Energy spectrum, persistent current and electron localization in quantum rings

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Abstract

Energy spectra of quasi-one-dimensional quantum rings with a few electrons are studied using several different theoretical methods. Discrete Hubbard models and continuum models are shown to give similar results governed by the special features of the one-dimensionality. The energy spectrum of the many-body system can be described with a rotation-vibration spectrum of a 'Wigner molecule' of 'localized' electrons, combined with the spin-state determined from an effective antiferromagnetic Heisenberg Hamiltonian. The persistent current as a function of magnetic flux through the ring shows periodic oscillations arising from the 'rigid rotation' of the electron ring. For polarized electrons the periodicity of the oscillations is always the flux quantum Φ₀. For nonpolarized electrons the periodicity depends on the strength of the effective Heisenberg coupling and changes from Φ₀ first to Φ₀/2 and eventually to Φ₀/N when the ring gets narrower.
I. INTRODUCTION

Recent experimental developments in manufacturing quantum dots and rings with only a few electrons have made quantum rings an ever increasing topic of experimental and theoretical research. In a quantum ring the electrons move in a ring-shaped quasi-one-dimensional confinement. The one-dimensionality makes the electrons strongly correlated. Among the quantum effects seen in such systems are the Aharonov-Bohm oscillations and persistent currents.

Many properties of the quantum rings can be explained with single-electron theory, which in a strictly one-dimensional (1D) system is naturally very simple. On the contrary, the many-particle fermion problem in 1D systems is surprisingly complicated due to enhanced importance of the Pauli exclusion principle. It is then customary to say that strictly 1D systems are not ‘Fermi liquids’ but ‘Luttinger liquids’ with specific collective excitations (for reviews see).

We consider two models for quantum rings. In the continuum model the electrons move in an external two-dimensional potential (shown schematically in Fig. 1a) usually considered to be harmonic:

$$V(r) = \frac{1}{2}m_e\omega_0^2(r - R)^2,$$

where $R$ is the radius of the ring and $\omega_0$ the strength of the radial confinement. The electron-electron interaction is the normal long-range Coulomb interaction. If the number of electrons is small, the many-electron states in this external potential can be solved (numerically) exactly using standard configuration interaction (CI) methods.

Another theoretical approach to quantum rings has been a model where the ring consists of discrete lattice sites, as shown in Fig. 1b. The many-particle Hamiltonian can be approximated with the Hubbard model

$$H = -t \sum_{i=1}^{L} \sum_{\sigma} \left( e^{-i2\pi\phi/L} c_{i+1,\sigma}^\dagger c_{i,\sigma} + e^{i2\pi\phi/L} c_{i,\sigma}^\dagger c_{i+1,\sigma} \right) + U \sum_{i=1}^{L} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow},$$

where $t$ and $U$ are the Hubbard parameters determining the hopping between neighbouring sites and the on-site energy, $L$ is the number of electrons and the number of sites, respectively, and $\phi$ is the magnetic flux through the ring (in units of the flux quantum $\Phi_0 = h/e$). The advantage of the discrete model is that the many-body problem is much easier than that of Eq. (1), and can be solved exactly in some limiting cases.
The two theoretical approaches, although seemingly very different, give in many cases qualitatively similar results. The aim of this work is to compare these models quantitatively and study the reasons for the similarities of these two approaches (for an introductory review see Ref. 17).

II. ENERGY SPECTRA: ROTATIONAL AND VIBRATIONAL STATES

Figure 2 shows the energy spectra of quantum rings with six electrons, calculated from the continuum model and from the lattice model with eight sites. In both cases the excitation spectrum contains a low energy band of rotational states with energy increasing in the continuum model roughly as $\frac{\hbar^2 M^2}{2I}$, where $M$ is the total angular momentum and $I$ the moment of inertia $I = N \mu_e R^2$. The low energy electron spectrum thus corresponds to rigid rotation of a ring of six electrons while the higher bands correspond to vibrational excitations. Moreover, the energy splitting (due to spin) can be quantitatively described with an antiferromagnetic Heisenberg model. Thus one arrives at the following model Hamiltonian

$$H_{\text{eff}} = \frac{\hbar^2}{2I} M^2 + J \sum_{\langle i,j \rangle} S_i \cdot S_j + \sum_{\nu} \hbar \omega_\nu n_\nu,$$

(3)

where the last term describes vibrational states of electrons localized on the ring (in Fig. 2 the vibrational states are the ones not marked with the spin number).

Figure 2 shows that nearly exactly the same low energy spectrum can be obtained from the Hubbard model with suitably chosen parameters. It is known that in the limit of large $U$ the half-filled Hubbard model ($N = L$) approaches the antiferromagnetic Heisenberg model, explaining the correct spin structure of the model Hamiltonian above. However, the correspondence seems to go even further: If $L > N$ the rigid rotations and vibrational states also appear in agreement with the continuum model.

The similarity of the discrete lattice model with contact interaction and the continuum model with long-range interaction can be traced back to the special properties of one-dimensional systems. The strong contact interaction effectively prevents electrons to pass each other and the 'kinetic energy repulsion' makes the strong $\delta$-function interaction look like a $1/r^2$ interaction as evident from the Calogero-Sutherland model$^{17,18,19}$. Nevertheless, it is surprising that the similarity survives to quasi-one-dimensional rings considered in Fig.
The 'localization' of electrons along the ring happens at all electron numbers. Similar traces of electron localization can be found in the energy spectra of two-dimensional quantum dot\(^{20}\). Figure 3 shows the energy spectra of quantum rings and dots with four electrons. In both cases the classical localization geometry is a square. Indeed the low-energy spectrum is similar for a ring and for a dot. The Hubbard model gives again qualitatively the same spectra as the continuum model (not shown here)\(^{11,17}\).

III. PERIODICITY OF THE PERSISTENT CURRENT

The persistent current of a quantum ring can be determined from the flux dependence of the total energy\(^{17}\)

\[
I(\Phi) = -\frac{\partial E}{\partial \Phi},
\]

where \(\Phi\) is the magnetic flux through the ring. Since the discrete Hubbard model gives the same energy levels as the continuum model, we can use it to study the persistent current. The Hamiltonian (2) can be solved numerically for small number of electrons and sites. Due to the phase factors the energy levels, and consequently the persistent current, will be periodic functions of the flux.

Figure 4 shows the spectrum of a Hubbard ring of four electrons in eight sites, as a function of \(\Phi\) for different values of \(U\). For \(U = 0\) the ground state energy has a periodicity \(\Phi_0\). When \(U\) increases the period changes first to \(\Phi_0/2\) and eventually to \(\Phi_0/N\). This happens at all electron numbers and in a similar fashion for continuum\(^{21}\) and discrete\(^{17}\) rings. The increase of the strength of the radial confinement, \(\omega_0\) in Eq. (1), of the continuum model corresponds to the increase of the on-site energy \(U\) of the Hubbard model. In both cases the ring becomes more strictly one-dimensional in the sense that electrons are prevented to pass each other.

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FIG. 1: Two models of quantum rings, a continuum ring and a ring consisting of discrete lattice sites.

FIG. 2: Many-particle spectra of six electrons in a continuum ring and in a Hubbard ring with eight sites. The numbers indicate the total spin of the state.
FIG. 3: Many-particle spectrum of four electrons in a ring and a dot, shown in the insets ($U = 40t$).

FIG. 4: Flux-dependence of the many-particle spectrum of a Hubbard ring with eight sites and four electrons.