad (3.5)$$

Here the total interaction energy $U_{\text{tot}}$ is meant to be evaluated on the instanton trajectory, $\Delta U_{\text{tot}}$ stands for the difference of its values at a given $\tau = \tau(x)$ and at $\tau = \infty$. Matrix $\omega$ is such that $\omega^2 = M^{-1/2} \Xi M^{-1/2}$, where $\Xi$ is the matrix of the second derivatives $\Xi_{ij} = \delta_{ij} \delta_{X_i X_j} U_{\text{tot}}$. Finally, the constant $E$ of dimension of energy is such that at $x \to a$, the solution of Eq. (3.5) matches the expected Gaussian form, $\phi(x) \propto \exp[-(x-a)^2/2l^2]$, where $l = [\hbar^2/\mu \dot{\epsilon}_x^2 U_{\text{tot}}(a)]^{1/4} \sim r_s^{-1/4} a \ll a$ is the amplitude of the zero-point motion in $x$.

Due to space limitations, we quote only the final results of the derivation [14]:

$$g(x) = \frac{a}{l} \left[ \frac{1}{2\pi} \text{det} \Omega(a) \right]^{1/2} \exp \left[ -\sqrt{2} \eta \right], \quad a \ll a_B << a, \quad a_B = \frac{\hbar}{m^*}. \quad (3.6)$$

Here the action $S(x)$ is defined to be the value of the integral in Eq. (3.3) when its lower limit is replaced by $\tau = \tau(x)$. The parameters $\eta$ and $\kappa$ in Eq. (2.2) are given by

$$\eta = \frac{2 S(0)}{\sqrt{2r_s}} = 2 \int_0^a dx \left[ \frac{\epsilon a}{e^2} \Delta U_{\text{tot}}(x) \right]^{1/2}, \quad \kappa = \frac{2^{5/4}}{\sqrt{\pi}} \left[ \left( \frac{\text{det} \Omega(0)}{\text{det} \Omega(x)} \right)^{3/4} \right]. \quad (3.8)$$

In comparison, the FLA [4], it amounts to setting $\Omega \to \Omega(x = a)$ and $X^* \to 0$ everywhere.

For $N = 3$, the instanton trajectory can be found in quadratures because the symmetry dictates $X^*_3 = 0$. For $N > 3$ listed in Table 1, $X^*$ were found numerically by minimization $S$ using standard algorithms. In all cases the displacement of electrons along the instanton trajectories were found to reach some finite but numerically small fractions of $a$ at $\tau = 0$. This collective electron motion lowers the effective tunneling barrier and causes $\eta$ to drop below its FLA value, although only by 0.7%, see Table 1. We estimate that the result for $N = 8$ coincides with the thermodynamic limit, i.e., quantum wire within the accuracy of the calculation.

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

<table>
<thead>
<tr>
<th>$N$</th>
<th>3</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>$\infty$</th>
<th>$\infty$-FLA</th>
</tr>
</thead>
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<tr>
<td>$\eta$</td>
<td>2.8009</td>
<td>2.7988(2)</td>
<td>2.7979(2)</td>
<td>2.7978(2)</td>
<td>2.7978(2)</td>
<td>2.8168</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>0.3448</td>
<td>0.318(6)</td>
<td>0.326(6)</td>
<td>0.332(7)</td>
<td>0.336(7)</td>
<td>0.336</td>
</tr>
</tbody>
</table>

To find the prefactor $\kappa$ function $\text{tr} \Omega(x)$ was computed by solving Eq. (3.5) numerically. To reduce the calculational burden, we set $X^*(\tau) \to 0$ instead of using the true instanton trajectory. The error in $\kappa$ incurred thereby, about $\sim 2\%$, was estimated from comparison with known exact results for a related model [14]. The resultant $\eta$ and $\kappa$ are listed in Table 1. In comparison, the FLA [4] underestimates $\kappa$ by about 50%. It gets $\eta$ correctly but only for $N = 3$ (where the displacement of the third electron along its instanton trajectory indeed vanishes).

### 4. RELATION TO EXPERIMENTS

Our results have direct implications for the energy spectroscopy of spin-splitting in nanoscale quantum rings and dots [1–3]. In longer 1D wires, $J$ determines the velocity $v_e = (\pi/2)Ja/\hbar$ of spin excitations,
which can be measured by tunneling [7], photoemission [8], or deduced from the enhancement of the spin susceptibility and electron specific heat [10]. Our result for \( v \) reads (cf. Table 1)

\[
\frac{v_s}{v_F} = 5.67 \left( \frac{\pi}{L} \right) \eta^{3/4} e^{-\sqrt{2\eta}}, \quad \eta = 2.7978(2),
\]

where \( v_F = (\pi/2)\hbar/n/m \) is the Fermi velocity.

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Note added.— After completion of Ref. [14], we learned that Klironomos et al. [15] independently computed \( \eta = 2.79805(5) \), but not the prefactor \( \kappa \). These authors also considered a correction to \( \eta \) due to a finite radius of the wire \( R \). We can show that as \( R \) increases, the ratio \( \pi/L \) in Eq. (4.1) is replaced by a more complicated expression that tends to unity at \( R > a_B \).

References