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Basic Modelling of Transport in Two-Dimensional Wave-Mechanical Nano-Dots and Billiards with Balanced Gain and Loss Mediated by Complex Potentials.

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Abstract: Non-Hermitian quantum mechanics with parity-time symmetry is presently gaining great interest, especially within the fields of photonics and optics. Here we give a brief overview of low-dimensional semiconductor nanodevices using the example of a quantum with in- and output leads, which are mimicked by imaginary potentials for gain and loss, and how wave functions, particle flow, coalescence of levels and associated breaking of parity-time symmetry may be analyzed within such a framework. Special attention is given to the presence of exceptional points and symmetry breaking. Related features for musical string instruments and “wolf-notes” are outlined briefly with suggestions for further experiments

1. Introduction

Following Dirac one prescribes in standard non-relativistic quantum mechanics (QM) that the Hamiltonian H , the sum of kinetic energy T and potential energies V of a system, is a Hermitian operator. This ensures that its energy eigenvalues turn out real and correspond to experimental observations [1]. More generally, observables, as for example the momentum of a particle, are to be represented by Hermitian operators with expectation values that equal the outcomes of measurements. All information about an eigenstate is contained in the associated wave function $\Phi(\mathbf{r},t)$, which tells that the number of particles in a system is conserved. As well known, the predictive power of this version of QM is overwhelming. If so, are there cases when non-Hermitian Hamiltonians would make sense and when would it be useful?

The answer is yes! Hence complex potentials have been employed since long in more phenomenological models to describe, for example, absorption in inelastic

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nuclear scattering in which particles need not be conserved [2,3]. A negative imaginary potential, let us say iV_I , gives rise to complex eigenvalues and to loss of particles for negative V_I , i.e. effectively there is a particle sink in the system [1,2]. At the same time wave functions are complex. This kind of model is usually referred to as the optical model and is used, besides nuclear physics, also in other fields as atomic and molecular physics, nanotransport and more to describe lossy processes. Neither particles nor energies may be conserved.

Complex wave functions as above also tell that there is a flow of particles into the region of a sink. If we now let V_I be positive in some region this scenario reverses. The imaginary potential then acts as a source of particles and the associated flow is away from the source. Suppose now that we have two regions in which the imaginary potential is positive in one of them and negative in the other. If so there will be a flow from source to sink, i.e. a transport process with both gain and loss. Intuitively we may associate this picture with the current flow between input and output leads in, for example, real electrically biased molecular and semiconductor nanodevices [4,5].

The continuity equation for probability density $\rho=|\Phi(\mathbf{r},t)|^2$ and current $\mathbf{J}$ reads [5]

$$(1)$$

where the right-hand side serves to add or withdraw particles depending on its sign. Suppose that there is a symmetry in the system which guarantees that gain and loss are perfectly balanced in such a way that the term on the right-hand side of equation (1) equals zero when integrated over all space. In this case the total number of particles is conserved and energy levels are real. In more general terms we here deal with Parity-Time (PT) symmetry for which eigenvalues may be real in spite of non-Hermiticity [6,7]. Presence of PT symmetry requires that the potential is complex with $V(\mathbf{r})=V^*(-\mathbf{r})$ and that the system is symmetric under the combined PT operations of parity (P) and time-reversal (T). These symmetry operations translate to $\mathbf{p} \rightarrow -\mathbf{p}$, $\mathbf{r} \rightarrow -\mathbf{r}$ for parity and $\mathbf{p} \rightarrow -\mathbf{p}$, $\mathbf{r} \rightarrow \mathbf{r}$, $i \rightarrow -i$ for time reversal. At PT symmetry gain and loss are exactly balanced, a symmetry that may be broken under parametric change. The break-up of symmetry is accompanied by exceptional points (EP) and underlying level crossings [8].

The purpose of the following text is to outline briefly how the above model with balanced gain and loss may be used to simulate wave functions and transport of particles between injector and collector in, for example, low-dimensional semiconductor nanodevices and billiards. By using complex potentials to emulate leads or various interactions with an environment which are generally hard to catch one may drastically reduce computational demands when modelling real systems, which now become effectively embedded in the surroundings and are of finite size

(see, for example, [8] and refs. within). Below we will focus on the special two-dimensional (2D) open quantum dot in figure 1 which was fabricated and analysed experimentally already in 2003 by Bird et al. [9]. This particular system, shown in figure 1a has since then served a “prototype” in a series of experimental and theoretical studies as, for example, in [5,8,10-16] and also as detailed below.

As mentioned, our main ambition is to outline the nature of quantum wave functions and particle flow in a special kind of low-dimensional semiconductor quantum dots and how to simulate such features using easy-to use but effective numerical methods. The underlying wave dynamics is, however, generic (see for example [17,18]). Analogous phenomena are therefore also found in optical structures and photonics [19], dielectric microcavities [20], LRC circuits, magnetic waveguides, acoustics, oscillatory classical systems and other open systems with loss and gain as covered more recently in [21,23] and refs within. The studies of PT symmetry with gain and loss are ever expanding because of importance in basic science and technology., in particular in optics and photonics where imaginary potentials may be implemented naturally via meta-materials and complex refractive indices. For example “Parity-Time Symmetry in Optics” has been listed among the ten top physics discoveries of the last ten years [24].

The remaining text is the following. In Section 2 we discuss simulated wave functions and currents in the 2D quantum dot in figure 1 and the relation to microwave emulations. The analysis therefore refers to the region of small imaginary potentials V_I which we refer to as the “linear region” or “small bias”. In Section 3 we discuss the same system but for arbitrary V_I and exceptional points and break-down/recovery of PT symmetry that occur in this “non-linear” more strongly biased regime. In Section 4 we extend the presentation to the case of four ports. In Section 5 we draw attention to related phenomena that have for a long time been known for musical instruments, more specifically string instruments for which one talks about how to master nasty “wolf tones”, unpleasant to both performers and audience. We end up by briefly mentioning a few related classical systems that would display the same type of phenomena.

2. Simulations of wave functions and currents in a weakly biased 2D quantum dot and emulation by microwaves.

Consider the PT symmetric 2D quantum dot in figure 1b. In this Section we let the interaction with the environment be very weak. i.e, V_I is finite but small. If so, the eigenstates of this well embedded dot are to a good approximation the same as for the dot in perfect isolations. Eigenvalues are real while wave functions turn complex because V_I is now finite. The admixture of real and imaginary components is weak in this case, yet there is a transport of particles taking place between the two “pseudo leads” in figure 1b. One may, of course, ask if such a current is an artefact of a too simple model or if it does reproduce real measurements. In general, it is beyond present techniques to measure particle and current distributions with high precision on

the scale of quantum dots as here. There is, however, a beautiful way out of this. As mentioned in the introduction wave phenomena turn out to be generic [17,18]. In the actual case the 2D quantum dot may be mapped onto a flat 2D macroscopic microwave billiard of the same shape [5, 10-16]. Entrance and exit antennas placed in the two opposite stubs, as in figure 1b, effectively act as the “source and the drain” for the microwaves. In addition, there is a movable, essentially non-perturbing probe for scanning the field in the interior region. In this way there is a one-to-one correspondence between the observed TM mode and the quantum-mechanical wave function [17]. The underlying equation for this mode is the Helmholtz equation with appropriate boundary conditions.

If we now turn to the quantum dot in figure 1b we obviously deal with the same type of problem as above but this time on a nanoscale. Instead of solving a Helmholtz kind of equation we now deal with the stationary Schrödinger equation. In the present situation the two equations turn out to be identical in form and differ only in the parameter values involved. We thus assume that particles are non-interacting and confined by steep walls according to the geometry in figure 1b. In the interior of the dot the real part of the potential is set equal to zero. This would correspond to a perfectly isolated dot. By adding the plus and minus imaginary regions in figure 1b we finally make contact with the dot and obtain a current between the fictitious input and output leads. As already mentioned we assume that the imaginary potentials are weak, i.e. $|V_I|=V$ in figure 1b is small. Shifts with V of energy levels/resonances are therefore also small. Dirichlet boundary conditions are used for the steep walls defining the dot. At the ends of the two input and output stubs we have, however, chosen Neumann conditions as this choice would be consistent with in- and outward flows of particles.

It is convenient to solve for the eigenstates and associated properties by means of the Finite Difference Method (FDM) [25]. Typical examples of resonance states and current flow lines computed in this way are shown in figure 2. Without going into details here we conclude that numerical outcomes of the present model for our quantum dot are in surprisingly good agreement with its microwave analogue [5,10-14]. The model is validated in the same way in a number of additional studies dealing wave function and current statistics, chaos, quantum stress tensors and other related features [26,27]. In summary, the present non-Hermitian model with PT symmetry appears robust and reliable. It is simple to use when simulating, for example, the details of electron flow and particle distributions within nanodevices, one by one as here or networked into more complex structures. It may be extended in a standard way to include particle interactions as in [4] and time-dependent processes (FDMTD) [25]. These points have also been raised for a related PT symmetric model based on absorbing boundary conditions in [28] and references within. It still remains, however, to work out the details of the conductance for the present dot and how to relate that to a real physical voltage bias as indicated in [4].

3. Modelling of more strongly biased 2D quantum dot and breakdown of PT symmetry.

In previous Section we have discussed the case of low bias, i.e. small values of V_1 . In this case the states are in practice a weak mix of the even and odd unperturbed, non-interacting states. To a good approximation one may therefore determine the predominant pairing of such states and the eigenvalues of our particular quantum dot by a 2x2 matrix equation (see, for example [8] and refs. within),

$$(E_1 - E) c_1 + i V_{int} c_2 = 0 \quad (2a)$$

$$i V_{int} c_1 + (E_2 - E) c_2 = 0 \quad (2b)$$

where E_1 and E_2 are the unperturbed levels of the dot, c_1 and c_2 the mixing parameters and E is an eigenvalue of the embedded system. The interaction element equals $V_{int} = \langle 1 | V_1 | 2 \rangle$ with V_1 as defined in figure 1b, i.e. there is a linear dependence on $|V_1| = V$ which we write as γV where γ is a positive constant; hence $V_{int} = \gamma V$ in equation 2. At small bias the eigenvalues are real in spite of the Hamiltonian being non-Hermitian. With increasing bias the two levels eventually coalesce into an exceptional point (EP) beyond which the two levels turn complex, one being the complex conjugate of the other. This happens for $V = \Delta E / (2\gamma)$ with $\Delta E = E_2 - E_1$ being positive. The real parts are now degenerate while the complex parts form a symmetric pair taking plus and minus imaginary values (see, for example, [8]). This situation prevails beyond the EP. Observation of PT -symmetry breaking of this kind was observed for the first time in complex optical potentials [29]. It has also been found to take place in, for example, mutually coupled modes of a pair of active LRC circuits [30] and more.

The above scenario of the two coalescing levels is common but not universal. A full simulation of all levels in the present quantum dot [15] shows that there may be more than one EP for a subset of levels, i.e. if there is a symmetry breaking at a first EP PT symmetry may resurface at a second EP on further increase of bias. Suppose that the two levels in equations 2a and 2b would depend on V as $E_1 \rightarrow E_1 + \alpha V$ and $E_2 \rightarrow E_2 - \beta V$ with V , α and β positive, i.e., there is a change in the level separation with bias. If so there is the possibility of two EPs as above, one at $V_1 = \Delta E / (\alpha + \beta + 2\gamma)$ and the other one at the higher value $V_2 = \Delta E / (\alpha + \beta - 2\gamma)$. In between these two EPs one thus has a pair of complex energies provided $(\alpha + \beta - 2\gamma) > 0$. If not, there is only the EP at V_1 that is physically relevant. If $(\alpha + \beta) = 0$ we recover the first case discussed above. Evidently there is a delicate balance among the parameters α , β and γ if there will be a single EP or pairs of EPs. Figures 3 and 4 illustrate these two principle cases. The full FDM calculations in [15] confirm this overall scenario. See also the comprehensive discussion in [8] on the two-level problem and EPs.

As described in Section 2 particle probability distributions and currents may be emulated experimentally by macroscopic microwave billiards in the case of low bias. It remains to show, however, that also the case of stronger bias and the occurrence of EPs may be demonstrated in practice in a similar way. It also remains, as in previous section, how a real voltage bias and conductance may be worked out, this time in the presence of exceptional points. Here we leave this interesting problem for future studies, hopefully in conjunction with experiments.

4. Energy levels in a quantum dot with four ports

The present PT-symmetric model quantum dot with two ports as above may be expanded to multiple spatial mirror symmetries and ports. An example of such a system is shown in figure 5 as briefly discussed in [16.]. In this case the quantum dot has four leads/ports, each with an imaginary potential applied at the end. The potentials are now pairwise independent which yields a two independent parameters that may be changed, V and W (cf. figure 1b). The energy levels of this system are now longer lines but rather two-dimensional sheets as in figure 6. When two such sheets coalesce they do not, in general, form EPs but rather Exceptional Lines (ELs). It is obvious, and not surprising, that the eigenvalue dynamics in this system is more complex than for two ports. ELs represent a new aspect of this kind of system that invites to further studies., for example, by means of microwaves as above.

5. Interacting vibrations in classical string instruments: Relation between “wolf tunes” and exceptional points.

In the sections above we have discussed how wave mechanical states in an embedded dot may vary and interact pairwise under the variation of a bias. A typical feature is that such levels may coalesce at some critical bias in the form an EP beyond which levels become complex. We have also emphasized that wave phenomena are generic and outlined how 2D quantum dots may be mapped onto macroscopic microwave resonators with the same geometric shape. Figure 7 showing our particular quantum dot together with an ancient lyre is apparently suggestive and it is pleasing to find that there are related observations in the field of musical string instruments. Vibrational modes may be tuned to interact in a similar fashion as above to produce a version of EPs named “wolf tunes”, the name referring to the howling sounds, for example from cellos and violins, painful to both audience and performer. “Wolf tunes” are, as we will describe here, closely related to EPs and coalescence of states, which for this reason may be referred to as “quantum wolves” [16]. It is also interesting to find that related literature predates the non-Hermitian “ PT era” (see [31-33] and references cited) and that the two fields have progressed independently, as it seems one not knowing about the other. Much of the literature refers to string instruments like violins and cellos. Here we will, however, focus on pianos with hammer excitations rather than bows.

The lyre in figure 7 with its characteristic resonances is suggestive when put side-by-side with our quantum dot. Here the lyre may not be ideal, however, for detailed experimentation. On the other hand, in a grand piano there are numerous strings suspended in a large solid frame. The strings may be tuned individually. Weinreich [32,33] has used this possibility to tune pairs of strings in a high-precision Steinway grand piano. Frequencies were observed as well as modelled as one normal mode was kept constant while the second one was tuned over an interval, at one point in coincidence with the first one. The overall set-up evidently reminds the two-level interactions discussed above and it is most pleasing that the same generic behaviour is obtained for the two cases, a quantum dot and a Steinway. A most fortunate feature is that the levels/frequencies and level separation may be tuned individually. Typical results for a two-level system as obtained from the basic model in section 2 are shown in figure 8. The overall agreement with observations is good. In the present case we have assumed that the interaction V_{int} in equation 2 remains constant through the entire interval, which renders high symmetry as actually observed [33]. This choice is, however, not critical for a general understanding of the consecutive formation of EPs.

Not for reasons of music but for further basic research of interacting resonances and EPs it should be rewarding to explore also multiple strings in analogy with, for example, three-dimensional square waveguide arrays with diagonally-balanced gain/loss distribution [34]. One may also speculate how to engage similar arrays of tuneable organ pipes, glass tubes and other resonating glass vessels with liquids as, for example, verrophones. In addition to basic research, studies of this kind should be refreshing also in the area of education and novel educational collective projects.

6. Summary and concluding remarks

Non-Hermitian quantum mechanics and PT symmetry has been described briefly in connection with low-dimensional quantum dots with balanced gain and loss. By introducing injectors and collectors in terms of fictitious imaginary potentials/leads we propose that wave functions and transport of particles across the device may be simulated straightforwardly using numerical finite-difference methods (FDM/ FDTM). Comparisons with available experimental emulations by means of microwave billiards show that this approach is reliable and robust, at least at the weak biasing that applies in this case, i.e. below the onset of exceptional points. Particle interactions do not enter in this stage. At higher bias the model predicts that PT symmetry may be broken as well as restored depending on the particular features of an eigenstate. Associated with this there are exceptional points (EPs) at which energy levels coalesce and become complex. In view of experiments it would, of course, be of fundamental interest if such a behaviour could be validated, for example, employing microwave billiards as above. Another challenge is to develop the present model with respect to particle interactions using DFT including versions with real time dependence and in this fashion tie it to realistic devices, one by one or devices

embedded in more elaborate systems.

We have also emphasized the generic features of the wave phenomena presented here. In particular we draw attention to musical string instruments for which one talks about “wolf tones” rather than the closely related EPs. As it seems this relationship has passed unnoticed in the literature. We propose that studies of this kind could be extended to arrays of tuneable organ pipes, glass tubes and various resonating glass vessels. Such studies would be interesting *per se* but would also be of value in the teaching of physics.

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Figure 1. Left panel: Electron micrograph a two-dimensional semiconductor quantum dot (Q) in contact with an environment (P) via two openings to allow for a current to flow between the two P electron reservoirs as an external voltage is applied. A voltage applied to the metallic top gates (in grey) depletes electrons below the gates and the thereby shapes the remaining electron gas into the pattern in black (Figure reproduced from [9]). Right panel: Emulation of the embedded quantum dot Q in (a) by a cavity with fictitious “input and output leads” defined by the imaginary potentials $iV_I = iV$ and $iV_I = -iV$, respectively, indicated by the marked areas in the leads. (Figure (a) copied from [8], copyright IOP).

Figure 2. Typical results from FDM simulations of two different resonance states in the model quantum dot in figure 1 (arbitrary units). The left graphs show the probability density distributions and the right ones the corresponding current flowlines (cf. [5]).

The upper panel is reminiscent of a ‘particle-in-a-box’ state with $n_x = 4$ and $n_y = 4$ that is distorted by the leads and the rounding of corners (x horizontal direction; y vertical ditto). Because of the imaginary potential is small in the present case one may therefore view the resonance state as a weak admixture of even and odd unperturbed states. The accumulation of density in the leads shows that the cavity is well open. The two lower graphs illustrate the same features as above, but now one resembling ‘particle-in-a-box’-like states with $n_x = 2$ and $n_y = 7$. As above the quantum dot is well open.

Figure 3 The figure shows a typical case for a pair of EPs. Real (top graph) and imaginary (lower graph) parts of the complex eigenvalues of the two-level model in

(fig 3 continued)

equation 2. The dashed lines illustrate the the underlying crossing non-interacting levels $E=E_1+\alpha V$ and $E=E_2-\beta V$ with $\alpha=1$, $\beta=-0.8$ and $\gamma=0.2$ (arb. Units) .

(fig 4 continued)

Figure 4. The figure shows a typical case for a single EP. Real (top graph) and imaginary (lower graph) parts of the complex eigenvalues of the two-level model in equation 2; here $\alpha=0.1$, $\beta=-0.1$ and $\gamma=0.2$ (arb. units). This behaviour is observed for LRC circuits [30].

Figure 5 A quantum dot with four leads, each with an imaginary potential applied at the four ends. The potentials are now pairwise independent which yields a two independent parameters that may be changed, V and W (cf. figure 1b) Dimensions are given in arbitrary units.

Figure 6. A window of energy levels (in arb. units) of the four-port system for different values of the two independent pairs of imaginary potentials. In both figures, which are rotated with respect to each other to better visibility, the creation of exceptional lines (ELs) are clearly observed.

Figure 7. The open two-dimensional quantum dot considered in this article (left) and an ancient lyre (right). Both of them are resonators suggesting that they share similar physics.

Figure 8. Simulation according to equation 2 of two piano strings when the motions of the strings are coupled by a constant value for V_{int} (corresponding to the special case of a “purely resistive support” in [32,33]). The top graph indicates the mistuning of or difference between uncoupled modes (dashed crossing lines) and coupled modes (full curves); E_2 is kept constant with $\beta=0$ while E_1 is tuned relative E_2 as $E_1+\alpha V$

(Fig 8 Continued)

where $\alpha=1$. The two EPs define the window of level coalescence associated with “wolf tunes”. The lower graph shows the corresponding “damping”.