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Conductance of nano-systems with interactions coupled via conduction electrons: Effect of indirect exchange interactions

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November 6, 2006

Abstract. A nano-system in which electrons interact and in contact with Fermi leads gives rise to an effective one-body scattering which depends on the presence of other scatterers in the attached leads. This non local effect is a pure many-body effect that one neglects when one takes non interacting models for describing quantum transport. This enhances the non-local character of the quantum conductance by exchange interactions of a type similar to the RKKY-interaction between local magnetic moments. A theoretical study of this effect is given assuming the Hartree-Fock approximation for spinless fermions of Fermi momentum $k_{\rm F}$ in an infinite chain embedding two scatterers separated by a segment of length L_c. The fermions interact only inside the two scatterers. The dependence of one scatterer onto the other exhibits oscillations of period $\pi/k_{\rm F}$ which decay as $1/L_c$ and which are suppressed when L_c exceeds the thermal length $L_{\rm T}$. The analytical results given by the Hartree-Fock approximation are compared with exact numerical results obtained with the embedding method and the DMRG algorithm.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 72.10.-d Theory of electronic transport; scattering mechanisms – 73.23.-b Electronic transport in mesoscopic systems

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1 Introduction

The coupling of nano-objects via conduction electrons was discovered long ago, in the case of spins of magnetic ions, or of nuclei, which results indirectly from the interaction of such spins with those of conduction electrons in metals. After tracing out the degrees of freedom of the conduction electrons, one gets an effective spin Hamiltonian characterized by an oscillatory long range interaction, the RKKY-interaction [1,2,3,4], which plays a crucial role in understanding the large variety of possible ordered spin structures in magnetic crystals. If $\boldsymbol{I}_i$ is a local magnetic moment in a metal, the conduction electrons give rise to an interaction energy between these moments, which can be described by an Hamiltonian of the form:

$$H_{\rm RKKY} = \sum_i \sum_{j<i} J_{ij} \boldsymbol{I}_i \cdot \boldsymbol{I}_j. \qquad (1)$$

The coupling term between two moments separated by a distance R_{ij} behaves as

$$J_{ij} \propto \frac{2k_{\rm F}R_{ij}\cos(2k_{\rm F}R_{ij}) - \sin(2k_{\rm F}R_{ij})}{R_{ij}^4} \qquad (2)$$

in $d = 3$ dimensions, $k_{\rm F}$ being the Fermi momentum of the conduction electrons. In $d = 1$ dimension, this gives a long range $1/R$ interaction with oscillations of periodicity $\pi/k_{\rm F}$.

We show in this work that a similar phenomenon characterizes also the quantum conductance of nano-systems in which electrons interact, coupled via metallic wires. This phenomenon is very general and does not require to include the spin degrees of freedom. Combining Landauer's formulation [5] of quantum transport and the Hartree-Fock approximation, as reviewed in Ref. [6,7], we will show that the scattering matrix of an interacting system depends on what is embedded at a distance R of the interacting system in the attached leads, this dependence decaying as $1/R^d$ with oscillations of periodicity $\pi/k_{\rm F}$. This non local character of the quantum conductance is another example of the effect of indirect exchange interactions between interacting nano-systems via conduction electrons, as the RKKY-interaction between local magnetic moments.

To study this phenomenon, we take an infinite chain where spinless fermions do not interact outside two identical regions where the scattering is a pure many body effect due to Coulomb repulsions. The chain is described by a one dimensional tight binding model with nearest neighbor hopping $t_h = 1$. A nearest neighbor repulsion of strength U acts only between two consecutive sites, in two regions which are connected by $L_{\rm c}$ sites where the par-

ticles do not interact. This model is simple enough to be analytically solved at a mean field level, using the Hartree-Fock (HF) approximation. To simplify the calculations, we add positive compensating potentials which exactly cancels the Hartree terms of the HF equation. But the exchange term modifies the hopping term coupling the two internal sites of each scatterers, in such a way that it takes a value v instead of t_h. In the HF approximation, v is given by a self-consistent equation. Having v, it is straightforward to obtain the scattering matrix $S_1(v)$ of one scatterer at the Fermi energy of the infinite non interacting chain. Using the combination law of the one-body S-matrices in series, one can get the scatteringmatrix $S_2(v)$, and hence the dimensionless conductance $g_2^{k_{\rm F}}$ (in units of e^2/h) of these two many-body scatterers in series, in the HF approximation.

For such a system where two identical many-body scatterers are coupled by a perfect wire of $L_{\rm c}$ sites where the electrons do not interact, our main result is to show that the value of v characterizing one scatterer differs from its value when there is no second scatterer by an oscillatory term of period $\pi/k_{\rm F}$ which decays as $1/L$c. In certain limits, v can be given in a simple form as a function of $U, L_{\rm c}$ and $k_{\rm F}$. For instance, for a half-filled chain ($k_{\rm F} = \pi/2$) and weak interactions, the effective hopping term v reads

$$v = 1 + \frac{2}{2-\pi+2\pi/U} + \frac{(-1)^{L_{\rm c}}}{L_{\rm c}}\left(\frac{1}{2-\pi+2\pi/U}\right)^2 + \dots \tag{3}$$

In this limit, this expression shows how the effective hopping term v characterizing a single scatterer decays as $1/L_c$ towards its value when it is not in series with another one, with the even-odd oscillations characteristic of a half-filled chain. Using Eq. (3), it is straightforward to show how the scattering matrix $S_1(v)$ of a single scatterer is modified by the presence of a second scatterer. We underline that this non local effect is a pure many-body effect that one neglects when one takes non interacting models for describing quantum transport. This non local effect was first numerically discovered in a previous work [8], using the embedding method [9,10,11,12,13,14,15,16] and the DMRG algorithm [17,18] valid for one dimensional fermions. In this work, we give a simple theory of this effect based on the HF approximation, which turns out to qualitatively describe this non local effect for all values of U, including its suppression in the limit when $U \to \infty$. The HF approximation becomes quantitatively accurate for small strengths U of the interaction. Moreover, we will also show that this non local effect vanishes when the length $L_{\rm c}$ of the coupling wire exceeds the thermal length $L_{\rm T}$ characterizing free fermions in one dimension.

The paper is organized as follows:

In section 2, we consider a single scatterer with a nearest neighbor repulsion of strength U embedded in an infinite chain. In the first sub-section, the HF equation of this simple model is written, leading us to study a chain where the hopping term between the two central sites is equal to v instead of $t_h = 1$. This one body model is solved in the second sub-section, allowing us to obtain the implicit equation giving v in the HF approximation. The system being symmetric upon reflection, we use scattering phase shifts and Friedel sum rule for this purpose. In the third sub-section, the conductance of this single scatterer is studied as a function of the strength U of the nearest neighbor repulsion, the HF behavior being compared to the exact results given by the embedding method and the DMRG algorithm. In the fourth sub-section, the Friedel oscillations of the particle density around the scatterer are described. In a last sub-section, a correlation function inside the attached leads is calculated at a distance p from the scatterer, which will be useful for describing the case of two scatterers in series. This function is shown to decay as $1/p$ with oscillations of periodicity $\pi/k_{\rm F}$ towards an asymptotic value characterizing the chain without scatterer.

In section 3, we study the conductance of two scatterers in series, coupled by a scattering free wire of L_c sites. In the first sub-section, simple analytical expressions are given in the limit where the strength U of the interaction acting inside the two scatterers remains small. Notably, we show that the effective hopping term v characterizing each scatterer differs from the value obtained in the section 2 by a correction which decays as $1/L_c$ with oscillations of periodicity $\pi/k_{\rm F}$. In the second sub-section, the Hartree-Fock equation is solved exactly for arbitrary values of U, allowing us to show that the weak U-expansion assumed in the first sub-section remains valid till $U \approx t_h$. The effective hopping term v characterizing a single scatterer being modified when it is in series with another, the implication of this non local effect upon the conductance is illustrated in the third sub-section, the HF curves describing the conductance oscillations of the two scatterers in series being similar to the curves numerically obtained in Ref. [8].

In section 4, the results for two scatterers in series given by the HF theory are compared to the exact numerical values given in Ref. [8]. The HF theory turns out to give a good qualitative description of the non local effect, which becomes quantitatively accurate when $U < t_h$ for the very small scattering regions which we have considered.

In section 5, we show that this non local effect is suppressed at a temperature T, when the length L_c of the coupling wire exceeds the thermal length $L_{\rm T} \propto v_{\rm F}/T$ of free fermions in one dimension, $v_{\rm F}$ being the Fermi velocity.

We conclude in section 6 by a summary of the main results, underlining their relevance for a theory of the non local character of quantum transport measurements, and suggesting straightforward extensions of this theory outside one dimension.

2 Transmission through a single many-body scatterer

2.1 Microscopic model and exchange energy

To study the indirect exchange interaction via conduction electrons between nano-systems in which the electrons in-

teract, we begin to study the simplest many-body scatterer, taking a tight-binding model of spinless fermions which do not interact, unless they occupy the two central sites 0 and 1 of an infinite chain, which costs a nearest neighbor repulsion energy U. Assuming the Hartree-Fock approximation, this leads us to study an analytically solvable one body model where the hopping term between the two central sites is modified by the interaction, modification which has to be calculated self-consistently. The many-body scattering system is described by an Hamiltonian $H = H_{kin} + H_{int}$. The kinetic and interaction terms respectively read

$$\begin{aligned} H_{kin} &= -\sum_{p=-\infty}^{\infty} t_{\rm h}(c_p^\dagger c_{p-1} + c_{p-1}^\dagger c_p) \\ H_{int} &= U\left[n_1 - V_+\right]\left[n_0 - V_+\right] . \end{aligned} \tag{4}$$

The hopping amplitude $t_{\rm h} = 1$ between nearest neighbor sites sets the energy scale, c_p ($c_p^\dagger$) is the annihilation (creation) operator at site p, and $n_p = c_p^\dagger c_p$. The potential V_+ is due to a positive background charge which exactly cancels the Hartree term of the HF equation. The conduction band corresponds to energies $-2 < E = -2\cos k < 2$ (k real). H is invariant under reflections ($p-1/2 \to -p+1/2$) and exhibits particle-hole symmetry if the chain is half filled. In this case, $V_+ = 1/2$, the Fermi momentum $k_{\rm F} = \pi/2$ and one has a uniform density without Friedel oscillations around the central region where the fermions interact.

In the HF approximation, one assumes a variational ground state which is a Slater determinant of one-body wave-functions $\psi_\alpha(p)$ of energies $E_\alpha < E_F$. Since in our model the negative charge inside the scatterer is exactly compensated by a positive background charge, the Hartree term is cancelled and we have just to take into account the exchange term in the Hartree-Fock equation [19,20] giving the $\psi_\alpha(p)$:

$$-\psi_\alpha(p+1) - \psi_\alpha(p-1) - \sum_{p'} t_{p,p'}^{\rm HF}\psi_\alpha(p') = E_\alpha\psi_\alpha(p). \tag{5}$$

The exchange term

$$t_{p,p'}^{\rm HF} = \sum_{E_\beta<E_F} U_{p,p'}\psi_\beta^*(p')\psi_\beta(p) \tag{6}$$

with the taken nearest neighbor repulsion

$$U_{p,p'} = U\left\{\delta_{p,0}\delta_{p',1} + \delta_{p,1}\delta_{p',0}\right\}, \tag{7}$$

is very simple. It is zero, excepted between the two central sites where the fermions interact, where it yields an increase of the strength of the hopping term coupling the two central sites by an amount

$$t_{0,1}^{\rm HF}(U) = U\sum_{E_\alpha<E_F}\psi_\alpha^*(1)\psi_\alpha(0) = U\left\langle c_1^\dagger c_0\right\rangle. \tag{8}$$

The Hartree-Fock equation describes a tight-binding model which is represented in Fig.1, where the hopping

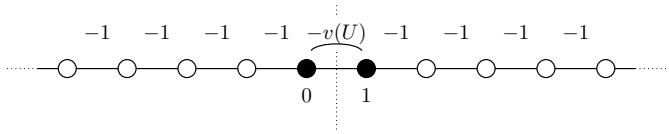

Fig. 1. Effective one body model obtained assuming the Hartree-Fock approximation for a single many body scatterer (Hamiltonian (4)). The hopping term (indicated above) $v(U)$ between the sites at $p = 0$ and $p = 1$ (indicated below) depends on U and $k_{\rm F}$.

term between the two central sites is no longer equal to $t_h = 1$, but takes an interaction dependent value v, which is given by an implicit equation:

$$v = t_h + t_{0,1}^{\rm HF}(v) = 1 + t_{0,1}^{\rm HF}(v) \tag{9}$$

for $t_h = 1$.

2.2 Scattering phase shifts and density of states

The effective one-body model being symmetric upon the reflection ($p-1/2 \to -p+1/2$), its Hamiltonian has even and odd standing-wave solutions $\psi_k^0(p)$ and $\psi_k^1(p)$, which can be written [21] inside the conduction band as:

$$\begin{aligned} \psi_k^0(p) &= \sqrt{\frac{2}{L}}\cos\left(k(p-\frac{1}{2}) - \delta_0(k)\right) \\ \psi_k^1(p) &= \sqrt{\frac{2}{L}}\sin\left(k(p-\frac{1}{2}) - \delta_1(k)\right), \end{aligned} \tag{10}$$

at the left side of the scatterer ($p \le 0$) and

$$\begin{aligned} \psi_k^0(p) &= \sqrt{\frac{2}{L}}\cos\left(k(p-\frac{1}{2}) + \delta_0(k)\right) \\ \psi_k^1(p) &= \sqrt{\frac{2}{L}}\sin\left(k(p-\frac{1}{2}) + \delta_1(k)\right), \end{aligned} \tag{11}$$

at its right side ($p \ge 1$). The normalization factor $\sqrt{\frac{2}{L}}$ corresponds to a chain of length $L \to \infty$. The scattering when $v \ne 1$ gives rise to two phase shifts $\delta_0(k)$ and $\delta_1(k)$. Writing the Schrödinger equation inside the scatterer (sites 0 and 1) for the even and odd solutions, one gets:

$$\begin{aligned} -(2\cos k)\psi_k^{0,1}(0) &= -\psi_k^{0,1}(-1) - v\psi_k^{0,1}(1) \\ -(2\cos k)\psi_k^{0,1}(1) &= -v\psi_k^{0,1}(0) - \psi_k^{0,1}(2), \end{aligned} \tag{12}$$

which yields the following expressions for the even and odd phase shifts:

$$\tan\delta_0(k) = \frac{v-1}{v+1}\cot\left(\frac{k}{2}\right) \tag{13}$$

and

$$\tan\delta_1(k) = \frac{1-v}{v+1}\tan\left(\frac{k}{2}\right). \tag{14}$$

In addition, a value of $v > 1$ gives rise to two bound states located in the central region with energies outside the conduction band. The first one of energy

$$E_{\rm bs1} = -(v + v^{-1}) \tag{15}$$

has an even wave-function given by

$$\psi_{\rm bs1}(p) = \left(\sqrt{\frac{v - v^{-1}}{2}}\right) v^{-|p-1/2|}, \tag{16}$$

while the second of energy

$$E_{\rm bs2} = v + v^{-1} \tag{17}$$

has an odd wave-function given by

$$\psi_{\rm bs2}(p) = \left(\sqrt{\frac{v - v^{-1}}{2}}\right) (-1)^p v^{-|p-1/2|}. \tag{18}$$

When a scatterer is introduced in the chain ($v \neq 1$), this yields a correction $\delta\rho(E)$ to the density of states $\rho(E)$, which is given [22] for the even and odd components inside the conduction band by:

$$\delta\rho_{0,1}(E) = \frac{1}{\pi}\frac{\partial\delta_{0,1}(E)}{\partial E}. \tag{19}$$

$\delta\rho(E)$ satisfies [22] Friedel sum rule:

$$\frac{\delta_0(E_F) + \delta_1(E_F)}{\pi} = \int_{-\infty}^{E_F} \delta\rho(E)dE = \nu L_S \tag{20}$$

for a scatterer of length L_S embedded in a chain with a uniform filling factor ν. This implies that

$$\frac{\int_{-\infty}^{E_F} \delta\rho(E)dE}{\int_{-\infty}^{E_F} \rho(E, v=1)dE} = \frac{L_S}{L} \to 0 \tag{21}$$

when $L \to \infty$: The change $\delta\rho(k)$ of the density of real momenta k (inside the conduction band) vanishes in the limit of infinite lead length. When $L \to \infty$, the only change in the density $\rho(k)$ due to the scatterer comes from the bound states $\psi_{\rm bs}$ of imaginary momenta $K = {\rm i}k$ which are occupied outside the conduction band at zero temperature. For an arbitrary function $F(k)$ at zero temperature, this gives the relation:

$$\sum_{k<k_{\rm F}} F(k) = \frac{L}{2\pi}\int_0^{k_{\rm F}} F(k)dk + \sum_{\rm bs} F(K_{\rm bs}), \tag{22}$$

the last term being a sum over the occupied bound states.

2.3 $\langle c_1^\dagger c_0\rangle$ and conductance $g_1^{k_{\rm F}}(v)$

To obtain the implicit equation giving v, we need to calculate $\langle c_1^\dagger c_0\rangle$, which is the sum of contributions $A_{\rm cb}^{1,0}$ due to the conduction band and $A_{\rm bs}^{1,0}$ due to the occupied bound states. Assuming that $E_F < 2$, only the even bound state is occupied and:

$$\begin{aligned}
\left\langle c_1^\dagger c_0\right\rangle =& A_{\rm cb}^{1,0} + A_{\rm bs1}^{1,0} \\
A_{\rm cb}^{1,0} =& \frac{L}{2\pi}\int_0^{k_{\rm F}} dk \left\{\sum_{i=0}^{1} \psi_k^{i*}(1)\psi_k^i(0)\right\} \\
=& \int_0^{k_{\rm F}} \frac{dk}{\pi}\left\{\frac{4v\cos k\sin^2 k}{1 + v^4 - 2v^2\cos(2k)}\right\} \\
=& \frac{v^{-2}-1}{2\pi}\arctan\left(\frac{2v\sin k_{\rm F}}{v^2-1}\right) + \frac{\sin k_{\rm F}}{\pi v}, \\
A_{\rm bs1}^{1,0} =& \psi_{\rm bs1}^*(1)\psi_{\rm bs1}(0) = \frac{1-v^{-2}}{2}
\end{aligned} \tag{23}$$

Using this, one can calculate v as a function of the interaction strength U and of the Fermi momentum $k_{\rm F}$ by solving the implicit equation

$$v = 1 + U\langle c_1^\dagger c_0(v)\rangle. \tag{24}$$

Once the change of the effective hopping term v between the two central sites is obtained, it is straightforward to determine the transmission coefficient $t_1(v)$. At zero temperature, the Landauer conductance $g_1^{k_{\rm F}}(v)$ (in units of e^2/h) of the central region where the electrons interact is given by this effective one-body transmission coefficient $|t_1^{k_{\rm F}}(v)|^2$. Using the Landauer formula, one gets the transmission coefficient and the dimensionless conductance

$$\begin{aligned}
t_1^{k_{\rm F}}(v) =& \frac{v({\rm e}^{2{\rm i}k_{\rm F}} - 1)}{v^2 - {\rm e}^{-2{\rm i}k_{\rm F}}} \\
g_1^{k_{\rm F}}(v) =& |t_1^{k_{\rm F}}(v)|^2 = \frac{4v^2\sin^2 k_{\rm F}}{v^4 - 2v^2\cos(2k_{\rm F}) + 1}.
\end{aligned} \tag{25}$$

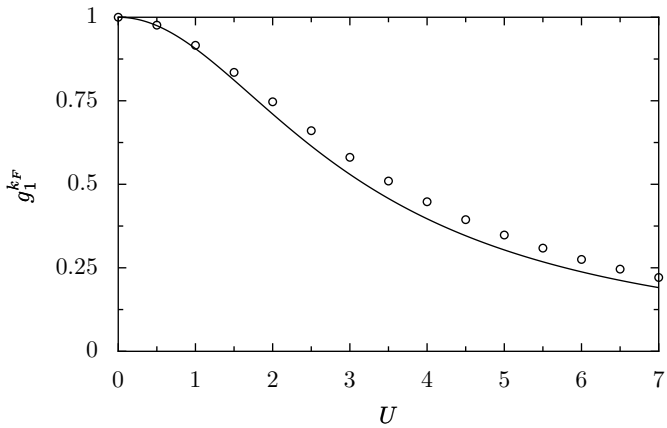

Fig. 2. Conductance $g_1^{k_{\rm F}}$ of a single scatterer as a function of the interaction strength U for $k_{\rm F} = \pi/2$. The solid line gives the HF behavior (Eq. (25)). The circles are the exact results obtained with embedding method and the DMRG algorithm.

The behavior of $g_1^{k_{\rm F}}$ as a function of the interaction strength U, obtained assuming the Hartree-Fock approximation (Eq. (25)) is shown in Fig. 2 for $k_{\rm F} = \pi/2$. An

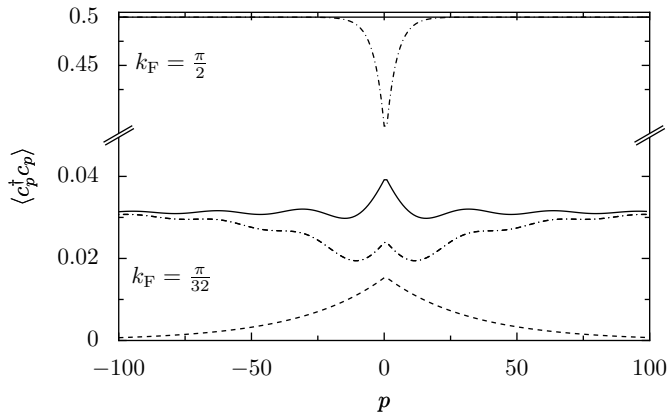

Fig. 3. Particle density $n_p = \langle c_p^\dagger c_p \rangle$ at sites p around a scatterer with an interaction strength $U = 0.4$. For $k_F = \pi/32$ (lower part of the figure): Contributions of the bound state (dashed line) and of the conduction band (dotted-dashed line) to n_p and Friedel oscillations of n_p around the average filling 1/32 (solid line). For $k_F = \pi/2$ (upper part of the figure): Contribution of the conduction band (dotted-dashed line) and total uniform density $n_p = 1/2$.

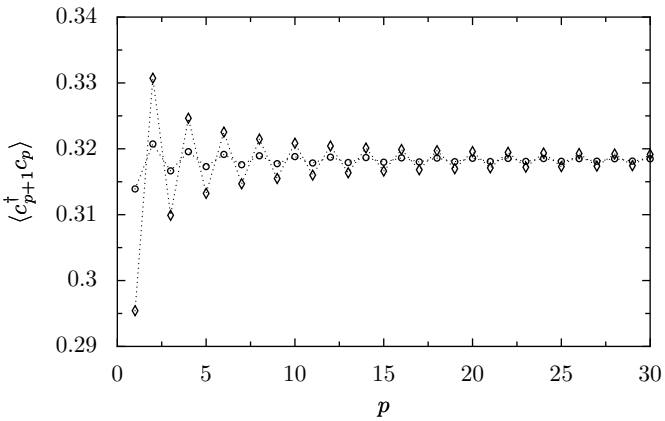

Fig. 4. Oscillatory decay of $\langle c_{p+1}^\dagger c_p \rangle$ towards its asymptotic value $1/\pi$ as a function of p for $k_F = \pi/2$, $U = 0.1$ (circles) and $U = 0.5$ (diamonds) obtained by using (28)-(30).

accurate value for $g_1^{k_F}$ can be obtained using the embedding method and the DMRG algorithm, as introduced in Refs. [9,10]. Using this exact method, we have also calculated $g_1^{k_F}$ at different interaction strengths U. The data are presented in Fig. 2, showing that the HF approximation is a good approximation for a very short interacting region of moderate interaction strength U.

2.4 Friedel oscillations of the density outside half-filling

For a half-filled chain, the system has particle-hole symmetry, and the density $n_p = \langle c_p^\dagger c_p \rangle$ must be equal to 1/2 at each site p. This is due to two opposite effects which compensate each other: a decrease of the contribution of the conduction band to the density that one can expect when there is a local repulsion acting inside the scatterer, and the contribution of the interaction-induced bound state to the density. These contributions are plotted separately in Fig. 3. For half-filling (upper part of Fig. 3), one gets an exact compensation of the two opposite effects for having a uniform density, and particle-hole symmetry is satisfied. Outside half-filling (lower part of Fig. 3), one gets large Friedel oscillations of the density around the scatterer, as shown in Fig. 3 for $k_F = \pi/32$ (filling factor 1/32). Since the Hartree term is exactly compensated in our model, those oscillations are only due to the exchange energy.

2.5 $\langle c_{p+1}^\dagger c_p \rangle$ outside the scatterer

The conductance $g_1^{k_F}(v)$ was obtained assuming infinite perfect leads outside the central scattering region. To know to what extend this condition does really matter, we calculate $\langle c_{p+1}^\dagger c_p \rangle$ outside the two sites where the electrons interact. When $p \geq 1$,

$$\left\langle c_{p+1}^\dagger c_p \right\rangle = A_{\rm cb}^{p+1,p} + A_{\rm bs1}^{p+1,p}, \tag{26}$$

where the contributions $A_{\rm cb}^{p+1,p}$ of the conduction band and $A_{\rm bs1}^{p+1,p}$ of the bound state to $\langle c_{p+1}^\dagger c_p \rangle$ read:

$$\begin{aligned} A_{\rm cb}^{p+1,p} =& \frac{L}{2\pi} \int_0^{k_F} dk \left\{ \sum_{i=0}^{1} \psi_k^{i*}(p+1)\psi_k^i(p) \right\} \\ =& \int_0^{k_F} \frac{dk}{\pi} \left\{ \cos k - G(v,k) \right\} \\ G(v,k) =& \left(v^2 - 1\right) \frac{v^2 \cos(2kp - k) - \cos(2kp + k)}{1 + v^4 - 2v^2 \cos(2k)} \\ A_{\rm bs1}^{p+1,p} =& \frac{v^2 - 1}{2} v^{-2p-1}. \end{aligned} \tag{27}$$

After integration, one obtains:

$$\left\langle c_{p+1}^\dagger c_p \right\rangle = \frac{\sin k_F}{\pi} + \frac{v^2 - 1}{\pi(2p+1)} X(k_F, p, v) \tag{28}$$

where the function $X(k_F, p, v)$ is defined as:

$$X(k_F, p, v) = {\rm Im} F(k_F, p, v) \tag{29}$$

$$F(k_F, p, v) =_2 F_1(1, \frac{1}{2} + p, \frac{3}{2} + p, v^2 {\rm e}^{2{\rm i}k_F}) {\rm e}^{{\rm i}k_F(2p+1)},$$

${}_2F_1(\alpha, \beta, \gamma, z)$ being the Gauss hypergeometric function

$${}_2F_1(\alpha, \beta, \gamma, z) = \sum_{n=0}^{\infty} \frac{(\alpha)_n (\beta)_n}{(\gamma)_n n!} z^n \tag{30}$$

with $(x)_n = \prod_{m=0}^{n}(x + m)$. Using an expansion of the Gauss hypergeometric function valid in the limit $p \to \infty$:

$${}_2F_1(1, \frac{1}{2} + p, \frac{3}{2} + p, v^2 {\rm e}^{2{\rm i}k_F}) \to \frac{1}{1 - v^2 {\rm e}^{2{\rm i}k_F}}, \tag{31}$$

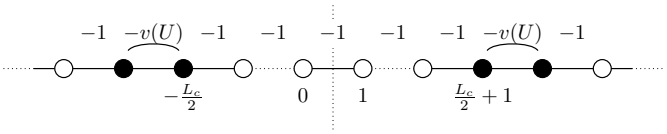

Fig. 5. Effective one body model describing two identical many-body scatterers (Hamiltonian (33)) coupled by L_c sites where the electrons do not interact.

one obtains for the behavior of $\langle c^\dagger_{p+1}c_p\rangle$ far from the scatterer a simpler expression:

$$\left\langle c^\dagger_{p+1}c_p\right\rangle \to \frac{1}{\pi}\left\{\sin k_{\rm F} + \frac{H^v_{k_{\rm F}}(p)}{2p+1}\right\} \tag{32}$$

where $H^v_{k_{\rm F}}(p)$ is an oscillatory function given by

$$H^v_{k_{\rm F}}(p) = \frac{(v^2-1)\left[-v^2\sin(k_{\rm F}(2p-1)) + \sin(k_{\rm F}(2p+1))\right]}{1+v^4-2v^2\cos(2k_{\rm F})}.$$

Outside the region where the electrons interact, $\langle c^\dagger_{p+1}c_p\rangle$ exhibits oscillations of periodicity $\pi/k_{\rm F}$ which have a slow power law decay towards an asymptotic value $\sin k_{\rm F}/\pi$. Those oscillations are illustrated in Fig. 4 for $k_{\rm F}=\pi/2$ and two values of U.

3 Transmission through two many-body scatterers coupled via conduction electrons

We now consider an infinite tight binding chain with the same kinetic Hamiltonian than defined in Eq. (4), but with an interaction Hamiltonian:

$$\begin{aligned} H_{int} =& U(n_{\frac{L_c}{2}+2} - V_{1+})(n_{\frac{L_c}{2}+1} - V_{2+}) \\ &+ U(n_{-\frac{L_c}{2}} - V_{2+})(n_{-\frac{L_c}{2}-1} - V_{1+}). \end{aligned} \tag{33}$$

This Hamiltonian describes two nano-systems where the electrons interact, as previously studied, which are coupled via an ideal lead of L_c sites where the electrons do not interact. Two positive background potentials V_{1+} and V_{2+} are introduced to compensate the Hartree terms of the HF equation. The total Hamiltonian is symmetric under the reflection $p-1/2 \to -p+1/2$. At half-filling, one has particle-hole symmetry, $V_{1+} = V_{2+} = 1/2$ and the density $n_p = 1/2$ is uniform. As before, the exchange leads to a modified effective hopping term v in the HF-approximation. Because of reflection symmetry, this modification must be the same for the two scatterers. The corresponding one-body model is sketched in Fig. 5. However, when there are two scatterers in series, the value of v characterizing each scatterer becomes different from the value of v obtained in the previous section when there is a single scatterer. This is due to the indirect exchange interaction which takes place between two scatterers coupled via conduction electrons. This indirect exchange interaction gives rise to an effect upon the quantum conductance of two nano-systems in series, which vanishes only if the length L_c of the coupling wire becomes infinite. We first study this effect in the limit when $U \to 0$, before solving exactly the Hartree-Fock equation. We give only the results for L_c even. The extension to the case where L_c is odd is straightforward. Moreover, for $k_{\rm F}=\pi/2$ and odd values of L_c, the conductance of the two scatterers in series $g_2^{\pi/2}=1$, independently of v. Because of this, we just need v for the even value of L_c, at half-filling.

3.1 Expansion in the weak interaction limit

For writing the self-consistent equation giving the effective hopping term v of one scatterer in series with another, we need to calculate the ground state expectation value of $\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(v,v)\rangle_2$ inside one scatterer when another identical scatterer is located at the sites $-\frac{L_c}{2}-1$ and $-\frac{L_c}{2}$. This value depends of the two modified hopping terms which characterize each scatterer, and which are equal because of reflection symmetry. In the limit of a weak interaction strength U, $v\to 1^+$ $(v>1)$ and one can expand:

$$\begin{aligned} \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(v,v)\right\rangle_2 &= \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(1,1)\right\rangle_2 \\ &+ (v-1)\left\{\frac{\partial}{\partial v}C_2(L_c,v)\right\}_{v\to 1^+} + O\left((v-1)^2\right) \end{aligned} \tag{34}$$

where

$$C_2(L_c,v) = \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(1,v)\right\rangle_2 + \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(v,1)\right\rangle_2.$$

We note that the above expansion involves only terms with a single scatterer, for which one can write

$$\begin{aligned} \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(1,1)\right\rangle_2 &= \left\langle c^\dagger_1 c_0(1)\right\rangle \\ \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(v,1)\right\rangle_2 &= \left\langle c^\dagger_1 c_0(v)\right\rangle \\ \left\langle c^\dagger_{\frac{L_c}{2}+2}c_{\frac{L_c}{2}+1}(1,v)\right\rangle_2 &= \left\langle c^\dagger_{L_c+3}c_{L_c+2}(v)\right\rangle. \end{aligned} \tag{35}$$

Using Eqs. (23) and (28), one gets when $v\to 1$ $(v>1)$

$$\begin{aligned} \frac{\partial}{\partial v}\left\langle c^\dagger_1 c_0(v)\right\rangle &\to \frac{1}{2} - \frac{\sin k_{\rm F}}{\pi} \\ \frac{\partial}{\partial v}\left\langle c^\dagger_{p+1}c_p(v)\right\rangle &\to \frac{2X(k_{\rm F},p,1)}{\pi(2p+1)}, \end{aligned} \tag{36}$$

the function $X(k_{\rm F},p,v)$ being defined in Eq. (29).

In the weak interaction limit, the effective hopping term v characterizing each of the two scatterers in series is given by the self-consistent equation:

$$1-v \approx -U\left\{\frac{1}{\pi} + (v-1)\frac{\partial}{\partial v}C_2(L_c,v)\right\}_{v\to 1^+} \tag{37}$$

where $C_2(L_c,v) = \langle c^\dagger_1 c_0(v)\rangle + \langle c^\dagger_{L_c+3}c_{L_c+2}(v)\rangle$. One eventually obtains:

$$v \approx 1 + \left\{\frac{\pi(2-U)}{2U} - \frac{2X(k_{\rm F},L_c+2,1)}{2L_c+5} + \sin k_{\rm F}\right\}^{-1}. \tag{38}$$

when $U \to 0$. One can see that the indirect exchange interaction gives rise to a correction which decays with a power law as the length L_c of the coupling wire increases. This is when $L_c \to \infty$ that the scatterers become decoupled, and characterized by a value for the effective hopping term which coincides with the value given by Eq. (24) for a single scatterer in the limit $U \to 0$:

$$v(L_c = \infty, U \to 0) \approx 1 + \frac{2}{2\sin k_{\rm F} - \pi + 2\pi/U}. \quad (39)$$

Equation (38) can be written in a simpler form for a half-filled chain. Expressing $X(k_{\rm F}, L_c + 2, 1)$ for $k_{\rm F} = \pi/2$ one obtains for the effective hopping term the equation (3) given in the introduction.

3.2 Exact solution of the Hartree-Fock equation

Let us solve now the HF-equation for v without assuming that $v \to 1^+$. The effective one-body model described in Fig. 5 has even and odd standing-wave solutions $\psi_k^0(p)$ and $\psi_k^1(p)$, which can be written inside the conduction band as:

$$\begin{aligned} \psi_k^0(p) =& \sqrt{\frac{2}{L}} \cos\left(k(p - \frac{1}{2}) - \delta_0(k)\right) \\ \psi_k^1(p) =& \sqrt{\frac{2}{L}} \sin\left(k(p - \frac{1}{2}) - \delta_1(k)\right), \end{aligned} \quad (40)$$

at the left side of the two scatterers ($p \le -\frac{L_c}{2} - 1$) and

$$\begin{aligned} \psi_k^0(p) =& \sqrt{\frac{2}{L}} \cos\left(k(p - \frac{1}{2}) + \delta_0(k)\right) \\ \psi_k^1(p) =& \sqrt{\frac{2}{L}} \sin\left(k(p - \frac{1}{2}) + \delta_1(k)\right), \end{aligned} \quad (41)$$

at the right side of the two scatterers ($p \ge \frac{L_c}{2} + 2$). Between the two scatterers ($-\frac{L_c}{2} \le p \le \frac{L_c}{2} + 1$), the even and odd standing-wave solutions $\psi_k^0(p)$ and $\psi_k^1(p)$ read

$$\begin{aligned} \psi_k^0(p) =& \sqrt{\frac{2}{L}} a_0 \cos\left(k(p - \frac{1}{2})\right) \\ \psi_k^1(p) =& \sqrt{\frac{2}{L}} a_1 \sin\left(k(p - \frac{1}{2})\right), \end{aligned} \quad (42)$$

The expressions for the factors a_0 and a_1 are given in Appendix.

When $v \neq 1$, the scattering gives rise to two phase shifts $\delta_0(k)$ and $\delta_1(k)$, which are given by

$$\tan\delta_0(k) = \frac{(v^2 - 1)\left(\cos(k(L_c + 2)) + \cos k\right)}{(v^2 - 1)\sin(k(L_c + 2)) + (v^2 + 1)\sin k} \quad (43)$$

and

$$\tan\delta_1(k) = \frac{(1 - v^2)\left(-\cos(k(L_c + 2)) + \cos k\right)}{(v^2 - 1)\sin(k(L_c + 2)) - (v^2 + 1)\sin k} \quad (44)$$

respectively.

In addition, a value of $v > 1$ can give rise to four bound states located around the scatterers with energies outside the conduction band. We just write those below the conduction band ($E_{\rm bs} < -2$). There is an even bound state of energy $E_{\rm bs0} = -2\cosh K_0$, K_0 being the real solution of the equation:

$$v^2 + v^2 \exp(K_0(L_c + 1)) = 1 + \exp(K_0(L_c + 3)). \quad (45)$$

Its wave function reads

$$\psi_{\rm bs0}(p) = A_0 \exp\left(K_0(p + \frac{L_c + 1}{2})\right) \quad (46)$$

at the left side of the two scatterers ($p \le -\frac{L_c}{2} - 1$),

$$\psi_{\rm bs0}(p) = A_0 \exp\left(-K_0(p - \frac{L_c + 3}{2})\right) \quad (47)$$

at the right side of the two scatterers ($p \ge \frac{L_c}{2} + 2$), and

$$\psi_{\rm bs0}(p) = A_0 b_0 \cosh\left(K_0(p - \frac{1}{2})\right) \quad (48)$$

between the two scatterers ($-\frac{L_c}{2} \le p \le \frac{L_c}{2} + 1$). The expression for the factor b_0 is given in Appendix.

If L_c is large enough, the equation:

$$v^2 - v^2 \exp\left(K_1(L_c + 1)\right) = 1 - \exp\left(K_1(L_c + 3)\right) \quad (49)$$

has a real solution for K_1. In this case, there is also an odd bound state below the conduction band of energy $E_{\rm bs1} = -2\cosh K_1$. Its wave function is given by

$$\psi_{\rm bs1}(p) = -A_1 \exp\left(K_1(p + \frac{L_c + 1}{2})\right) \quad (50)$$

at the left side of the two scatterers ($p \le -\frac{L_c}{2} - 1$),

$$\psi_{\rm bs1}(p) = A_1 \exp\left(-K_1(p - \frac{L_c + 3}{2})\right) \quad (51)$$

at the right side of the two scatterers ($p \ge \frac{L_c}{2} + 2$), and

$$\psi_{\rm bs1}(p) = A_1 b_1 \sinh\left(K_1(p - \frac{1}{2})\right) \quad (52)$$

between the two scatterers ($-\frac{L_c}{2} \le p \le \frac{L_c}{2} + 1$). The expression for the factor b_1 is given in Appendix.

The condition

$$\sum_{p=-\infty}^{\infty} |\psi_{\rm bs0,1}(p)|^2 = 1 \quad (53)$$

gives the normalization factors $A_{0,1}$. The obtained expressions are somewhat involved and given in Appendix.

Using Eq. (22), one can calculate

$$\begin{aligned} \left\langle c_{p+1}^\dagger c_p \right\rangle_2 =& \frac{L}{2\pi} \int_0^{k_{\rm F}} dk \left\{ \sum_{i=0}^{1} \psi_k^{i*}(p+1)\psi_k^i(p) \right\} \\ &+ \sum_{\rm bs} \psi_{\rm bs}^*(p+1)\psi_{\rm bs}(p) \end{aligned} \quad (54)$$

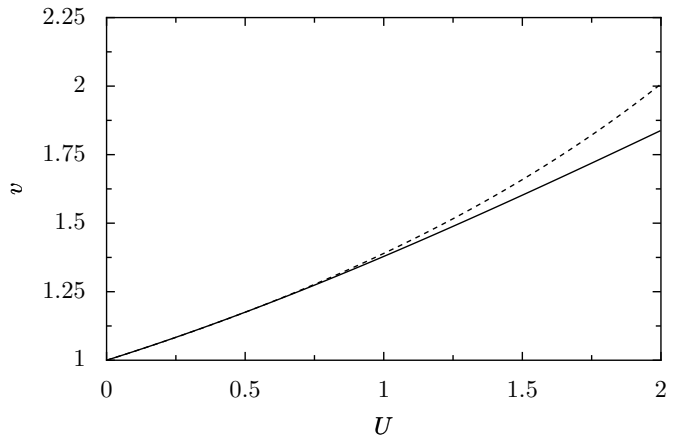

Fig. 6. Two scatterers in series: Value v of the effective hopping term as a function of U. v characterizes each of the scatterers for $L_c = 4$ and $k_{\rm F} = \pi/2$. The solid line gives the exact HF value obtained from Eq. (54) and the dashed line gives the approximated value (Eq. (38)).

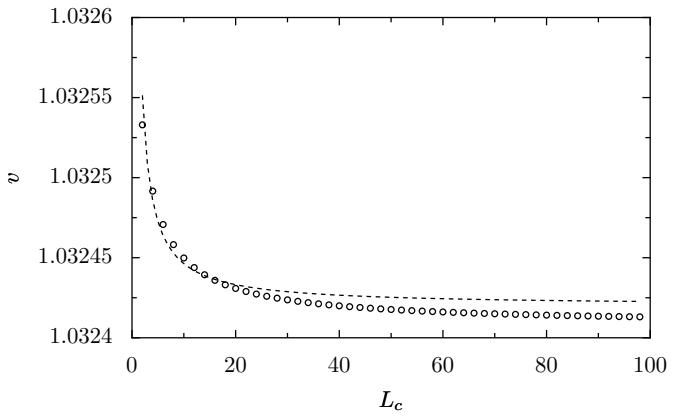

Fig. 7. Two scatterers in series: v as a function of even values of L_c for $U = 0.1$ and $k_{\rm F} = \pi/2$. The circles give the exact HF value obtained from Eq. (54) and the dashed line gives the approximated value (Eq. (38)). The even-odd oscillations characteristic of $k_{\rm F} = \pi/2$ are not shown, v for odd L_c being not plotted.

for $p = \frac{L_c}{2} + 1$ to obtain the HF equation giving v for two scatterers in series. The above integrals have been calculated using Mathematica.

We compare in Fig. 6 and Fig. 7 the exact HF value of v obtained with formula (54) to the approximated value given by formula (38) in the limit $v \to 1^+$. One can see that the approximated value is accurate enough for the values of U where one can trust the HF approximation. Fig. 7 shows the effect of indirect exchange interaction upon the value v of the effective hopping, and how this effect disappears when $L_c \to \infty$, for even L_c only.

3.3 Density oscillations and quantum conductance for two many-body scatterers in series

Once the self-consistent value for v is obtained, one can calculate the Friedel oscillations of the density $n_p = \langle c_p^\dagger c_p \rangle$

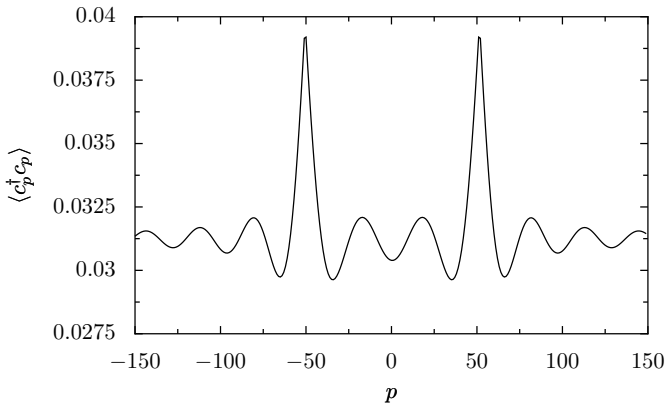

Fig. 8. Two scatterers in series: Friedel oscillations of the density $n_p = \langle c_p^\dagger c_p \rangle$ for $U = 0.4$, $L_c = 100$ and $k_{\rm F} = \pi/32$.

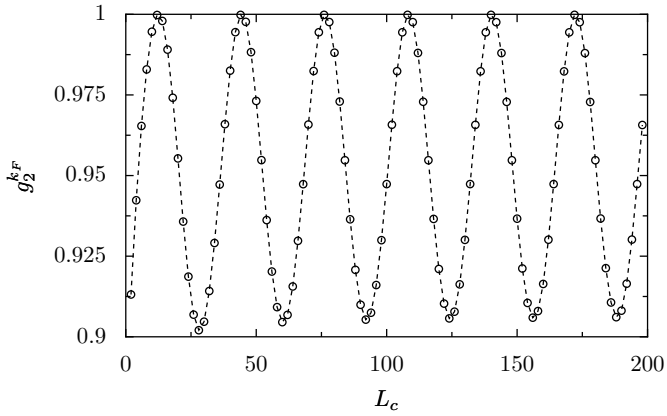

Fig. 9. Two scatterers in series: total conductance $g_2^{k_{\rm F}}(L_c, U)$ as a function of L_c for $U = 0.4$ and $k_{\rm F} = \pi/32$. Only the values given by the exact solution of the Hartree-Fock equation where L_c is even are plotted.

around the two scatterers. Outside half-filling, our model exhibits Friedel oscillations of the density which are illustrated in Fig. 8 for $U = 0.4$, $L_c = 100$ and $k_{\rm F} = \pi/32$.

The transmission coefficient $t_1^{k_{\rm F}}$ of a single scatterer as a function of v and $k_{\rm F}$ is given by Eq. (25). $r_1^{k_{\rm F}}$ denoting its reflection coefficient, the transfer matrices $M_1^{k_{\rm F}}$ and $M_{L_c}^{k_{\rm F}}$ through a single scatterer and the coupling lead read:

$$M_1^{k_{\rm F}} = \begin{pmatrix} (1/t_1^{k_{\rm F}})^* & r_1^{k_{\rm F}}/t_1^{k_{\rm F}} \\ (r_1^{k_{\rm F}}/t_1^{k_{\rm F}})^* & 1/t_1^{k_{\rm F}} \end{pmatrix} \tag{55}$$

and

$$M_{L_c}^{k_{\rm F}} = \begin{pmatrix} e^{{\rm i}k_{\rm F}L_c} & 0 \\ 0 & e^{-{\rm i}k_{\rm F}L_c} \end{pmatrix} . \tag{56}$$

From the matrix $M_2^{k_{\rm F}} = M_1^{k_{\rm F}} M_{L_c}^{k_{\rm F}} M_1^{k_{\rm F}}$, and current conservation ($1 = |t_1^{k_{\rm F}}|^2 + |r_1^{k_{\rm F}}|^2$), one obtains the transmission coefficient $t_2^{k_{\rm F}}$ and the dimensionless conductance $g_2^{k_{\rm F}}$ of two scatterers in series, coupled by L_c sites where

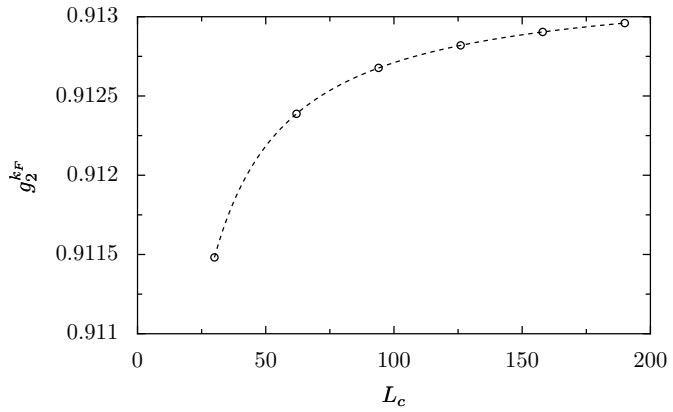

Fig. 10. Two scatterers in series: Minimum values of $g_2^{k_F}(L_c, U)$ for the successive conductance oscillations occurring when $U = 0.4$ and $k_F = \pi/16$, underlining the power law decay of their amplitudes as a function of L_c. The dashed line is a numerical fit $0.91324 - 0.05267/L_c$.

the electrons do not interact:

$$\begin{aligned} t_2^{k_F}(v) &= -\frac{2iv^2 e^{2ik_F}\sin^2 k_F}{d^{k_F}(v)} \\ g_2^{k_F}(v) &= \frac{4v^4\sin^4 k_F}{|d^{k_F}(v)|^2}, \end{aligned} \tag{57}$$

where

$$\begin{aligned} d^{k_F}(v) =& e^{-ik_F}\sin[k_F(L_c+3)] - 2v^2\sin[k_F(L_c+2)] \\ &+ v^4 e^{ik_F}\sin[k_F(L_c+1)]. \end{aligned}$$

The presence of L_c dependent corrections to v shows that the transmission coefficient $t_1^{k_F}$ of one scatterer depends on the distance L_c from the other scatterer. Accordingly, this non-local effect affects the conductance $g_2^{k_F}$ of two scatterers in series. We show in Fig. 9 the total conductance $g_2^{k_F}$ of two scatterers in series for a low filling factor ($k_F = \pi/32$), obtained by the exact solution of the Hartree-Fock equation. One can see the large period $\pi/k_F = 32$ of the conductance oscillations, though the values for odd L_c are not plotted. The conductance oscillations are larger when L_c is small, due to the effect of the exchange energy. The $1/L_c$-decay of the conductance oscillations towards its asymptotic L_c-independent value is underlined in Fig. 10 obtained with $k_F = \pi/16$.

4 Comparison with exact DMRG results

Exact values of the conductance of a one dimensional scatterer in which electrons interact can be obtained using the embedding method and the DMRG algorithm, as explained in previous works [8,9,10,11]. We have compared in Fig. 5 the HF results and the exact DMRG results for a single very short scatterer. The difference was negligible for small values of U. Nevertheless, the HF values differ [7] more and more from the exact values when the size of the scatterer in which the electrons interact increases. The difference should become more pronounced for two scatterers in series. We study the ability of the HF approximation to describe two interacting nano-systems in series for a half filled chain ($k_F = \pi/2$).

If the scattering matrix of one scatterer is not modified by the presence of other scatterer as for non-interacting systems, the conductance $g_2^{\pi/2}$ of two scatterers in series for $k_F = \pi/2$ shows even-odd oscillation as a function of the size L_c of the coupling wire: $g_2^{\pi/2} = 1$ when L_c is odd, and is given by [8]

$$g_2^{\pi/2} = \left(\frac{g_1^{\pi/2}}{g_1^{\pi/2} - 2}\right)^2 \tag{58}$$

when L_c is even. Here $g_1^{\pi/2}$ is the conductance of a chain with a single scatterer. In the presence of electron-electron interaction, however, the scattering matrix of one scatterer can be affected by the other scatterer as shown in the previous subsection.

In Ref. [8], the exact values of $g_1^{\pi/2}$ and $g_2^{\pi/2}$ were obtained separately, using the embedding method: $g_1^{\pi/2}$ being calculated for an infinite chain embedding a single scatterer, $g_2^{\pi/2}$ for an infinite chain embedding two scatterers. It was found that $g_2^{\pi/2} = 1$ if L_c is odd, as predicted. But if L_c is even, $g_2^{\pi/2}$ was related to $g_1^{\pi/2}$ by formula (58) only in the limit $L_c \to \infty$. For small sizes L_c, formula (58), with $g_1^{\pi/2}$ obtained for a single scatterer surrounded by infinite leads without other scatterers, overestimates $g_2^{\pi/2}$ by an amount

$$\delta g_2^{\pi/2}(L_c) = \frac{A(U, k_F)}{L_c} \tag{59}$$

characterized by a function $A(U, k_F)$ given in Fig. 11 for $k_F = \pi/2$.

Using the HF approximation, we have shown that the parameter v characterizing a single scatterer becomes modified if another scatterer is put in series. Hence, the conductance $g_1^{\pi/2}$ of one scatterer in series with another differs from its value when it is alone. If one ignores this difference, as previously using the DMRG algorithm, taking for $g_1^{\pi/2}$ its value without the second scatterer and using formula (58), one overestimates also $g_2^{\pi/2}$ by an amount which is described by formula (59), but with a different function $A(U, k_F)$ given in Fig. 11. One can see that the HF approximation reproduces qualitatively the DMRG results, giving a function $A(U, k_F)$ characterizing the correction $\delta g_2^{\pi/2}(L_c)$ which first increases before decreasing as U varies. When U is small enough, the HF approximation reproduces quantitatively the DMRG results: $A_{HF}(U, k_F) \approx A_{DMRG}(U, k_F)$. When U becomes larger, the decay of $A_{DMRG}(U, k_F)$ is not quantitatively reproduced by the HF approximation. A more suitable description could be obtained using a perturbative approach adapted to the limit $U \gg t_h$, as used in Ref. [23]. For intermediate U, there is no simple analytical approach, making

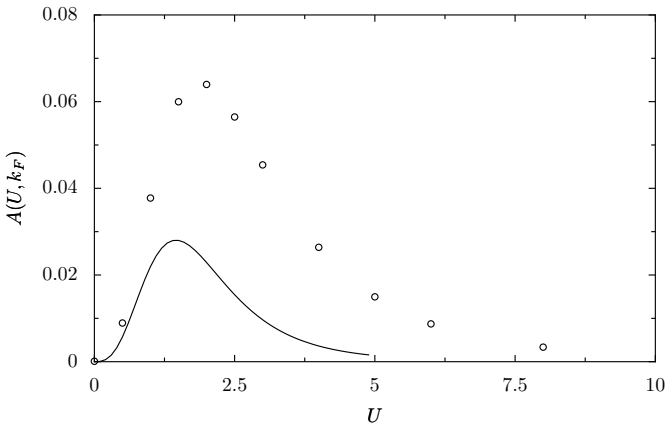

Fig. 11. Function $A(U, k_{\rm F})$ characterizing the interaction induced correction $\delta g_2^{k_{\rm F}}(L_c)$ to $g_2^{k_{\rm F}}$ of (58) for two interacting nano-systems in series (formula (59)) at $k_{\rm F} = \pi/2$. The exact values obtained from the embedding method and the DMRG algorithm are shown by circles, the values obtained from the HF approximation by a solid line.

the use of numerical renormalization methods (NRG [22, 24] or DMRG) necessary.

5 Temperature dependent scale $L_{\rm T}$ of the indirect exchange interactions

We have shown that the indirect exchange interaction between two scatterers gives rise to corrections to the value of the quantum conductance $g_2^{k_{\rm F}}$ which slowly decays as L_c increases at zero temperature. We are going to show that this effect is suppressed when the length of the wire coupling the two scatterers exceeds $L_{\rm T}$, which is the scale on which an electron propagates at the Fermi velocity during a time $\hbar/k_B T$, i.e. the thermal length characteristic of free fermions in one dimension. Since our approach is essentially valid in the limit of weak values of U, it is sufficient to consider the weak interaction limit discussed in subsection 3.1 for a temperature $T = 0$. In this limit, the effect was given by the deviation of $\langle c_{p+1}^\dagger c_p\rangle$ from its uniform value $\sin k_{\rm F}/\pi$, deviation induced inside the leads by an embedded scatterer. To show that this deviation is exponentially suppressed above $L_{\rm T}$ is enough for proving that the effect of the indirect exchange interaction upon $g_2^{k_{\rm F}}$ vanishes when $L_c > L_{\rm T}$.

At finite temperature $k_B T = \beta^{-1}$, the Fermi-Dirac function $f(E, \mu_{\rm F})$ gives the occupation number of the level of energy E at a Fermi chemical potential $\mu_{\rm F}$:

$$f_\beta(E, \mu_{\rm F}) = \frac{1}{{\rm e}^{\beta(E-\mu_{\rm F})} + 1}. \tag{60}$$

When one has a single scatterer embedded in an infinite perfect lead, the temperature modifies [20] the value of $\langle c_1^\dagger c_0\rangle$ inside the scatterer. Instead of having Eq. (23), one now has:

$$\langle c_1^\dagger c_0\rangle_\beta = A_{\rm cb}^{1,0}(\beta, \mu_{\rm F}) + A_{\rm bs}^{1,0}(\beta, \mu_{\rm F}) \tag{61}$$

where the contribution of the conduction band reads:

$$\begin{aligned} A_{\rm cb}^{1,0}(\beta, \mu_{\rm F}) =& \frac{L}{2\pi}\int_0^\pi dk f_\beta(E_k, \mu_{\rm F})\left\{\sum_{i=0}^{1}\psi_k^{i*}(1)\psi_k^i(0)\right\} \\ =& \int_0^\pi \frac{dk}{\pi} f_\beta(E_k, \mu_{\rm F})\left\{\frac{4v\cos k\sin^2 k}{1+v^4-2v^2\cos(2k)}\right\}, \end{aligned}$$

the contribution of the two bound states becoming

$$\begin{aligned} A_{\rm bs}^{1,0}(\mu_{\rm F}) =& \sum_{\rm bs} f_\beta(E_{\rm bs}, \mu_{\rm F})\psi_{\rm bs}^*(1)\psi_{\rm bs}(0) \\ =& \{f_\beta(E_{\rm bs1}, \mu_{\rm F}) - f_\beta(E_{\rm bs2}, \mu_{\rm F})\}\,\frac{1-v^{-2}}{2}. \end{aligned}$$

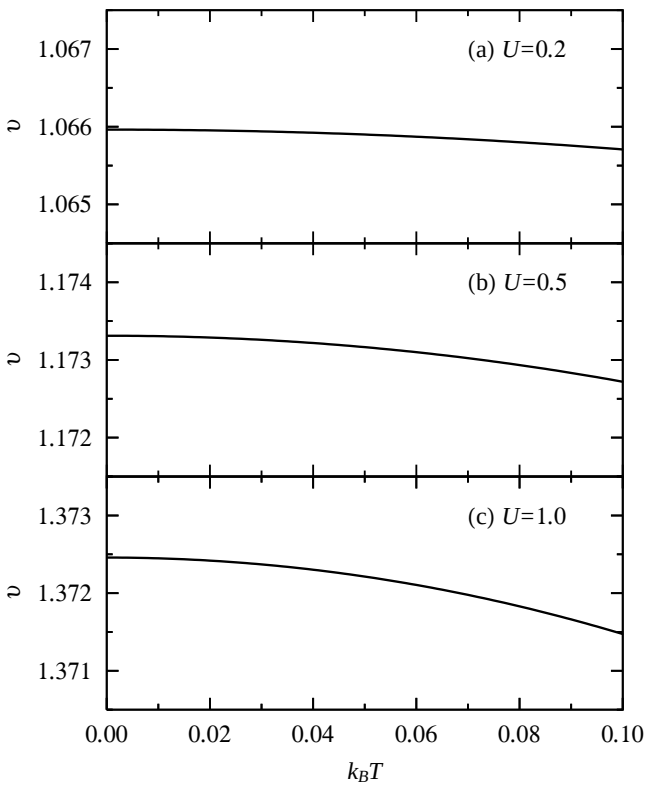

Fig. 12. v given by Eq. (62) as a function of the temperature $T = \beta^{-1}$ for different values of U and $\mu_{\rm F} = 0$.

The effective hopping term v is given by the implicit equation:

$$v = 1 + U\langle c_1^\dagger c_0(v)\rangle_\beta, \tag{62}$$

and becomes dependent on the temperature T and on $\mu_{\rm F}$.

Assuming a half-filled chain ($\mu_{\rm F} = 0$ due to particle-hole symmetry), v given by Eq. (62) has been calculated numerically for weak values U of the interaction strength. The T dependence of v is shown in Figs. 12. One can see that this dependence remains weak when the temperature $k_B T \leq 0.1$ and U is small.

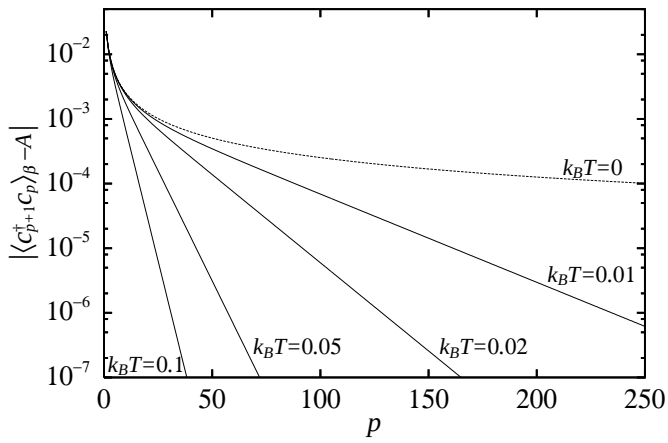

Fig. 13. $\left|\left\langle c^\dagger_{p+1}c_p\right\rangle - A\right|$ as a function of p for $U = 0.5$ and $\mu_{\rm F} = 0$ (half-filling). A is the asymptotic value when $p \to \infty$.

The equation (28) giving $\langle c^\dagger_{p+1}c_p\rangle$ outside the part where the electrons interact ($p \geq 1$) becomes at a temperature T:

$$\begin{aligned}\left\langle c^\dagger_{p+1}c_p\right\rangle_\beta &= \frac{L}{2\pi}\int_0^\pi dk f_\beta(E_k,\mu_{\rm F})\left\{\sum_{i=0}^{1}\psi^{i*}_k(p+1)\psi^i_k(p)\right\} \\ &\quad + \sum_{\rm bs} f_\beta(E_{\rm bs},\mu_{\rm F})\psi_{\rm bs}(p+1)\,\psi_{\rm bs}(p) \qquad (63)\\ &= \frac{1}{\pi}\int_0^\pi dk f_\beta(E_k,\mu_{\rm F})\left\{\cos k - G(k,v)\right\} \\ &\quad + \left\{f_\beta(E_{\rm bs1},\mu_{\rm F}) - f_\beta(E_{\rm bs2},\mu_{\rm F})\right\}\frac{v^2-1}{2}v^{-2p-1},\end{aligned}$$

the function $G(k,v)$ being defined in Eq. (27).

By using numerical integration, we have calculated $\langle c^\dagger_{p+1}c_p\rangle_\beta$ as a function of p for different temperatures T and $\mu_{\rm F} = 0$. The data show that $\langle c^\dagger_{p+1}c_p\rangle_\beta$ exhibits oscillations which have a faster decay when the temperature increases. If A is the asymptotic value of $\langle c^\dagger_{p+1}c_p\rangle_\beta$ when $p \to \infty$, we show in Fig . 13 how the absolute value of the difference between $\langle c^\dagger_{p+1}c_p\rangle_\beta$ and A decays when p increases for different values of T. One can see that the decay towards its asymptotic value of $\langle c^\dagger_{p+1}c_p\rangle_\beta$ becomes exponential:

$$\left|\left\langle c^\dagger_{p+1}c_p\right\rangle_\beta - A\right| \propto \exp\left(-\frac{p}{L_{\rm T}}\right) \qquad (64)$$

when p is large.

In Fig. 14 the decay length $L_{\rm T}$ is shown as a function of T. One can see that L_T decays when the temperature increases as:

$$L_{\rm T} = \frac{1}{\pi k_B T}. \qquad (65)$$

Since we have taken $t_{\rm h} = 1$ and the lattice spacing $s = 1$ in our calculations, one can identify this decay length with the length on which a free fermion of speed $v_F = \hbar^{-1}\partial E_F/\partial k_{\rm F} = 2/\hbar$ propagates during a time $\hbar/(k_BT)$ in one dimension. Ignoring a multiplicative factor $1/(2\pi)$, $L_{\rm T}$ is the usual thermal length of free fermions in one dimension.

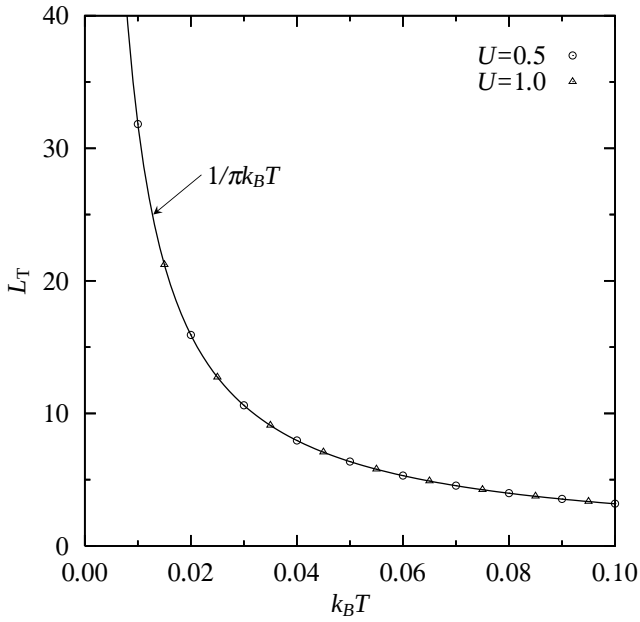

Fig. 14. Thermal length $L_{\rm T}$ as a function of the temperature T obtained from the exponential decays of $\langle c^\dagger_{p+1}c_p\rangle_\beta$ shown in Fig. 13. The points obtained using two values of U = (0.5 and 1) and T form a single solid curve $L_{\rm T} = 1/(\pi k_B T)$.

6 Conclusion

Extending the Landauer formulation of quantum transport to nano-systems inside which electrons interact, we have studied a one dimensional spinless model which is simple enough to be analytically solved assuming the Hartree-Fock approximation. We have shown that the scattering becomes non local when the many-body effects inside the scatterer are taken into account. Using two identical nano-systems in which interaction gives rise to scattering and which are coupled by a non-interacting lead of length L_c, the Hartree-Fock approximation have allowed us to map the many-body scatterers onto effective one-body scatterers which depend on the other scatterer through the indirect exchange interaction via the conduction electrons of the coupling lead. The non local character of the scattering is only due to exchange terms in the studied model, a positive background charge compensating the Hartree contribution. We have shown that the HF theory provides a qualitative understanding of the non local effects found in Ref.[8], quantitatively reproducing the exact behaviors in the weak interaction limit.

Eventually, we point out that we have restricted our HF study to a purely one dimensional limit where powerful renormalization methods (DMRG, NRG) are available.

Though it has allowed us to compare the HF results to exact numerical results, this is the worst limit for using the HF approximation. To extend the HF study to the many channel case, where the electron dynamics will be more two or three dimensional does not present particular difficulties [7]. Moreover, the HF approximation is believed to become more accurate outside one dimension. A HF study of this many channel limit is in progress and will be published in another work.

We believe that the interaction induced enhancement of the sensitivity of the quantum conductance to the nature of the attached leads can be relatively easily observed. A more detailed study of a possible experiment will be discussed in a separate work.

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8 Appendix

For two scatterers in series, one uses even and odd standing wave functions. The factors a_0 and a_1 for the even and odd functions of energy inside the conduction band read:

$$\begin{aligned} a_0 =& \frac{v|\sin k|}{\sqrt{\alpha_0}}, \\ \alpha_0 =& \left\{(v^2-1)\cos\left(\frac{k}{2}(L_c+1)\right)\right\}^2 \\ &+ \sin k\left\{v^2\sin k + (v^2-1)\sin(k(L_c+2))\right\}, \\ a_1 =& \frac{v|\sin k|}{\sqrt{\alpha_1}}, \\ \alpha_1 =& \left\{(v^2-1)\sin\left(\frac{k}{2}(L_c+1)\right)\right\}^2 \\ &+ \sin k\left\{v^2\sin k - (v^2-1)\sin(k(L_c+2))\right\}. \end{aligned}$$

The factors b_0 and b_1 for the even and odd functions of energy outside the conduction band read:

$$\begin{aligned} b_0 =& \frac{v}{\mathrm{e}^{K_0/2}\cosh\frac{K_0(L_c+3)}{2}}, \\ b_1 =& \frac{v}{\mathrm{e}^{K_1/2}\sinh\frac{K_1(L_c+3)}{2}}. \end{aligned}$$

Using the auxiliary functions $A_\pm(L_c, K)$

$$A_\pm(L_c, K) = 2 + L_c \pm \frac{\sinh(k(L_c+2))}{\sinh K},$$

the normalization factors A_0 and A_1 for the even and odd bound states of energy below the conduction band read:

$$\frac{A_0}{\sqrt{2}\mathrm{e}^{\mathrm{i}K_0/2}} = \left\{2 + 2\coth K_0 + \frac{v^2 A_+(L_c, K_0)}{\left(\cosh\frac{K_0(L_c+3)}{2}\right)^2}\right\}^{-1/2},$$

$$\frac{A_1}{\sqrt{2}\mathrm{e}^{\mathrm{i}K_1/2}} = \left\{2 + 2\coth K_1 - \frac{v^2 A_-(L_c, K_1)}{\left(\sinh\frac{K_1(L_c+3)}{2}\right)^2}\right\}^{-1/2}.$$

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