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Tuning the transmission phase by the dot size

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HIGHLIGHTS

- The transmission phase increase on resonances is calculated for few electrons rectangular quantum dots.
- Electronic correlations induce a quasi–liner decrease of the transmission phase with the dot size.
- Ground state spin transitions are reflected in jumps of the transmission phase.

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ABSTRACT

The phase shift of the electron's wave function after a tunneling event (i.e. the transmission phase) was at first measured for its fundamental or applicative relevance for quantum circuitry, but later the phase study self-motivated due to a number of unexpected results. One such result was the reduced increment of the phase on some resonances - with only fractions of π - in the few-electrons "mesoscopic" regime. In this paper we address such a regime for a rectangular quantum dot and compute the total phase increase on the first four resonances by means of accurate configuration–interaction method and a generalized Friedel sum rule as proposed by Rontani (2006) [17]. Our findings confirm that the electronic correlations reduce the on-resonance phase growth which is also found to decrease quasi–linearly with the dot size, the decrease being more pronounced as the number of electrons on the dot is raised. Sudden jumps (of small amplitude) of the phase are found to accompany ground states spin transitions.

1. Introduction

Since the wave functions in quantum mechanics are complex quantities, measuring – or calculating – the phase of the electron has emerged as a natural key direction in the mesoscopic physics of the last two decades. The phase of the wave function, rather than just the amplitude, plays an important role for instance in the bonding of molecular orbitals or in quantum interference phenomena. The focus of this paper will be the study of the electron's phase shift after tunneling through a quantum dot, with potential applications in quantum circuitry, the motivation residing also in some intriguing experimental results, which are yet to be explained. The textbook model of an electron tunneling through a double barrier predicts an increase of the transmission phase (i.e. the phase of the complex quantity t from the te^{ikx} transmission term) with precisely π on each resonance and a constant value between resonances (see for illustration Fig. 14 from [1]), however the experimental results have been very different from that expectation.

The first transmission phase measuring experiments [2,3] have been performed by inserting a quantum dot in one arm of a mesoscopic interferometer and it was shown that the transmission phase can be directly related to the shift of the Aharonov–Bohm oscillations, making it rigourously identifiable. The mentioned experiments have revealed an unexpected result, namely a universal π lapse of the phase between all pairs of resonances, contradicting not only an intuitive Friedel sum rule [4] or the simple double barrier model, but also more elaborate models (see the early review [1]). As time passed, the phase lapse problem received an well-deserved appellative of "longest standing puzzle in mesoscopic physics" [5], efforts being still on-going for a convincing explanation (see, e.g., [6–13] and references therein).

Later, Avinun–Kalish et al. [14] have shown that the universal phase lapse behavior occurs only for large number of electrons ($N \gtrsim 10$) while in the few-electrons regime – named by the authors "mesoscopic"- the phase lapses are not omnipresent. Nevertheless, the mesoscopic regime revealed some equally intriguing puzzles of its own, among which the reduced evolution of the phase on some resonances and the presence of on-resonance non-monotonic evolutions (of dip-like shapes). Some theoretical papers already addressed the mesoscopic regime [15–18]. A reduced variation of the transmittance phase for a electron

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tunneling through a quantum dot with a magnetic impurity was found in [19].

The focus of our paper will be on the mesoscopic regime, with the emphasis on the magnitude of the transmission phase evolution on resonances, for a wide interval of dot sizes. Multi-electrons regime and the phase lapse problem between resonances fall outside of our scope here.

Electron–electron interaction gives rise to a large variety of mesoscopic phenomena. If few electrons are weakly confined in large quantum dots, Wigner crystallization [20–22] and particles-like behavior may occur, while in the opposite situation of extreme confinement interaction effects are negligible compared to the kinetic energies involved. Quite remarkably, it is the intermediate regime that corresponds to the experimental set-up [14], giving raise to complex interplay between confinement and interaction effects, which we shall addressed in the context of transmission phase calculations. For this purpose, we shall consider a rectangular quantum dot of variable size, the motivation for shape choosing residing in a better resemblance with the lithographycally defined dots [14], also avoiding particular degeneracies of circular or parabolical confinements.

Our approach will then follow [17,18], by performing spectral calculations in the few-electrons regime and extract relevant phase information via the Friedel sum rule. The spectra are calculated using the configuration–interaction method, which is known to give highly accurate results of controlled precision, or numerically exact results for discrete systems with small number of sites and electrons [18,23–37]. Exact diagonalization is performed on the full set of Slater determinants, separated in subspaces with the same electrons number, no approximations or truncations being done in this part of calculations. Most importantly, the method has convergence properties in respect to the size of the single particle basis (used for the Slater determinants) which can be increased till the main results – spectrum and wave functions coefficients – undergo negligible changes.

The results indicate that the overall increase of the phase across a single resonance decrease almost linearly with dot size, discontinuities being found in case of ground states spin transitions.

The outline of the paper is as follows: Section 2 presents the configuration–interaction method for calculating the eigenfunctions which are then used in Section 3 to calculate the total increase of the phase on resonances. Section 4 concludes the paper.

2. Few-electrons eigenfunctions calculation by use of configuration–interaction method

The system we consider in this paper is a rectangular quantum dot – depicted in Fig. 1, and prior to the many–body calculations one has to determine the single-particle eigenfunctions and eigenenergies. For a wide variety of shapes, even complex ones, there exist in literature recipes for exact or highly accurate eigenvalues and eigenfunctions calculations (see, e.g. [38] and references therein). For the 2D rectangle they are simply:

$$\Psi_{m,n}(x,y)=\frac{2}{L\sqrt{\gamma}}\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi y}{\gamma L}\right),\ \epsilon_{m,n}=\frac{\pi^2\hbar^2}{2m_e}\left(\frac{m^2}{L^2}+\frac{n^2}{(\gamma L)^2}\right), \quad (1)$$

with the usual notations, L and γL being the rectangle sides and the integer longitudinal and transversal quantum numbers $m, n \geq 1$ naturally label the modes. In the following, we shall switch to a single parameter notation $\{(m,n)\} \Leftrightarrow \{a\}$, strictly for simplicity of exposure, existing no risk of confusion – and the order being given by the respective eigenenergies, starting with the ground state.

The interacting dot Hamiltonian can be generically written in the second quantization:

$$H^D=\sum_{a=1}^{N}\sum_{\sigma}\epsilon_a c^{\dagger}_{a\sigma}c_{a\sigma}+\frac{1}{2}\sum_{a,b,c,d=1}^{N}\sum_{\sigma\sigma'}V_{abcd}c^{\dagger}_{a\sigma}c^{\dagger}_{b\sigma'}c_{c\sigma'}c_{d\sigma}, \quad (2)$$

with

$$V_{abcd}=\int_r\int_{r'}dr\ dr'\Psi^*_a(r)\Psi^*_b(r')U_{r,r'}\Psi_c(r')\Psi_d(r), \quad (3)$$

the single-particle energies ϵ_a and eigenmodes Ψ_a being those from Eq. (1) (relabeled with only one index, in order of increasing energy) and the Coulomb interaction coefficient is: $U_{r,r'}=e^2/(4\pi\epsilon|r-r'|)$. It is interesting to notice on the spot that the Coulomb terms depend on the dot size as $1/L$ while the kinetic terms in Eq. (1) depend as $1/L^2$. As such, interaction effects are expected to be negligible at very high confinement (low values of L) and dominant at large dot sizes.

After calculating the Coulomb elements (Eq. (3)), the diagonalization procedure for the Hamiltonian (Eq. (2)) can be performed for sub-spaces with set number of electrons placed in all possible ways in the chosen number of single particles states. The configuration–interaction method proceeds by increasing the single-particle basis (given by N in Eq. (2)) until convergence is attained for the quantities of interest such as the ground state energy and coefficients of the eigenfunctions. The maximum number of single particles states used in this paper will be 28 (including the spin), which ensure good convergence for the presented results.

For a rectangular dot with sides ratio $\gamma = 0.8$ (see Fig. 1), the expansion of the ground state wave function for two, three and four electrons is given in Table 1, assuming two different values of the "long" side L [expressed in units of the Bohr radius $a_0=4\pi\epsilon\hbar^2/(e^2m_e)$, which has the values $a_0=0.053$ nm in vacuum and $a_0=10$ nm in GaAs]. Note that the coefficients are given, including the sign – relative to the dominant coefficient-, and not the square modules which show in fact the states occupancies. For length considerations, only coefficients higher then 0.1 -corresponding to a spectral weight of 1%- have been given. Still it is important to mention that for high values of L, and increase effect of interaction, contributions much lower than 1% can become important as there are very numerous terms with such coefficients. In the numerical calculations, all contributions are considered.

The effect of interaction is relatively small for $L = 4a_0$ when the occupation of higher Slater determinants is reduced for all studied electrons numbers. By increasing the size of the dot, the interaction becomes more dominant which reflects in the occupancy of higher states. The maximum size considered in this paper is $L = 12a_0$, corresponding to roughly 120 nm for the case of GaAs heterostructures. This size exceeds the dot sizes used in usual phase measuring experiments (in [14] we estimate $L < 100$ nm), corresponding therefore to higher role of correlations. Moreover, the dots in experiment are not truly 2D, as is the case in our model, making confinement effectively less. All these aspects allow us to conclude that the lengths range studied in this paper

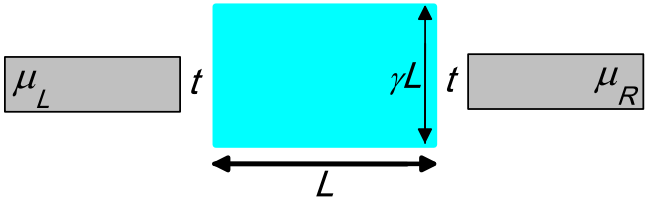

Fig. 1. Sketch of a rectangular quantum dot with sides ratio γ which is connected to leads by a hopping t. The numerical calculations will be performed for $\gamma = 0.8$. Even if the dot is connected to the Left and Right leads, some transmission phase properties can be extracted from the spectral properties of the isolated dot – see description in text.