Quantum mechanical scattering by time-periodic potentials

Summary of the Ph.D. thesis

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Introduction

Scattering processes are of fundamental importance in several areas of physics providing fundamental information, e.g., on the nature of the relevant interaction. In general, scattering is a process when an object (an elementary particle, light) interacts with an other object, then moves towards a possibly different direction with respect to the original trajectory. The interaction can be originated from a mechanical collision or another acting force (e.g. Coulomb force) which can be usually derived from a potential. There is a special class of time-periodic scattering processes when we assume that the time dependence of the scattering potential contains a single frequency. Such excitation can be a beam of light (e.g. laser) or a gate-voltage applied to a solid-state device. For strong excitations, the highly inelastic photon-induced processes that involve the absorption/emission of one or a few photons, can be appropriately described by using classical, periodic fields. In this intensity regime, Floquet's theory [1, 2] is proved to be one of the most efficient methods.

Quantum scattering by time-harmonic potentials is an important and vivid research area. It provides deep understanding of a rich variety of interesting phenomena in strongly driven quantum systems. Optical control, laser assisted scattering or transport processes are remarkable examples showing that the presence of an alternating field can lead to strongly inelastic processes. The optical control of quantum mechanical particles offers a wide variety of promising applications, including ultrafast electronics [3, 4], imaging [5, 6], or quantum computation [7, 8]. Recently, laser assisted scattering has received a growing importance in various branches of research aiming, for instance, the generation of ultrashort (even attosecond) electron pulses [9, 10], four-dimensional imaging and ultrafast electron microscopy [11, 12], or photon-induced near field electron microscopy [6, 13]. Much of the theoretical works published so far studied also the electron transport through time-dependent potentials. Developments in the experimental techniques during the last decades allow that the results have the possibility of direct applications in the rapidly expanding field of meso- and nanoscale quantum devices [14, 15].

Objectives

The objective of the thesis was to examine the role of the time-periodic excitation in quantum mechanical scattering problems. If this excitation can not be considered as a small perturbation, anharmonic responses are observable.

Beside exploring the fundamental effects, our aim was also to examine the specific properties of the quantum systems in question and to seek possible applications. We studied two one-dimensional models in which we inquire the response of a de Broglie plane wave to a time-periodic excitation. In the case of relativistic particles, based on the linear dispersion relation of graphene, we can model the electron transport in graphene with an applied periodic gate-voltage. Here, we wanted to examine what kind of practical applications could there be for a periodic excitation, which show the known relativistic effects, like Klein paradox. As for nonrelativistic particles, the solid-state physical analogy could be the dynamics of the electrons in the conduction band with an applied optical field. Of course, the description of the dynamics of a beam consisting of charged particles naturally arises in both cases. After understanding the physical background, it was important question how the filtering of the energy can be achieved for the outgoing particles.

Additionally, our aim was to study a three-dimensional model, in which charged particles (e.g., electrons) are scattered on a nano-particle which is modeled by a hard sphere. Beside the possibility of the optical control, we intended to examine the dynamics in the presence of an electromagnetic field. The main quantity to be calculated here was the differential cross section, whose analysis could give us an insight into the dynamics of the scattering process.

Methods

Periodic systems can be effectively described by Floquet's theory [1, 2]. The mathematical foundations of this approach were originally developed in 1883 by G. Floquet to study ordinary differential equations with periodic coefficients. Regarding quantum systems, Floquet's theory was first used in the context of laser-atom interaction by J. H. Shirley in 1965. He considered a quantum system with two discrete states interacting with a semiclassically treated oscillating field with a single frequency [2]. The advantage of this method is that the dynamical equation can be reduced to an infinite-dimensional linear algebraic system of equations, and the interaction is taken into account in a nonperturbative way. With this approach, the fundamental quantum effects like the interference of matter waves in strong external fields can be examined as well as the appearance of harmonics.

Time-periodic systems are described by a Hamiltonian $H(t) = H(t+T)$, where the time period $T = 2\pi/\omega$ and ω is the angular frequency of the excitation. Based on Floquet's theorem, the wave function can be written in the form $|\Psi(t)\rangle = \exp(-i\epsilon t/\hbar)|\Phi(t)\rangle$, where $|\Phi(t)\rangle$ is the so-called Floquet state, whose periodicity is the same as the Hamiltonian, i.e., $|\Phi(t)\rangle = |\Phi(t+T)\rangle$. The Floquet quasienergy ϵ is a real parameter and is defined up to the integer multiples of $\hbar\omega$. In other words, it can be reduced to a zone with a width of $\hbar\omega$. As an analogy to solid-state physics, this zone and the quasienergy ϵ correspond to the first Brillouin zone and to the quasi wave vector, respectively. Due to their periodicity, the Floquet states can be expanded into Fourier series, which is the reason why the eigenvalue equations can be transformed into an infinite dimensional matrix equation. If the wave function have a Floquet form and the boundary conditions are also taken into account, the system is well-defined. Practically, the linear system of equations are solved by including only a finite number of the Floquet channels.

Scientific results

In the following, I present a brief summary of the new scientific results discussed in the thesis which are collected in five thesis points. The publications connected to my statements are listed at the end of this booklet and cited in each title.

T1. Scattering of charged particles in a Ramsey-like setup: transmission resonances [P3]

— I constructed a quantum mechanical model in which charged particles (e.g. electrons) are scattered by a time-oscillating electric field in a spatially separated (Ramsey-like) setup [16]. I analyzed the cycle-averaged transmission probabilities as the function of the energy of the incoming electrons E_0, and identified transmission resonances in the spectrum.

— In order to interpret the results, I created a model, based on a classical physical consideration, by replacing the oscillating electric fields with static potential barriers of heights equal to the ponderomotive energy of the electron.

— I proved that the static double-barrier system is a proper first approximation in finding the transmission resonances. For low values of E_0, the oscillating model has transmission resonances around the energy eigenvalues of the static model. I concluded that the localized states, which exist between the two potential barriers, are the reason for the appearance of the resonances.

T2. Scattering of charged particles in a Ramsey-like setup: phase dependence [P3]

— In the model examined in [P3], I also analyzed the dependence of the cycle-averaged transmission probability $\langle T \rangle$ on the separation distance d and the phase difference φ_0 between the two optical fields. I found that $\langle T \rangle$ is quasi-periodic in d, and the transmission probability can change as much as 50% as a function of φ_0.

— With the examination of the space- and time-dependent probability density and current, I analyzed the scattering process in the case of low and high transmission probabilities, and I interpreted the dynamics in these limiting cases using classical terms.

— I showed that in order to control the transmission by changing the phase φ_0, the parameters of the electric fields must correspond to a ponderomotive potential close to the energy of the particle beam.

T3. Describing laser-assisted electron scattering with spherical Gordon-Volkov states [P2]

— Based on the work of Varró and Ehlotzky [17], I investigated the electron scattering on a hard sphere in the presence of a laser field.

I derived the spherical Gordon-Volkov states using the translational addition theorem of spherical harmonics [18, 19]. I reduced the Fourier spectrum of these states to a series of hypergeometric functions. The resulting analytic expression significantly simplifies the calculation of the spectrum.

— I examined the differential cross sections for different Floquet channels in the weak-field limit. I found that the Floquet channels indexed by $n \neq 0$ get more populated for increasing electric field strengths. For increasing electron energies, E_0, new scattering channels open up similarly to the model presented in [P3].

T4. Relativistic electron scattering on an oscillating potential barrier: cycle-averaged transmission probabilities [P1]

— I studied the scattering of relativistic electrons on an oscillating potential barrier in one dimension. By examining the cycle-averaged transmission probabilities $\langle T \rangle$, I observed that the Klein paradox is also visible in the oscillating case similarly to the one-dimensional relativistic static scattering. That is, the transmission probability approaches 1 for increasing potential heights V_0.

— I also showed that when the barrier heights are within the band gap of $2mc^2$, the cycle-averaged transmission probability can take non-zero values, if the oscillation amplitude is large enough or the oscillation is localized in a narrow region.

T5. Relativistic electron scattering on an oscillating potential barrier: wave-packet generation, Fano-type resonances [P1]

— In the model studied in [P1], in order to understand the details of the transmission spectrum, I examined the space- and time-dependent probability density and current. I identified the effect of "temporary trapping" inside the oscillating potential barrier.

— For a low incoming electron energy E_0, I discovered Fano-type resonances [20] in the transmission probability. Using the Dirac equation, I calculated the bound states and the corresponding energies of the static relativistic potential barrier, which I identified to be the reason for the appearance of these resonances.

Publications

Refereed research papers related to the thesis:

[P1] L. Zs. Szabó, M. G. Benedict, A. Czirják, and P. Földi, *Relativistic electron transport through an oscillating barrier: Wave-packet generation and Fano-type resonances*, Phys. Rev. B **88** (7), 075438 (2013); doi:10.1103/PhysRevB.88.075438

[P2] S. Varró, L. Zs. Szabó, and A. Czirják, *Laser-assisted electron scattering on a nano-sphere*, Nucl. Instr. Meth. Phys. Res. B **369**, 29 (2016); doi:10.1016/j.nimb.2015.10.064

[P3] L. Zs. Szabó, M. G. Benedict, and P. Földi, *Scattering of charged particles on two spatially separated time-periodic optical fields*, Phys. Rev. A **96** (6), 063419 (2017); doi:10.1103/PhysRevA.96.063419

Additional refereed research papers:

[A4] A. Szenes, B. Bánhelyi, L. Zs. Szabó, G. Szabó, T. Csendes, and M. Csete, *Enhancing diamond color center fluorescence via optimized plasmonic nanorod configuration*, Plasmonics **12** (4), 1263 (2017); doi:10.1007/s11468-016-0384-1

[A5] A. Szenes, B. Bánhelyi, L. Zs. Szabó, G. Szabó, T. Csendes, and M. Csete, *Improved emission of SiV diamond color centers embedded into concave plasmonic core-shell nanoresonators*, Sci. Rep. **7** (1), 13845 (2017); doi:10.1038/s41598-017-14227-w

[A6] I. Magashegyi, L. Zs. Szabó, and P. Földi, *Ultrashort laser-pulse-driven currents in conductors: one-dimensional model for local excitation in the single-electron picture with quadratic dispersion*,

J. Opt. Soc. Am. B **35** (5), A116 (2018);
doi:10.1364/JOSAB.35.00A116

References

[1] G. Floquet, *Sur les équations différentielles linéaires à coefficients périodiques*, Ann. École Norm. Sup. **12**, 47 (1883); url:https://eudml.org/doc/80895

[2] J. H. Shirley, *Solution of the Schrödinger equation with a Hamiltonian periodic in time*, Phys. Rev. **138** (4B), B979 (1965); doi:10.1103/PhysRev.138.B979

[3] F. Krausz and M. I. Stockman, *Attosecond metrology: from electron capture to future signal processing*, Nat. Photonics **8**, 205 (2014); doi:10.1038/nphoton.2014.28

[4] E. Gruber, R. A. Wilhelm, R. Pétuya, V. Smejkal, R. Kozubek, A. Hierzenberger, B. C. Bayer, I. Aldazabal, A. K. Kazansky, F. Libisch, A. V. Krasheninnikov, M. Schleberger, S. Facsko, A. G. Borisov, A. Arnau, and F. Aumayr, *Ultrafast electronic response of graphene to a strong and localized electric field*, Nat. Commun. **7**, 13948 (2016); doi:10.1038/ncomms13948

[5] A. Feist, N. Bach, N. Rubiano da Silva, T. Danz, M. Möller, K. E. Priebe, T. Domröse, J. G. Gatzmann, S. Rost, J. Schauss, S. Strauch, R. Bormann, M. Sivis, S. Schäfer, and C. Ropers, *Ultrafast transmission electron microscopy using a laser-driven field emitter: Femtosecond resolution with a high coherence electron beam*, Ultramicroscopy **176**, 63 (2017); doi:10.1016/j.ultramic.2016.12.005

[6] B. Barwick, D. J. Flannigan, and A. H. Zewail, *Photon-induced near-field electron microscopy*, Nature **462**, 902 (2009); doi:10.1038/nature08662

[7] D. Kim, S. G. Carter, A. Greilich, A. S. Bracker, and D. Gammon, *Ultrafast optical control of entanglement between two quantum-dot spins*, Nat. Phys. **7** (3), 223 (2011); doi:10.1038/nphys1863

[8] R.-B. Liu, W. Yao, and L. J. Sham, *Quantum computing by optical control of electron spins*, Adv. Phys. **59** (5), 703 (2010); doi:10.1080/00018732.2010.505452

[9] P. B. Corkum and F. Krausz, *Attosecond science*, Nat. Phys. **3**, 381 (2007); doi:10.1038/nphys620

[10] S. Varró and Gy. Farkas, *Attosecond electron pulses from interference of above-threshold de Broglie waves*, Laser Part. Beams **26** (1), 9 (2008); doi:10.1017/S0263034608000037

[11] W. E. King, G. H. Campbell, A. Frank, B. Reed, J. F. Schmerge, B. J. Siwick, B. C. Stuart, and P. M. Weber, *Ultrafast electron microscopy in materials science, biology, and chemistry*, J. Appl. Phys. **97** (11), 111101 (2005); doi:10.1063/1.1927699

[12] A. H. Zewail, *Four-dimensional electron microscopy*, Science **328** (5975), 187 (2010); doi:10.1126/science.1166135

[13] S. T. Park, M. Lin, and A. H. Zewail, *Photon-induced near-field electron microscopy (PINEM): theoretical and experimental*, New J. Phys. **12** (12), 123028 (2010); doi:10.1088/1367-2630/12/12/123028

[14] W. Lu and C. M. Lieber, *Nanoelectronics from the bottom up*, Nat. Mater. **6**, 841 (2007); doi:10.1038/nmat2028

[15] S. Kohler, J. Lehmann, and P. Hänggi, *Driven quantum transport on the nanoscale*, Phys. Rep. **406** (6), 379 (2005); doi:10.1016/j.physrep.2004.11.002

[16] N. F. Ramsey, *A molecular beam resonance method with separated oscillating fields*, Phys. Rev. **78** (6), 695 (1950); doi:10.1103/PhysRev.78.695

[17] S. Varró and F. Ehlotzky, *Scattering by a hard sphere in a laser field*, Z. Phys. D **8** (3), 211 (1988); doi:10.1007/BF01436943

[18] S. Stein, *Addition theorems for spherical wave functions*, Quart. Appl. Math. **19**, 15 (1961); doi:10.1090/qam/120407

[19] O. R. Cruzan, *Translational addition theorems for spherical vector wave functions*, Quart. Appl. Math. **20**, 33 (1962); doi:10.1090/qam/132851

[20] U. Fano, *Effects of configuration interaction on intensities and phase shifts*, Phys. Rev. **124** (6), 1866 (1961); doi:10.1103/PhysRev.124.1866