Parity Effects in Stacked Nanoscopic Quantum Rings

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The ground state and the dielectric response of stacked quantum rings are investigated in the presence of an applied magnetic field along the ring axis. For odd number $N$ of rings and an electric field perpendicular to the axis, a linear Stark effect occurs at distinct values of the magnetic field. At those fields energy levels cross in the absence of electric field. For even values of $N$ a quadratic Stark effect is expected in all cases, but the induced electric polarization is discontinuous at those special magnetic fields. Experimental consequences for related nanostructures are discussed.

Considerable progress has been made in precise measurements of the dielectric response of solids at low temperatures. New physical effects have been found due to these advances. An example are certain multicomponent glasses where it has been found that at ultra-low temperatures $T < 100\text{mK}$ the dielectric response is strongly magnetic field dependent. The interactions between the different tunneling systems in the glasses consisting of groups of atoms (or single atoms) are sufficiently strong so that large groups of them form a coherent state with a Aharonov-Bohm phase. Here we are considering a stack of symmetrical ring molecules (quantum rings) with one (unpaired) electron per ring. Electrons in different rings interact with each other. For simplicity we restrict that interaction to neighboring rings, but the conclusions of the present investigation do not depend on this simplification. The purpose of this communication is to point out that a stack of such quantum rings shows an interesting even-odd effect with respect to the number $N$ of rings in the stack. In particular we want to show the following.

(i) The dielectric response of an even number of rings to an electric field in the plane of the rings is considerably smaller than in the case of an odd number.

(ii) The induced electric polarization $P(\phi)$ as a function of magnetic flux $\phi$ through the rings is a continuous function of $\phi$ when the number of rings is odd while it shows discontinuities in the case when $N$ is even.

In order to prove the above statements we start from a Hamiltonian for the cofacially stacked rings in an axial magnetic field and a perpendicular electric field with simplified electron interactions. The interactions are assumed to take place only between neighboring rings and we assume for them a simple angular dependence. In analogy to previous works on glasses, we write for a system of $N$ rings

$$H = H_0 - E\phi_0 \sum_j \cos \theta_j,$$

$$H_0 = \frac{\hbar^2}{2mr^2} \sum_j \left( i \frac{\partial}{\partial \theta_j} + \frac{\phi}{\phi_0} \right)^2 + J \sum_{j=1}^{N-1} \cos(\theta_{j+1} - \theta_j).$$

Here $r$ is the radius of a ring, $m$ is the particle mass, $\phi_0 = \hbar c/e$ is the flux quantum, $J > 0$ is the coupling strength of particles in neighboring rings, $E$ is the size of the electric field in the plane of the rings and $p = er$ is a dipole moment. The following considerations do not depend on the special form of the interaction chosen here provided the interaction is repulsive. In order to simplify the notation we shall use the abbreviation $u = \hbar^2/(2mr^2)$. First we consider the case of $E = 0$. Then the total angular momentum commutes with $H_0$ and hence is a good quantum number. Disregarding the spin indices which are not important in this context, the eigenfunction of $H_0$ can be classified by two indices $M, \alpha$, i.e., the azimuthal total angular momentum quantum number, and $\alpha$. The quantum number $\alpha$ describes the different states of a given angular momentum $M$. In the absence of any interactions, i.e., for $J = 0$ the eigenstates are highly degenerate, but this degeneracy is lifted by the interactions. It is easy to show from Eq. (2) that in the presence of a magnetic field through the rings the eigenenergies are given by

$$E_{M,\alpha}(\phi) = E_{M,\alpha}(0) + uN \left( \frac{\phi}{\phi_0} - \frac{M}{N} \right)^2 - \frac{uM^2}{N},$$

where $E_{M,\alpha}(0)$ are the eigenenergies in the absence of an applied magnetic field. As a function of $\phi$ the eigenenergy $E_{M,\alpha}(\phi)$ and in particular the ground-state energy $E_{M,G}(\phi)$ have the form of a parabola centered at $\phi/\phi_0 = M/N$. As for the ground state we need to consider therefore $M$ values only within the range $0 \leq M \leq N$ when $\phi$ varies between $0 \leq \phi \leq \phi_0$. Because of the $\phi$ dependent term in Eq. (3), energy levels cross each other at fluxes

$$\phi_{M,M'}^* = \frac{\phi_0}{2u(M - M')} \left( E_{M,\alpha}(0) - E_{M',\alpha'}(0) \right).$$

When we consider the ground states ($\alpha = G$), then with increasing flux a cross-over will take place from the state with $E_{M,G}(\phi)$ to the one with $E_{M+1,G}(\phi)$, starting from $E_{0,G}(\phi)$. This is a conjecture at this point which is equivalent to the assumption that

$$\frac{\partial^2 E_{M,G}(0)}{\partial M^2} = E_{M+1,G}(0) + E_{M-1,G}(0) - 2E_{M,G}(0) > 0. \quad (5)$$

We do not provide a proof here of that inequality but merely mention that in the case of strong interactions, i.e., for $J \to \infty$ this is immediately seen. The system
behaves like a single quantum ring with a particle of mass \(Nm\) and a charge \(Ne\). The ground-state energy is
\[
E_{M,G} = \frac{\hbar^2}{2Nm^2} \left( N\phi_0 - M \right)^2 + \cdots ,
\]
where the remaining terms neither depend on \(M\) nor on \(\phi\). From Eqs. (6,7) we obtain a ground state with \(N\) level crossing points \(\phi(1) < \phi(2) < \cdots < \phi(N)\). At these points the ground state is degenerate.

When an electric field \(E\) is turned on, the degeneracies are lifted provided the corresponding matrix element \(\langle \Psi_{M+1,G} | \sum_j \cos \theta_j | \Psi_{M,G} \rangle\) differs from zero. We want to show that this is indeed the case when \(N\) is odd while when \(N\) is even the matrix element vanishes. For this purpose we introduce an reflection operator (with respect to the \([xy]\)-plane in the middle of the stack of rings) \(P\) and a rotational operator \(R_\pi\). They are defined through
\[
P\Psi(\theta_1, \theta_2, \ldots, \theta_N) = \Psi(\theta_N, \theta_{N-1}, \ldots, \theta_1),
\]
\[
R_\pi \Psi(\theta_1, \theta_2, \ldots, \theta_N) = \Psi(\theta_1 + \pi, \theta_2 + \pi, \ldots, \theta_N + \pi).
\]
Note that \([P, H_0] = [R_\pi, H_0] = 0\) and furthermore that \([P, R_\pi] = 0\). Both \(P\) and \(R_\pi\) have eigenvalues \(\pm 1\). Because of the repulsive interactions the probability of finding particles in neighboring rings by an angle \(\pi\) apart exceeds the case of finding these with the same angles. This implies that
\[
P\Psi_{M,G} = \Psi_{M,G} \ (N = \text{odd})
\]
\[
R_\pi \Psi_{M,G} = \Psi_{M,G} \ (N = \text{even}),
\]
otherwise we have the unphysical condition \(\Psi_{M,G}(\theta, \theta + \pi, \theta + \cdots) = 0\). For an illustration see Fig. 2.

When \(N\) is even we may also write \(P\Psi_{M,G} = R_\pi \Psi_{M,G}\) and furthermore \(R_\pi \Psi_{M,G} = e^{i\pi M} \Psi_{M,G} = (-1)^M \Psi_{M,G}\). Therefore, by inserting \(P^2 = 1\) into the matrix element \(\langle \Psi_{M+1,G} | \sum_j \cos \theta_j | \Psi_{M,G} \rangle\) we find for these \(N\) values
\[
\langle \Psi_{M+1,G} | P^2 \sum_j \cos \theta_j | \Psi_{M,G} \rangle
\]
\[
= (-1)^{2M+1} \langle \Psi_{M+1,G} | \sum_j \cos \theta_j | \Psi_{M,G} \rangle = 0.
\]
This implies that for \(N=\text{even}\) the ground state remains degenerate at the crossing points of fluxes \(\phi(1), \ldots, \phi(N)\) even when an electric field is applied in the plane of the rings.

Next we consider the electric polarization \(P(\phi)\) which is defined by \(P(\phi) = p_0 \sum_j \langle \Psi_G(\phi) | \cos \theta_j | \Psi_G(\phi) \rangle\), where \(|\Psi_G(\phi)\rangle\) is the ground state in the presence of the magnetic flux \(\phi\). In the more general case, a thermodynamic average has to be taken instead. At flux \(\phi\) away from the special cases \(\phi(1), \ldots, \phi(N)\) an electric field causes a quadratic Stark effect. But in the vicinity of \(\phi(1), \ldots, \phi(N)\) a linear Stark effect is expected, provided the electric field \(E\) splits the degenerate states as is the case for odd values of \(N\). Therefore the polarization is quite different in the two cases.

In the regime of a quadratic Stark effect we can apply non-degenerate second-order perturbation theory. For small values of \(\phi\) the ground-state energy shifts due to the electric field is
\[
\Delta E = (E_{p0})^2 \sum_{M = \pm 1} \sum_\alpha \frac{|\langle \Psi_{M,\alpha} | \sum_j \cos \theta_j | \Psi_{0,G} \rangle|^2}{E_{0,G}(\phi) - E_{M,\alpha}(\phi)}.
\]
We abbreviate the matrix element \(W_\alpha = |\langle \Psi_{1,\alpha} | \sum_j e^{i\theta_j} | \Psi_{0,G} \rangle|^2\) and set \(\Delta_\alpha = E_{1,\alpha}(\phi) - E_{1,G}(\phi)\). When \(N\) is odd the leading contribution comes from \(\alpha = G\) with \(\Delta_\alpha = 0\). In contrast, when \(N\) is even we have \(W_G = 0\) and the leading contribution has \(\Delta_\alpha = \infty\) and therefore is smaller. This is particularly the case in the strong interaction limit where
\[
P_{\text{odd}}(\phi) \approx \frac{E_{p0} W_G N}{u} \left( 1 + 4N^2 \left( \frac{\phi}{\phi_0} \right)^2 \right) \quad (\phi << \phi_0/N),
\]
\[
P_{\text{even}}(\phi) \rightarrow 0 \quad \text{for } J \rightarrow \infty.
\]
In the region of a linear Stark effect which is present only when \(N\) is odd, we find from degenerate perturbation theory \(\Delta E \approx -\frac{1}{2}E_{p0} \sqrt{W_G}\) and therefore
\[
P_{\text{odd}}(\phi) \approx \frac{1}{2}E_{p0} \sqrt{W_G}.
\]
For odd \(N\), the ground state in the presence of the electric field is non-degenerate for any \(\phi\) and therefore the corresponding wavefunction and the polarization \(P(\phi)\) are also continuous functions of \(\phi\). This is not the case for even \(N\). Since level crossings at fluxes \(\phi(1), \ldots, \phi(N)\) are not removed by an applied electric field, \(P(\phi)\) is generally discontinuous at these special values of the magnetic field.
Shown in Fig. 2 are numerical results for $P(\phi)$ of rings up to $N = 4$. Calculations have been done by diagonalization of the respective Hamiltonian which is a matrix of size up to 3000×3000. The basis which is used in the calculations consists of products of $N$ single-particle eigenfunctions of the single-particle Schrödinger equation in the presence of an electric field. For particular values $J/u = 2$ and $\mathcal{E}p_0/u = 0.1$ we find that $P_{\text{even}}$ is by about one order of magnitude smaller than $P_{\text{odd}}$. For $N = 3$ a quasiperiodic peak structure is observed. Note the discontinuities of the polarization for $N = 2, 4$ in accordance with the behaviour pointed out above.

Not only the dielectric response but also far-infrared spectroscopy may show even-odd ring number parity effects. For example, for stacks with an even number of rings the optical transition between the ground- and first excited state vanishes as seen from Eq. (11) while for odd values of $N$ one notices that $|A\rangle$ and $|B\rangle$ are no longer correlated with respect to each other, i.e., when $V(\theta) = V_j(\theta)$ for all $j$. Level crossings will exist if $V(\theta)$ satisfy the condition $\int_0^{2\pi} d\theta V(\theta) \exp(i\theta) = 0$. An example is a symmetric double-well potential. When the inter-ring interactions are larger than the potential barriers $V(\theta)$ and furthermore larger than the kinetic energy $\hbar \omega$, the ground state is a superposition of two configurations. One of it is indicated in Fig. 3 (a) and the other one is obtained by rotating all particles by $\pi$. In the two configurations labeled $|A\rangle$ and $|B\rangle$ the repulsive energy is minimized. Due to the kinetic energy both configurations are connected by a tunneling matrix element resulting in correlated tunneling paths of the particles (see Fig. 3 (a)). Within this classical path picture the two lowest lying eigenstates can be looked upon as those of a single quantum ring with an effective double well potential and effective charge (see Fig. 3 (b)). The flux dependent tunneling splitting is given by $t_{\text{eff}}(\phi) = t_{\text{eff}}(0) \cos(N \pi \phi/\phi_0)$. One notices that the flux $N\phi$ enters here because the correlated motion of the $N$ particles corresponds to an effective charge $Ne$ of the system. Level crossing takes place whenever $t_{\text{eff}}(\phi) = 0$. For odd values of $N$ one notices that $|A\rangle$ and $|B\rangle$ are reproduced when $P$ is acting on them. The same holds true for the states $|A\rangle \pm |B\rangle$. In distinction we find for even values of $N$ we choose $|A\rangle$ and $|B\rangle$ so that $P |A\rangle = |B\rangle$ holds. Therefore $P(|A\rangle \pm |B\rangle) = \pm (|A\rangle \pm |B\rangle)$ in that case. Then for even value of $N$ the degeneracy of the ground state at level-crossing points is not lifted by an electric field and no linear Stark effect does appear.

$$H_0 = \frac{\hbar^2}{2mr^2} \sum_{j=1}^{N} \left( \frac{\partial}{\partial \theta_j} + \frac{\phi}{\phi_0} \right)^2 + \sum_{i<j} U_{|i-j|}(\theta_i - \theta_j) + \sum_j V_j(\theta_j),$$

where $U_{|i-j|}(\theta_i - \theta_j)$ is a repulsive particle interaction and $V_j(\theta_j)$ is the azimuthal barrier potential of the $j$-th ring. When we consider only the (unpaired) electron in the highest occupied molecular orbital, $V(\theta)$ is the potential felt by it. The extension of the range of the inter-ring interaction $U_{|i-j|}(\theta_i - \theta_j)$ does not affect the invariance of it under the operation $P$.

In order for $H_0$ to be invariant under the operation $P$, it must hold that $V(\theta) = V_j(\theta)$. This is the case when the ring molecules are stacked without rotations with respect to each other, i.e., when $V(\theta) = V_j(\theta)$ for all $j$. Level crossings will exist if $V(\theta)$ satisfy the condition $\int_0^{2\pi} d\theta V(\theta) \exp(i\theta) = 0$. An example is a symmetric double-well potential. When the inter-ring interactions are larger than the potential barriers in $V(\theta)$ and furthermore larger than the kinetic energy $\hbar \omega$, the ground state is a superposition of two configurations. One of it is indicated in Fig. 3 (a) and the other one is obtained by rotating all particles by $\pi$. In the two configurations labeled $|A\rangle$ and $|B\rangle$ the repulsive energy is minimized. Due to the kinetic energy both configurations are connected by a tunneling matrix element resulting in correlated tunneling paths of the particles (see Fig. 3 (a)). Within this classical path picture the two lowest lying eigenstates can be looked upon as those of a single quantum ring with an effective double well potential and effective charge (see Fig. 3 (b)). The flux dependent tunneling splitting is given by $t_{\text{eff}}(\phi) = t_{\text{eff}}(0) \cos(N \pi \phi/\phi_0)$. One notices that the flux $N\phi$ enters here because the correlated motion of the $N$ particles corresponds to an effective charge $Ne$ of the system. Level crossing takes place whenever $t_{\text{eff}}(\phi) = 0$. For odd values of $N$ one notices that $|A\rangle$ and $|B\rangle$ are reproduced when $P$ is acting on them. The same holds true for the states $|A\rangle \pm |B\rangle$. In distinction we find for even values of $N$ we choose $|A\rangle$ and $|B\rangle$ so that $P |A\rangle = |B\rangle$ holds. Therefore $P(|A\rangle \pm |B\rangle) = \pm (|A\rangle \pm |B\rangle)$ in that case. Then for even value of $N$ the degeneracy of the ground state at level-crossing points is not lifted by an electric field and no linear Stark effect does appear.
operator and the kinetic energy is replaced by the charging energy of a superconducting grain. When the superconducting paring is of the conventional form, i.e., s-wave, spin singlet paring, the sign of \( J \) in Eq. (2) is negative. Therefore no parity effect is expected because Eq. (10) does not hold in that case. However, an array of \( \pi \) junctions should show a difference between an even and odd number of junctions since \( J > 0 \) in that case. This difference refers to the response of the superconducting phase to a perturbation acting on it.

A different parity effect which is sometimes called Leggett's conjecture has already attracted strong attention. In that case, the magnetic field response of \( N \) spinless fermions in a ring show diamagnetic (paramagnetic) when \( N \) is even (odd). In contrast, our parity effect refers to electric field response. In both cases, however, essential roles are played by certain symmetries in the systems. While in Leggett's conjecture the antisymmetry of the many-body wavefunctions of the fermions are responsible for the even-odd parity effect, the mirror reflection symmetry in the stack of rings is essential in the present parity effect.

In summary, we have presented here a theory of stacked quantum rings with repulsive inter-ring interactions in the presence of an applied magnetic field. Due to the mirror reflection symmetry, the electric polarization induced by an applied electric field shows a different behaviours for even and odd number of rings. A linear Stark effect at different magnetic fields is expected for odd number of rings while for even number of rings the quadratic Stark effect prevails. In the latter case the polarization is weakly flux dependent and may show discontinuities at special external magnetic fields. Nanoscopic semiconductor rings or stacks of ring molecules may show the symmetry effects discussed here.

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