

LETTER TO THE EDITOR

Conductance anomalies in quantum wiresT Rejec[†], A Ramšak^{†‡} and J H Jefferson[§][†]J Stefan Institute, SI-1000 Ljubljana, Slovenia[‡]Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia[§]DERA, St Andrews Road, Great Malvern, Worcestershire WR14 3PS, England

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Abstract. We study the conductance threshold of clean nearly straight quantum wires in which an electron is bound. We show that such a system exhibits spin-dependent conductance structures on the rising edge to the first conductance plateau; one near $0.25(2e^2/h)$, related to a singlet resonance, and one near $0.75(2e^2/h)$, related to a triplet resonance. As a quantitative example we solve exactly the scattering problem for two-electrons in a wire with planar geometry and a weak bulge. From the scattering matrix we determine conductance via the Landauer–Büttiker formalism. The conductance anomalies are robust and survive to temperatures of a few degrees. With increasing in-plane magnetic field the conductance exhibits a plateau at e^2/h , consistent with recent experiments.

Following the pioneering work in [1, 2] many groups have now observed conductance steps in various types of quantum wire. These first experiments were performed on gated two-dimensional electron gas (2DEG) structures, while a similar behaviour of conductance is exhibited in ‘hard-confined’ quantum wire structures, produced by cleaved edge over-growth [3], epitaxial growth on ridges [4], heteroepitaxial growth on ‘v’-groove surfaces, [5] and most recently in GaAs/Al_δGa_{1-δ}As narrow ‘v’-groove [6] and low-disorder [7] quantum wires.

These experiments strongly support the idea of ballistic conductance in quantum wires and are in surprising agreement with the now standard Landauer–Büttiker formalism [8, 9] neglecting electron interactions [10]. However, there are certain anomalies, some of which are believed to be related to electron–electron interactions and appear to be spin-dependent. In particular, already in early experiments a structure is seen in the rising edge of the conductance curve [1], starting at around $0.7G_0$ with $G_0 = 2e^2/h$ and merging with the first conductance plateau with increasing energy. Under an increasing in-plane magnetic field, the structure moves down, eventually merging with a new conductance plateau at e^2/h in very high fields [11, 12]. Theoretically this anomaly has not been adequately explained, despite several proposed scenarios, including spin-polarized sub-bands [13], conductance suppression in a Luttinger liquid with repulsive interaction and disorder [14] or local spin-polarized density-functional theory [15]. Recently we have shown that these conductance anomalies near $0.7G_0$ and $0.25G_0$ are consistent with an electron being weakly bound in wires of circular cross-section, giving rise to spin-dependent scattering resonances [16].

In this Letter we extend our previous work to planar quantum wires with a rectangular cross-section and also analyse the effects of an external in-plane magnetic field. We consider here, as an example, a small fluctuation in thickness of the wire in some region giving rise to a weak bulge. Such a system may be regarded as an ‘open quantum dot’ in which one electron is bound and inhibits the transport of conduction electrons via Coulomb repulsion. The problem is analogous to treating the collision of an electron with a hydrogen atom as, e.g., described

in [17] and studied 70 years ago by J R Oppenheimer and N F Mott [18]. The conductance is obtained from the transmission probabilities for individual channels via the usual Landauer–Büttiker formalism [8,9]. In the present two-electron problem, the relevant channels are singlet and triplet, with transmission amplitudes t_s and t_t , respectively, and corresponding transmission probabilities $\mathcal{T}_s(E) = |t_s|^2$ and $\mathcal{T}_t(E) = |t_t|^2$. The transmission amplitudes for particular spin configurations of the target (bound electron) and scattered electron are further expressed in terms of t_s and t_t as $t_{\uparrow\uparrow\rightarrow\uparrow\uparrow}(E) = t_t$, $t_{\downarrow\uparrow\rightarrow\downarrow\uparrow}(E) = \frac{1}{2}(t_s + t_t)$, and $t_{\downarrow\uparrow\rightarrow\uparrow\downarrow}(E) = \frac{1}{2}(t_s - t_t)$, where, for example, $t_{\downarrow\uparrow\rightarrow\uparrow\downarrow}(E)$ is the transition amplitude from $[\downarrow, \uparrow]$ to $[\uparrow, \downarrow]$ spin states of the [scattered,bound] electron. The conductance for unpolarized electrons is then the *average* over the initial and the *sum* over the final configurations, $G(E) = G_0\mathcal{T}(E)$, where

$$\begin{aligned} \mathcal{T}(E) &= \frac{1}{4} \left(|t_{\uparrow\uparrow\rightarrow\uparrow\uparrow}|^2 + |t_{\downarrow\uparrow\rightarrow\downarrow\uparrow}|^2 + |t_{\downarrow\uparrow\rightarrow\uparrow\downarrow}|^2 + |t_{\downarrow\downarrow\rightarrow\downarrow\downarrow}|^2 + |t_{\uparrow\downarrow\rightarrow\uparrow\downarrow}|^2 + |t_{\uparrow\downarrow\rightarrow\downarrow\uparrow}|^2 \right) \\ &= \frac{1}{4}\mathcal{T}_s(E) + \frac{3}{4}\mathcal{T}_t(E). \end{aligned} \quad (1)$$

At finite temperatures the conductance is calculated using a generalized Landauer–Büttiker formula [19]

$$G(E) = G_0 \int \mathcal{T}(\epsilon) \left[-\frac{\partial f(\epsilon - E, T)}{\partial \epsilon} \right] d\epsilon \quad (2)$$

where $f(\epsilon, T) = [1 + \exp(\epsilon/k_B T)]^{-1}$ is the usual Fermi function.

For simplicity, quantitative treatment of quantum wires is restricted to the geometry shown in figure 1, with confinement in the x - and y -direction and electron propagation in the z -direction. This is similar to wires produced in ‘ v ’-grooves as reported by Kaufman *et al* [6] with thicknesses in the range 10–20 nm. The wire shape under consideration is symmetric around the z -axis with constant potential, $V(x, y, z) = 0$ within a boundary shown in figure 1, and confining potential $V_0 > 0$ elsewhere. As shown in figure 1 the wire has thickness a_3 and a single bulge.

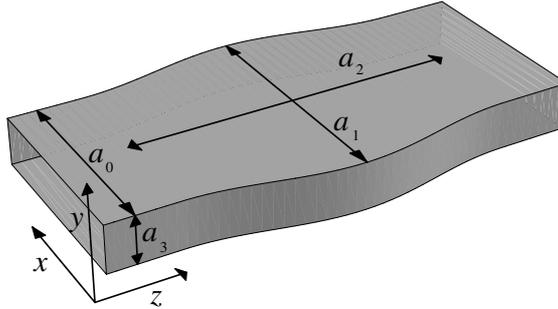


Figure 1. Geometry of a near perfect wire or ‘open quantum dot’, parametrized as $x_0(z) = \frac{1}{2}[a_0 + (a_1 - a_0) \cos^2 \pi z/a_2]$ for $|z| \leq \frac{1}{2}a_2$ and $x_0(z) \equiv \frac{1}{2}a_0$ otherwise.

In order to obtain precise results, we choose parameters appropriate to GaAs for the wire and $\text{Al}_\delta\text{Ga}_{1-\delta}\text{As}$ for the barrier with δ such that $V_0 = 0.4$ eV, which is close to the cross-over to an indirect gap. Band non-parabolicity is neglected and we use the GaAs effective mass, $m^* = 0.067m_0$, neglecting its variation across the boundary. The corresponding one-electron Schrödinger equation reads

$$-\frac{\hbar^2}{2m^*} \nabla^2 \Psi(x, y, z) + V \Psi(x, y, z) = (E_0 + E) \Psi(x, y, z) \quad (3)$$

where E is electron energy measured from the lowest transverse channel in the straight part of the wire with energy E_0 (which is V_0 -dependent, with $E_0 = \hbar^2/(8m^*)(a_0^{-2} + a_3^{-2})$ for $V_0 \rightarrow \infty$). The wave function is expanded in elementary modes or channels, $\Psi(x, y, z) = \sum_n \Phi_n(x, z) \chi(y) \psi_n(z)$, where the basis functions $\Phi_n(x, z)$ are orthogonal solutions of one-dimensional (1D) Schrödinger equations in the x -direction for fixed z . We choose $a_3 \ll a_0$ and hence only the lowest y -channel solution, $\chi(y)$, is relevant.

If such a wire is connected to metallic source-drain contacts, electrons can flow into the wire region. At least one electron will become bound in the bulge region of the wire. The number of bound electrons depends on both the Fermi energy and the relative size of the bulge (i.e. parameters a_1 and a_2). The single electron problem may be reduced to a quasi-1D N -component differential equation [20, 21]. From the solution of the scattering problem, the conductance is calculated from the usual Landauer–Büttiker formula. For $a_1/a_0 \gg 1$ many channels are needed, while for $a_1 \sim a_0$ the inter-channel mixing can be neglected and the conductance is very similar to that of a perfect straight wire with conductance steps in multiples of G_0 . For energies $E < 0$, the solutions of equation (3) are bound states.

We consider the interacting electron problem with wire parameters in a range which ensures that only one electron occupies a bound state and that restriction to a single channel near the conduction edge is an excellent approximation. This is the case when the bulge is sufficiently weak, with $a_1 \gtrsim a_0$. The electron wave function is then determined from a 1D Schrödinger equation for $\psi_0(z)$ as in [21]. Within the single-channel approximation we consider the interacting two-electron problem in which one electron is bound in the quantum dot region. It should be noted that the existence of a single-electron bound state is guaranteed in 1D and in this sense is a universal feature. With the chosen parameter range, a second electron cannot be bound due to the effective 1D Coulomb repulsion $U(z, z')$ between the electrons

$$U(z, z') = \frac{e^2}{4\pi\epsilon\epsilon_0} \iiint \frac{|\Phi_0(x, z) \Phi_0(x', z') \chi(y) \chi(y')|^2 dx dx' dy dy'}{\sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}}. \quad (4)$$

The dielectric constant is taken as $\epsilon = 12.5$, appropriate for GaAs. We solve the two-electron scattering problem exactly, subject to the boundary condition that the asymptotic states consist of one bound electron in the ground state and one free electron.

In figure 2(a) we show plots at zero temperature of $T_s(E)$ and $T_t(E)$ for a typical wire with the geometry of figure 1. The thin dotted line represents the non-interacting result, independent of spin. In figure 2(b) the conductance $G(E)/G_0$ is shown, as calculated from equation (2) for various temperatures. The resonances have a strong temperature dependence and, in particular, the sharper singlet resonance is more readily washed out at finite temperatures. However, it should be noted that resonances survive to relatively high temperatures, because the width of the wire, which dictates the energy scale, is small ($a_0 = 10$ nm) [21]. Note that for weak coupling, the energy scale is set by the x -energy of the lowest channel, $\sim a_0^{-2}$, and hence the conductance versus Ea_0^2 with Ua_0 fixed is roughly independent of a_0 (the scaling would be exact for $V_0 \rightarrow \infty$).

The effect of elevated temperatures is mainly to smear the resonances. The effect of a magnetic field on conductance is much more subtle [4, 11] and a complete general theory is not presently available. For the special case of an in-plane magnetic field (parallel to the x - z plane), however, an estimate can be obtained as follows. We assume that the bound electron in the initial state is polarized with spin \downarrow . This assumes that the bound electron will reach its lowest Zeeman state between scattering events, whereas the effect of the field on the electrons in the leads near the Fermi energy will be to simply change their densities of states, as in Pauli paramagnetism. Thus the energy of the localized electron will be lowered

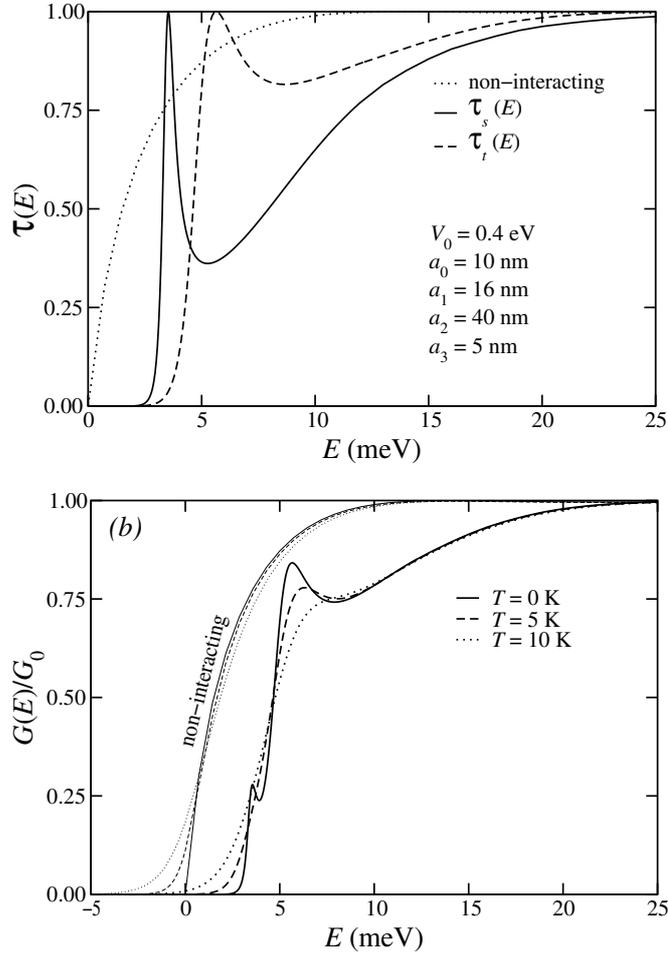


Figure 2. (a) Zero temperature singlet transmission probability $T_s(E)$, and triplet $T_t(E)$ with full and dashed lines, respectively. The energy E is measured from the lowest transverse channel in the straight part of the wire. The dotted line represents the corresponding non-interacting result. (b) Total conductance, $G(E)$, for the temperature range $T \leq 10$ K, where resonances are still discernible. The thin lines show the corresponding non-interacting result.

by $E_B = \frac{1}{2}g^*\mu_B B$, whereas the electron densities will be $\rho_\uparrow(E, B) = \rho_\uparrow(E - E_B, 0)$ and $\rho_\downarrow(E, B) = \rho_\downarrow(E + E_B, 0)$. Although the densities of up and down spin electrons are no longer equal in finite magnetic fields, the conductances of each spin species will be independent of their densities in the Landauer–Büttiker formula, due to the usual cancelation with group velocity. Hence, assuming that the transmission amplitudes have the same dependence on kinetic energy as in zero field, the conductance is $G(E, B) = G_0 T(E, B)$, where

$$\begin{aligned} T(E, B) &= \frac{1}{2} \left(|t_{\downarrow\downarrow \rightarrow \downarrow\downarrow}(E + E_B)|^2 + |t_{\uparrow\downarrow \rightarrow \uparrow\downarrow}(E - E_B)|^2 + |t_{\uparrow\downarrow \rightarrow \downarrow\uparrow}(E - E_B)|^2 \right) \\ &= \frac{1}{2} T_t(E + E_B) + \frac{1}{4} [T_s(E - E_B) + T_t(E - E_B)]. \end{aligned} \quad (5)$$

We have included the spin-flip term in this equation, which assumes that the scattered electron, which lies $2E_B$ below the Fermi energy, is not reflected by the collector. This

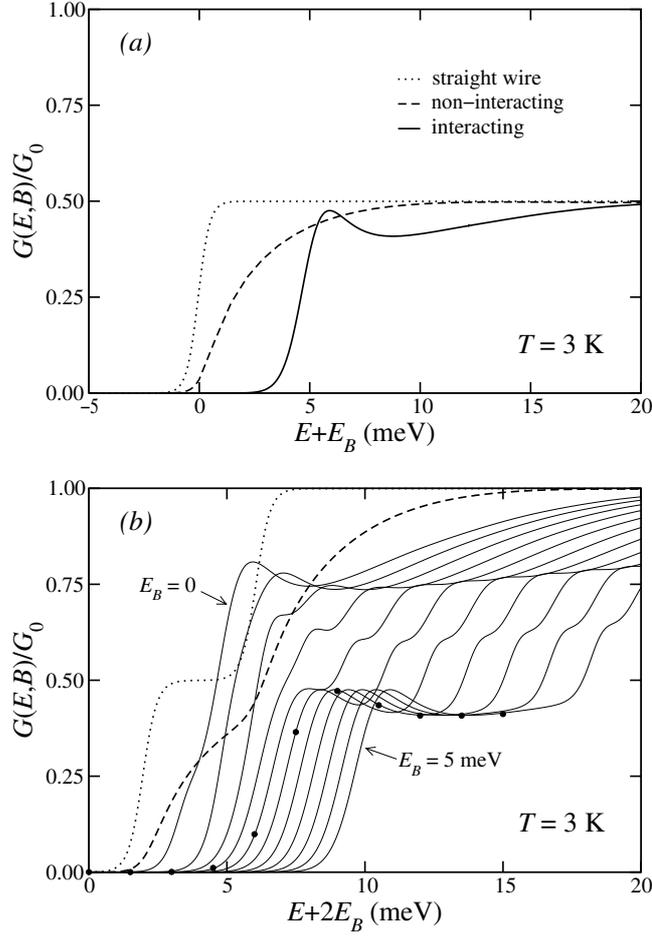


Figure 3. (a) $G(E, B)$ in a high magnetic field, equation (6), shown together with the non-interacting result (dashed) and the corresponding result for a perfectly straight wire (dotted). (b) $G(E, B)$ for $T = 3$ K and the geometry of the wire shown in figure 2. Successive traces represent results for E_B incremented in steps $\Delta E_B = 0.5$ meV and for clarity have been horizontally offset by $2E_B$. Also shown is the non-interacting result (dashed) and perfect straight wire result (dotted) for $E_B = 2$ meV.

necessitates inelastic processes in the collector and the approximation may break down in some circumstances which we shall not consider further here.

In any case, $t_{\uparrow\downarrow\rightarrow\downarrow\uparrow}(E - E_B) = t_{\downarrow\uparrow\rightarrow\uparrow\downarrow}(E - E_B) = 0$ when $E \leq E_B$, for which we get from equation (5)

$$G(E, B) = \frac{e^2}{h} T_1(E + E_B). \quad (6)$$

This is plotted in figure 3(a) for $T = 3$ K together with the corresponding results for non-interacting electrons and a straight wire. We see that these curves are very similar, with a plateau at e^2/h but with the interacting case displaced to the right (due to the Coulomb repulsion) and showing a slight dip, due to the broad triplet resonance. This curve is very similar to high-field experimental curves on gated 2DEG wires which show the ‘0.7’ anomaly [12], further supporting the view that an electron is weakly bound in the wire. In figure 3(b) $G(E, B)$ for

$T = 3$ K is presented for a magnetic field increasing from zero in steps with $\Delta E_B = 0.5$ meV, and for clarity the curves have been shifted by $2E_B$ to the right with increasing E_B . We present results for $a_0 = 10$ nm, but note that E_B also obeys the above mentioned scaling $E_B a_0^2$ with varying a_0 . Magnetic fields which would give substantial effects in e.g. narrow ‘v’-groove wires [6], would have to be very large, since $E_B = 1$ meV corresponds to large $g^* B \sim 35$ T. However, due to ‘ $E_B a_0^2$ ’ scaling, the corresponding value for a wider wire with $a_0 \sim 50$ nm would be only ~ 1.4 T. Also plotted in figure 3(b) for comparison are the corresponding results for the non-interacting electron case (dotted) and the perfectly straight wire (dashed), with $E_B = 2$ meV. In this figure we have indicated with a dot the points $E = E_B$. To the left of these points G satisfies equation (6), whereas at high energies $t_{\uparrow\downarrow\rightarrow\uparrow\downarrow}$ and $t_{\uparrow\downarrow\rightarrow\downarrow\uparrow}$ are non-zero in equation (5). As argued above, these parts of the curves should be treated with caution, though they are expected to be more reliable at lower fields.

In summary, we have shown that quantum wires with weak longitudinal confinement, or open quantum dots, can give rise to spin-dependent, Coulomb blockade resonances when a single electron is bound in the confined region. This is a universal effect in one-dimensional systems with very weak longitudinal confinement. The emergence of a specific structure at $G(E) \sim \frac{1}{4}G_0$ and $G \sim \frac{3}{4}G_0$ is a consequence of the singlet and triplet nature of the resonances, and the probability ratio 1:3 for singlet and triplet scattering and as such is a universal effect. A comprehensive numerical investigation of open quantum dots using a wide range of parameters shows that singlet resonances are always at lower energies than the triplets, in accordance with the corresponding theorem for bound states [22]. With an increasing in-plane magnetic field, the resonances shift their position and a plateau $G(E) \sim e^2/h$ emerges. The effect of a magnetic field is observable only in relatively wider quantum wires, due to the intrinsic energy scale $\propto a_0^{-2}$.

Finally, we speculate on how these results might change if more than one electron is confined longitudinally in the wire. This possibility could arise, for example, in long, near perfect wires with a long weak confinement region. Theoretically this becomes a more complicated spin-dependent scattering problem [17]. The conductance would then again show resonance anomalies with positions determined by the weights of the spin states. The generalized Landauer–Büttiker formula for such cases was discussed recently by Flambaum and Kuchiev [23], who also derived independently the formula for the singlet/triplet case discussed above and in [16]. In the case when two electrons are bound, i.e. a conduction electron scattering from two bound electrons in the confinement region, the relevant resonant states of three electrons will be doublets and quartets. When the length of the longitudinal confinement region is somewhat greater than a Bohr radius, we are in the quasi-1D strong correlation regime for which we expect a low lying manifold of spin states, well separated from higher-lying states and described by a Heisenberg model, as in a 1D quantum dot with 3 electrons. This spin manifold contains $2^3 = 8$ states, which split into two doublets and a quartet; we expect a doublet to be lowest in accordance with the Lieb–Mattis theorem. This is consistent with the exchange being antiferromagnetic, which is the case in a truly closed 1D quantum dot with 3 electrons, for which the quartet is highest in energy [24]. If this picture holds for the resonant bound states, then we should get two doublet resonances with weight 1/4 each, followed by the quartet at highest energy with weight 1/2. This latter resonance will give a conductance anomaly near e^2/h . Furthermore, this resonance will be broader than the doublet resonances since it is somewhat higher in energy than the two singlets and is thus expected to be more pronounced at finite temperatures. Conductance anomalies close to e^2/h have been observed very recently in long, clean and nominally straight wires [7]. This is consistent with the above scenario, though we must await detailed calculations in this strong correlation regime for a more complete picture.

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References

- [1] van Wees B J *et al* 1988 *Phys. Rev. Lett.* **60** 848
- [2] Wharam D A *et al* 1988 *J. Phys. C: Solid State Phys.* **21** L209
- [3] Yacoby A *et al* 1996 *Phys. Rev. Lett.* **77** 4612
- [4] Ramvall P *et al* 1997 *Appl. Phys. Lett.* **71** 918
- [5] Walther M, Kapon E, Hwang D M, Colas E and Nunes L 1992 *Phys. Rev. B* **45** 6333
Grundmann M *et al* 1994 *Semicond. Sci. Tech.* **9** 1939
Rinaldi R *et al* 1994 *Phys. Rev. Lett.* **73** 2899
- [6] Kaufman D *et al* 1999 *Phys. Rev. B* **59** R10433
- [7] Kane B E *et al* 1998 *Appl. Phys. Lett.* **72** 3506
Reilly D J 2000 *Preprint cond-mat/0001174*
- [8] Landauer R 1957 *IBM J. Res. Dev.* **1** 223
Landauer R 1988 *IBM J. Res. Dev.* **32** 306
- [9] Büttiker M 1986 *Phys. Rev. Lett.* **57** 1761
- [10] van Houten H, Beenakker C W J and van Wees B J 1992 *Semiconductors and Semimetals* ed R K Willardson, A C Beer and E R Weber (New York: Academic)
- [11] Thomas K J *et al* 1996 *Phys. Rev. Lett.* **77** 135
Thomas K J *et al* 1998 *Phys. Rev. B* **58** 4846
Thomas K J *et al* 1999 *Phys. Rev. B* **59** 12252
- [12] Thomas K J *et al* 1998 *Phil. Mag. B* **77** 1213
- [13] Fasol G and Sakaki H 1994 *Jpn J. Appl. Phys.* **33** 879
- [14] Maslov D L 1995 *Phys. Rev. B* **52** R14368
- [15] Wang Chuan-Kui and Berggren K-F 1998 *Phys. Rev. B* **57** 4552
- [16] Rejec T, Ramšak A and Jefferson J H 1999 *Preprint cond-mat/9910399*
- [17] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon)
- [18] Oppenheimer J R 1928 *Phys. Rev.* **32** 361
Mott N F 1930 *Proc. R. Soc. A* **126** 259
- [19] Bagwell P F and Orlando T P 1989 *Phys. Rev. B* **40** 1456
- [20] Nakazato K and Blaikie B J 1991 *J. Phys.: Condens. Matter* **3** 5729
- [21] Ramšak A, Rejec T and Jefferson J H 1998 *Phys. Rev. B* **58** 4014
- [22] Lieb E and Mattis D 1962 *Phys. Rev.* **125** 164
- [23] Flambaum V V and Kuchiev M Yu 1999 *Preprint cond-mat/9910415*
- [24] Jefferson J H and Häusler W 1996 *Phys. Rev. B* **54** 4936