Elements of Physics for the 21st century

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Internal structures of electrons and photons: The concept of excitons

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Abstract
The theoretical foundations of quantum theory are discussed and it is shown that both theories are not mutually exclusive. They can be combined, and a realistic approach can be established to derive both schemes. Integrating
them applies a wave equation. Including excitons, the field, in this context, is arbitrary due to internal energy. The consistent wave functions in quantum theory as well as in classical physics allow
expression of this, fundamental arbitrariness of the single wave function and mathematical formalism, providing formulations explicitly. These actions justify the initial assumption of the non-locality of actions, which can be referred to vanishing intrinsic field energy. Fundamental difficulties for a fully covariant description of finite systems seem to be related to the evolving properties of quantum field theory.

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Solving the Einstein–Podolsky–Rosen puzzle: The origin of non-locality in Aspect-type experiments

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So far no mechanism is known, which could connect the two measurements in an Aspect-type experiment. Here, we suggest such a mechanism, based on the phase of a photon’s field during propagation. We show that two polarization measurements are correlated, even if no signal passes from one point of measurement to the other. The non-local connection of a photon pair is the result of its origin at a common source, where the two fields acquire a well defined phase difference. Therefore, it is not actually a non-local effect in any conventional sense. We expect that the model and the detailed analysis it allows will have a major impact on quantum cryptography and quantum computation.

Keywords entanglement, Bell inequalities, coincidence measurements, Einstein–Podolsky–Rosen paradox

PACS numbers 03.65.Yd, 03.67.-a
Overview

• The problem

• Densities and wavefunctions

• Experiments:
  – Accelerations of electrons
  – Stern Gerlach experiments
  – Double slit interferometry
  – Bell-type experiments

• Towards a nuclear model based on densities
• Implies:
  – That electrons are point particles
  – That their electrostatic energy is infinite
  – That wavefunctions do not have physical reality
  – That measurements cannot be arbitrarily precise
Introducing: Scanning probe microscopy

What the scanning probe measures in all these experiments is the two dimensional distribution of the density of electron charge.
The Ag(111) surface with adatoms

Quantum Corral Ag on Ag(111)

Pixel: ~ 20pm

Numbers:

Temperature [1]: 5K
Distance of atoms: 290pm
Wigner-Seitz radius: 106pm
Band energy at $E_F$: 80meV
Maximum energy $\Delta E$: 80meV
Lateral resolution: 20pm
Vertical precision [2]: 0.05pm

Maximum energy and local uncertainty

- The maximum available energy for an electron at the Fermi level is the band energy of 80meV:

\[ \Delta p = p(80\text{meV}) = \sqrt{2mE} = 1.53 \times 10^{-25} \text{kgms}^{-1} \]

\[ \Delta x = \Delta x(\Delta p) \geq \frac{\hbar}{2 \cdot \Delta p} = 3.48 \times 10^{-10} \text{m} = 348 \text{pm} \]

- Statistical distribution of measurements of point-like electrons with this local uncertainty:
Statistical analysis of experiments

• Standard deviation of a measurement of x-coordinate:

\[
\sigma_x = \sqrt{\frac{1}{N} \sum_{i=1,\ldots,N} (x_i - \langle x \rangle)^2}, \quad \langle x \rangle = \frac{1}{N} \sum_{i=1,\ldots,N} x_i \quad (1)
\]

• Maximum standard deviation:

\[
\frac{\Delta z}{z_0} \leq 0.3\% \quad \Rightarrow \quad \Delta x(STM) \geq 3\sigma(\Delta E)
\]

• Result for surface state electron on Ag(111):

\[
\Delta x(STM) \approx 10\ pm \quad 3\sigma(\Delta E) \approx 800\ pm
\]

\[
\Rightarrow \Delta x(STM) \ll 3\sigma(\Delta E)
\]

Contradiction!
Result of the statistical analysis:

• Under the assumptions that
  1. The electron is a point-particle
  2. The uncertainty of location is related to the uncertainty of energy
• We find that
  1. The standard deviation in experiments is only about one percent of the theoretical value
  2. The uncertainty of location corresponds to an energy value of about 1000eV
• Conclusion:
  1. The electron is not a point-particle
  2. The uncertainty relations are violated by thousands of measurements every single day

Heisenberg, uncertainty, and the scanning tunneling microscope

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We show by a statistical analysis of high-resolution scanning tunneling microscopy (STM) experiments, that the interpretation of the density of electron charge as a statistical quantity leads to a conflict with the Heisenberg uncertainty principle. Given the precision in these experiments we find that the uncertainty principle would be violated by close to two orders of magnitude, if this interpretation were correct. We are thus forced to conclude that the density of electron charge is a physically real, i.e., in principle precisely measurable quantity.

Keywords scanning tunneling microscope, electron charge, density functional theory, uncertainty relations

PACS numbers 31.10.+z, 71.15.Mb
Wavefunctions and densities

1. A system is fully defined by its wavefunction of electrons.
2. A system is fully defined by its density of electron charge.

Erwin Schrödinger
Born Vienna 1887

Walter Kohn
Born Vienna 1923
One principle: the density of electrons is real

\[ \rho(z, t) = \frac{\rho_0(z)}{2(1 + \theta(z, t))} \]

\[ \lim_{v_{el} \to 0} \rho = \rho_0(z) \]

\[ \mathcal{E} = e_1 \epsilon_0 \]

\[ \mathcal{H} = e_2 \mathcal{H}_0 \]

Unconventional Approach to Orbital-Free Density Functional Theory Derived from a Model of Extended Electrons

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Abstract  An equation proposed by Levy, Perdew and Sahni (Phys. Rev. A 30:2745, 1984) is an orbital-free formulation of density functional theory. However, this equation describes a bosonic system. Here, we analyze on a very fundamental level, how this equation could be extended to yield a formulation for a general fermionic distribution of charge and spin. This analysis starts at the level of single electrons and with the question, how spin actually comes into a charge distribution in a non-relativistic model. To this end we present a space-time model of extended electrons, which is formulated in terms of geometric algebra. Wave properties of the electron are referred

Note: the vector components are a necessary consequence of energy variations of density components. Their velocity is equal to the velocity of the electron, and they are associated with the electron's spin density.
Wavefunctions $\psi$

\[ S = \mathcal{E} \mathcal{H} = e_1 e_2 \mathcal{E}_0 \mathcal{H}_0 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right). \]

\[ S = i e_3 S, \]

\[ S = \mathcal{E}_0 \mathcal{H}_0 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right), \]

\[ S = S_0 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi vt \right), \quad S_0 \equiv \mathcal{E}_0 \mathcal{H}_0. \]

\[ \psi = \rho^{1/2} + S^{1/2} e_1 e_2 = \rho^{1/2} + i S^{1/2} e_3. \]

\[ \psi^\dagger = \rho^{1/2} + S^{1/2} e_2 e_1 = \rho^{1/2} - i S^{1/2} e_3. \]

\[ \psi^\dagger \psi = \rho + S = \rho_0 = \text{constant} \]

Spin component

General form of a wavefunction

Born rule

1. The group velocity is equal to the velocity of the electron (de Broglie)
2. The frequency of the wave is proportional to the kinetic energy (Planck)
3. The total energy is the energy of its inertial mass (classical mechanics)
Many-body physics

Many-body Wavefunction
\[ \Psi = \rho^{1/2} + i e_S S^{1/2}, \]

Schrodinger Equation
\[ \left[ -\frac{1}{2} \nabla^2 + v_{ext} + v_{eff,0} + i e_v v_i \right] \Psi = \mu \Psi, \]

Density
\[ \rho_0 = \Psi^\dagger \Psi, \]

Spin density
\[ \Lambda(\mathbf{r}) = e_S S^{1/2}, \]

Bivector potential
\[ \Pi(\mathbf{r}) = e_v v_i, \]

Coupled Schrodinger equations
\[ \left[ -\frac{1}{2} \nabla^2 + v_0(\mathbf{r}) - \mu \right] \rho^{1/2}(\mathbf{r}) = \Pi(\mathbf{r}) \cdot \Lambda(\mathbf{r}), \]

Many body interactions
\[ \nu_0(\mathbf{r}) = v_{ext} + v_{eff,0}, \]

Advantage: the many-body wavefunction in this case has only 4 instead of 3N variables
Energy changes

• What happens if an electron accelerates (decelerates) in a static field?
  1. Its velocity will change
  2. Its density distribution will change
  3. Its field components will change
  4. The external field will change due to energy transfer

• Comprehensive description:

  \[ \mathbf{f} = -\nabla \phi = \rho_0 \frac{d\mathbf{v}_{el}}{dt}. \]

  ‘Local’ Ehrenfest theorem

• Internal changes:

  \[ \rho + S = \rho_0 = \text{constant}. \]

  \[ \dot{S} + \dot{\rho} = 0 \quad \rightarrow \quad \frac{d}{dt} (\psi_S^\dagger \psi_S)v = \rho_0 \frac{d\mathbf{v}_{el}}{dt}. \]

  Energy is shifted from mass components to field components

Wavelength changes because of energy redistribution
Electrons in static magnetic fields

\[ \rho_0 \frac{dv}{dt} = \rho_0 (E + v \times B). \]  
Free electrons: Lorentz forces

\[ S = e_s \cdot S \quad \frac{de_s}{dt} = \text{const} \cdot e_s \times \left( u \times \frac{dB}{dt} \right) \]  
Constrained trajectory: rotation of spin vectors

Stern-Gerlach experiments:

- **Standard model:**
  - Spin is isotropic
  - Measurement breaks spin isotropy
  - No process to explain symmetry breaking

- **New model:**
  - Spin is isotropic
  - Measurement induces spin components aligned to field
  - Measurement measures induced spin components
Double slit experiments

• Conventional model (Feynman path integrals)
  – A single particle splits into virtual particles
  – Each virtual particle passes one slit

The problem: No physical process is known which could account for the creation of virtual particles and their recombination after the interferometer.
Model due to Duane and Lande [1,2]

Duane-Lande model:
- Single wavelets interact with the slit system
- The interaction spectrum of the interferometer is discrete
- Wavelets acquire discrete lateral momenta

Note: The slit environment is composed of atoms in a regular crystal lattice. Such a system always has a discrete interaction spectrum depending on the chemical element and the crystal symmetry.

- Perform interference experiments at 4K

1W. Duane, Proc. Nat. Acad. Sci. 9, 158 (1923);
2A Lande, From Dualism to Unity in Quantum Physics, CUP (1960)
Quantum fiction: wave properties of large molecules\textsuperscript{1}

Quantum fact: fringes due to interactions between molecule and slit environment\textsuperscript{2}

\textsuperscript{1}Zeilinger group: Nature 401, 680 (1999)

\textsuperscript{2}Berninger et al.: PRA 76, 013607 (2007)
Aspect-type experiments

- **Assumptions:**
  1. Quantum theory is complete
  2. Correlation due to common source

\[
R(z_1) = \exp(\mathbf{e}_1 \cdot \mathbf{e}_2) e_3 z_1 2\pi/\lambda
\]

\[
R(z_2) = \exp(\mathbf{e}_1 \cdot \mathbf{e}_2) e_3 z_2 2\pi/\lambda
\]

\[
R(\varphi_1) = \exp(i z_1 2\pi/\lambda) = e^{i\varphi_1}
\]

\[
R(\varphi_2) = \exp(-i(z_2 2\pi/\lambda + \Delta)) = e^{-i(\varphi_2 + \Delta)}
\]

**Rotation**

\[
p(\varphi_i) = (\Re(R(\varphi_i)))^2
\]

\[
p(\varphi_1, \varphi_2) = [\Re[R(\varphi_1) \cdot R(\varphi_2)]]^2
\]

**Filtering**

\[
C^{++} = C^{--} = \cos^2(\varphi_1 - \varphi_2)
\]

\[
C^{+-} = C^{-+} = 1 - \cos^2(\varphi_1 - \varphi_2)
\]

\[
E(\varphi_1, \varphi_2) = 2 \cos^2(\varphi_1 - \varphi_2) - 1 = \cos 2(\varphi_1 - \varphi_2)
\]

**Coincidences**

Aspect 1982
Experimental results and Bell inequalities

\[ \varphi_1 = 0, \varphi_1' = 45, \varphi_2 = 22.5, \varphi_2' = 67.5, \]

\[ S(\varphi_1, \varphi_1') = E(\varphi_2, \varphi_2') \]

The problem:

J. S. Bell, Physics 1, 195 (1964), Eq. (2)

Two separate rotations at A and \(-B\) in geometric algebra

The key mistake of Bell was not to realize that rotations in space generate complex numbers.

Research Article

Solving the Einstein–Podolsky–Rosen puzzle: The origin of non-locality in Aspect-type experiments

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Electrons and neutrons

\[ n^0 \rightarrow p^+ + e^- + 0.782 \text{ MeV} \]

Scattering on neutrons\(^1\):

Question: Is there a high-density phase of electrons in nuclei?

Energetics

\[ W_e^0 = \frac{1}{2} \int_{r_e}^{\infty} \frac{1}{\epsilon_0} |E|^2 dV = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_e} \approx 11eV \]

\[ W_e^n = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_n} \approx 0.960 MeV \]

Electrostatic field: hydrogen electron

Electrostatic field: neutron electron (1.5fm)

The electrostatic field energy of a high density electron is sufficient to explain the excess mass of a neutron

\[ \rho(r) = \rho_0 e^{-2\alpha r} \quad \psi(r) = \sqrt{\rho_0} e^{-\alpha r} \quad \left( -\frac{\hbar^2}{2m} \Delta - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \right) \psi(r) = E \psi(r) \]

Density and wavefunction

Schrödinger equation

\[ \left( -\frac{\hbar^2\alpha^2}{2m} + \frac{2\hbar^2\alpha}{2mr} - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi(r) = E \psi(r) \]

Characteristic equation

\[ \frac{2\hbar^2\alpha}{2mr} - \frac{e^2}{4\pi\epsilon_0 r} = 0 \quad \Rightarrow \quad \alpha = \frac{me^2}{4\pi\epsilon_0 \hbar^2} \]

Solution
Length scales and energy scales

\[ \alpha = \frac{2.101 \times 10^{-58}}{\hbar^2} = (\hbar = 6.672 \times 10^{-34}) \]
\[ = 1.89 \times 10^{10} \, [m^{-1}] \]

\[ \hbar_n = x\hbar \quad \alpha_n = \frac{1.89 \times 10^{10}}{x^2} \, [m^{-1}] \]

\[ \psi(r) = \sqrt{\rho_0}e^{-\alpha_n r} \]

Length scale in atomic physics: depends on Planck’s constant

Constants in nuclear environment \((a_0 = \text{Bohr radius})\)

\[ a_n = x^2 \cdot a_0 \quad E_n = \frac{E_0}{x^2} \]

The decay length, the unit of length and the unit of energy all scale differently in a nuclear environment

\[ \left( -\frac{1}{2} \nabla^2 - \frac{1}{r} \right) \psi(r) = E \psi(r) \]

Schrödinger equation: nuclear units

\[ W_n = \frac{e^2}{4\pi \varepsilon_0 a_0} \left( -\frac{1}{2x^2} + \frac{a_0}{r_n} \right) = \left( \frac{a_0}{r_n} - \frac{1}{2x^2} \right) \times 27.211[\text{eV}] \]

Total energy

The total energy depends on the neutron radius and the scaling factor \(x\)
Fine structure constant and unit energy

\[ r_n = 1.37 \text{ fm:} \]

\[ x^2 = \frac{1}{18779} = \alpha_f^2 \]

\( \alpha_f \) equal to the scaling factor of nuclear units.

\[ a_n = \frac{a_0}{18779} = 2.81 \text{ [fm]} \]

\[ E_n = E_0 \times 18779 = 0.511 \text{ [MeV]} = m_e c^2 \]

Energy unit equal to the rest mass of electrons.

Neutron: Energetics
Nuclear shell model

• If neutrons are composite entities then
  – Nuclei are composed of protons and electrons
  – Protons are immersed in negative charge
  – Inter-proton distances are equal
Six things to remember

1. The uncertainty relations are violated by up to two orders of magnitude in thousands of experiments every single day.

2. Wavefunctions themselves are not real, but their components, mass and spin densities, are real.

3. Rotations in space generate complex numbers, which are not described in a Gibbs vector algebra.

4. Double slit interference experiments most likely show two features: a discrete interaction spectrum with the slit system and a thermal broadening due to environmental conditions.

5. Based on the experimental neutron radius we are led to conclude that the fine structure constant describes the nuclear energy scale.

6. Closed shell nuclei could be due to the geometrical arrangement of nuclear protons.
Three things I have learned

• Mathematics is not physics
  – Mathematical models must be based on a sound understanding of physical processes
  – Proper mathematicians will invent a new reality if the existing one contradicts their theorems

• It is easy to come up with complicated models
  – It is much more difficult to develop simple ones

• If it’s weird, it is probably wrong
Thank you for your attention
Electrons in electrostatic fields

\[
\frac{v_{el}^2}{2} = \omega_{el} = \omega_{ph} - \phi_m.
\]

**Photoelectric effect:** (Hertz effect, 1887): the kinetic energy of an electron subjected to electromagnetic fields of frequency \(\omega_{ph}\) is reduced by the electrostatic interaction within the metal \(\phi_m\).

\[
\omega_{el}(\phi_m) = \omega_{el}^0 - \phi_m.
\]

**Physical process:** the frequency of an electron is reduced in the presence of an electrostatic field.

**Consequence:**

**Modification of Schrödinger equation**

\[
-\frac{1}{2} \nabla^2 \psi_S = \frac{v_{el}^2}{2} \psi_S = \omega_0 \psi_S,
\]

\[
i \frac{\partial}{\partial t} \psi_S = (\omega_0 - \phi_m)\psi_S,
\]

\[
i \frac{\partial \psi_S}{\partial t} = \left[-\frac{1}{2} \nabla^2 + V\right] \psi_S.
\]
Energy and wavelength

\[ E_{\text{field}} = \frac{1}{2} \varepsilon_0 \mathcal{E}^2 + \frac{1}{2} \mu_0 \mathcal{H}^2 \]

\[ = \left( \frac{1}{2} \varepsilon_0 \mathcal{E}_0^2 + \frac{1}{2} \mu_0 \mathcal{H}_0^2 \right) \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t + \phi \right). \]

\[ \phi = \frac{\pi}{2} \implies E_{\text{field}} = \left( \frac{1}{2} \varepsilon_0 \mathcal{E}_0^2 + \frac{1}{2} \mu_0 \mathcal{H}_0^2 \right) \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) \]

\[ E_{\text{kin}} = \frac{1}{4} \rho_0 v_{\text{el}}^2 \left[ 1 + 2 \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) \right] - 1. \]

\[ E_{\text{tot}} = \frac{1}{4} \rho_0 v_{\text{el}}^2 + \frac{1}{4} \rho_0 v_{\text{el}}^2 \left[ 2 \cos^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) + 2 \sin^2 \left( \frac{2\pi}{\lambda} z - 2\pi \nu t \right) \right] - 1 \]

\[ = \frac{1}{2} \rho_0 v_{\text{el}}^2. \] Total energy density

\[ v_g = \frac{d\omega}{dk} = \frac{d(mv_{\text{el}}^2/2\hbar)}{d(mv_{\text{el}}/\hbar)} = v_{\text{el}}. \] Group velocity

1. The group velocity is equal to the velocity of the electron (de Broglie)
2. The frequency of the wave is proportional to the kinetic energy (Planck)
3. The total energy is the energy of its inertial mass (classical mechanics)
If the density of electron charge is a statistical quantity, then

- A measurement of location is a measurement of a statistical ensemble.
- And this statistical ensemble must comply with the uncertainty relations:


See in particular page 213, “Many gedankenexperiments have been designed to illustrate Heisenberg’s famous law; unfortunately, the false impression is often conveyed that his principle, which is actually a theorem about standard deviations in collectives of measurement results, imposes restrictions on measur-ability.” italics in the original text.
Existing nuclear models