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Emergence of four dimensional quantum mechanics from a deterministic theory in 11 dimensions

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Abstract. We develop a deterministic theory which accounts for the coupling of a high dimensional continuum of environmental excitations (called gravonons) to massive particle in a very localized and very weak fashion. For the model presented Schrödinger's equation can be solved practically exactly in 11 spacetime dimensions and the result demonstrates that as a function of time an incoming matter wave incident on a screen extinguishes, except at a single interaction center on the detection screen. This transition is reminiscent of the wave - particle duality arising from the "collapse" (also called "process one") postulated in the Copenhagen-von Neumann interpretation. In our theory it is replaced by a sticking process of the particle from the vacuum to the surface of the detection screen. This situation was verified in experiments by using massive molecules. In our theory this "wave-particle transition" is connected to the different dimensionalities of the space for particle motion and the gravonon dynamics, the latter propagating in the hidden dimensions of 11 dimensional spacetime. The fact that the particle is detected at apparently statistically determined points on the screen is traced back to the weakness and locality of the interaction with the gravonons which allows coupling on the energy shell alone. Although the theory exhibits a completely deterministic "chooser" mechanism for single site sticking, an apparent statistical character results, as it is found in the experiments, due to small heterogeneities in the atomic and gravonon structures.

1. Introduction

In the spirit of Feynman's statement [1] the double slit experiment contains the essence of quantum mechanics and its unresolved problems. In order to understand quantum mechanics we have to understand the double slit experiment with electrons, photons, matter waves. Modern experiments have clearly demonstrated that single massive particles (heavy rare gas atoms [2] and He clusters [3], fullerenes and their derivatives of high molecular weight [4]-[12], meso-tetraphenylporphyrin [6], phthalocyanine and its derivatives [5, 7, 8, 13]), when scattered from nano lattices and optical gratings, form diffraction patterns in quite the same way as particles of smaller mass and photons. The diffraction pattern can be understood as resulting from matter wave interfering with itself and is readily obtained as a solution of Schrödinger's equation. The formation of the interference pattern on the detection screen occurs, however, as a result of many repeated experiments. In each experiment a single particle is detected at a well defined local site on the screen. This transition from wave to particle behaviour is commonly claimed to be a "collapse" of the wave function, which itself cannot be understood by solving Schrödinger's equation or within any kind of well defined dynamics.



In this contribution we present an investigation of the diffraction of atoms and molecules from nano lattices from a novel theoretical point of view. From the experimental point of view diffraction has been observed for nearly any kind of atom or molecule, e.g. H [14], H₂ [15], He, Ne, Ar, Kr, Xe [2, 3, 16, 17], C₆₀, C₇₀ [4]-[9], [11, 12], phthalocyanine [5, 7, 10, 13]. Diffraction of He, Ne, H₂ has also been observed from crystalline structured surfaces [2, 18, 19, 20]. From the experimental findings it has to be concluded that right in front of the screen (surface) we have a wave front (wave function) which contains the diffraction pattern verified in the experimental outcome. The experimental observations are then: the diffracting particle *sticks* at a definite site on the surface, the stuck particle *stays* at least as long as the diffraction pattern has formed and finally the particle *moves* on the surface with a telegraph-signal like dynamics. This is the experimental finding which is referred to as the collapse of the wave function and as "wave - particle duality". Decoherence theory does not explain any of these observations.

The experimental outcome is at the same time interpreted as the sticking process which is believed to be accessible by standard quantum mechanical methods. From the experimental point of view collapse and sticking are identical phenomena, but sticking is considered to be completely inside the framework of the quantum mechanical formalism, whereas collapse is considered to be completely outside (cf. e.g. ref. [21]).

Within the Copenhagen interpretation the described experiments are considered as a manifestation of the wave - particle duality. The matter wave diffracts from the nano lattice and then collapses as a particle localized at a definite site on the screen. The collapse is considered outside the realm of the time dependent Schrödinger equation. This is not completely in accordance with the experimental point of view described above. In the Copenhagen interpretation the time dependent Schrödinger equation takes over again immediately after localization (collapse) and on cold flat surfaces this usually means a plane wave like motion parallel to the surface which is, however, not observed experimentally.

From the view of the time dependent Schrödinger equation alone wave packet calculations for H₂ dissociation and sticking on closed packed single crystal metal surfaces are feasible on six dimensional potential energy surfaces [22] and, after appropriate statistical averaging over initial states, in accordance with experimental results [23]. Wave packet calculations, however, cannot reproduce the telegraph like motion (diffusion) of H atoms and CO molecules on the surface. This has not yet been recognized as a significant problem.

Decoherence theory suggests that the time dependent Schrödinger equation could solve the problem, if coupling to the environmental degrees provided by the screen (surface) has to be included. It would calculate the reduced density matrix ρ_{red} which just comprises the degrees of freedom of the diffracted field (particle) after summing over the environmental degrees of freedom. Decoherence theory then claims that ρ_{red} becomes diagonal, the diagonal matrix elements specifying the probabilities for different outcomes of the experiment: sticking at various sites all over the surface or reflection into various directions.

Decoherence theory often treats localization as an exemplification of the quantum Zeno effect due to scattering of particles belonging to the environment [24]. The assumptions for this approach are: preparation of an initial state with an incoming particle from the environment; measurement of the system with the environmental particle in a definite state; probability interpretation of the transition rate in a definite final state and rate equations like the generalized Ehrenfest theorem or Fermi's golden rule. If the system (e.g. a particle) is initially in a delocalized zero energy state (e.g. Bloch state on an ordered surface) at zero temperature, then excited environmental states cannot be mixed in, because the total energy would not remain constant. If the system is initially in a localized gaussian at zero temperature of the environment, then it is not in a zero energy state. Mixing in of excited environmental modes is then possible, but would force the system to lower its energy, because of energy transfer from the system, which would mean delocalization of the system.

Within decoherence theory and especially the quantum Zeno effect, localization of a particle can only be obtained, if the environmental degrees are capable of localizing the particle. This is not the case for atoms or small molecules at cold surfaces, where experimentally localization is clearly observed. Hence decoherence theory cannot explain the experimental findings for localization of atoms and molecules on cold metal surfaces.

2. The Hamiltonian

The model Hamiltonian is:

$$\begin{aligned}
 H = & E_g n_g + \sum_p E_p n_p + \sum_w E_w n_w + \\
 & + \sum_p V_{gp} (c_g^+ c_p + c_p^+ c_g) + \sum_{p,w} V_{wp} (c_w^+ c_p + c_p^+ c_w) \\
 & + \varepsilon_0 n_0 + \sum_{\kappa_w, w} \varepsilon_{\kappa_w} n_{\kappa_w} + \sum_{\kappa_w, w} [V_{0, \kappa_w} n_w a_0^+ a_{\kappa_w} + V_{\kappa_w, 0} n_w a_{\kappa_w}^+ a_0] \quad (1)
 \end{aligned}$$

The environmental modes are existing in high dimensional spacetime (11 spacetime dimensions), have a high density of states and are called gravonons in the following. The meaning of the symbols in eq. (1) is: $n_g, n_p, n_w, n_0, n_{\kappa_w}$: number operators for gas particle at source, slits and screen, and gravonons; $c_i^+, c_i, a_0^+, a_0, a_{\kappa_w}^+, a_{\kappa_w}$: creation and annihilation operators for gas particle and gravonons; $E_g, E_w, E_p, \varepsilon_0, \varepsilon_{\kappa_w}$: energy quanta of gas particle and gravonons; $V_{gp}, V_{wp}, V_{0, \kappa_w}$: matrix elements for hopping of the gas particle and gravonon excitations. The gravonons are massive bosons which emerge in the limit of weak and local gravitational interaction in high (11) dimensional spacetime [25]. The coupling to gravonons is effective only within spacetime deformations called warp resonances represented by n_w, c_w^+, c_w , etc. In these warp resonances the gas particle is localized perpendicular and parallel to the screen surface. V_{0, κ_w} is calculated from the 11 dimensional gravitational potential $V_{grav}^{(11)}(r) = -\frac{G^{(11)}M}{\pi^{\frac{7}{8}}r^8}$. The physical nature of the gravonons as massive bosons, as well as the derivation of an effective Schrödinger equation in high dimensional spacetime yielding gravonons similar to the common quantum particles as its solution, are described in detail in ref. [25]. The gravonons are the only fields which reside not only in our 4 dimensional spacetime, but in the additional compactified hidden spacial dimensions.

The Hamiltonian is visualized in figure 1. The many-particle wave has the form: $|\Psi\rangle = C_0(t) |\phi\rangle \otimes |0\rangle + \sum_{w, \kappa_w} C_{w\kappa_w}(t) |w\rangle \otimes |\kappa_w\rangle$. $|\phi\rangle \otimes |0\rangle$ describes a tensor product of the particle in the wave $|\phi\rangle$ between source and screen and the gravonons in the initial configuration $|0\rangle$. $|w\rangle \otimes |\kappa_w\rangle$ has the particle in $|w\rangle$ at a specific point on the screen with gravonon excitations $|\kappa_w\rangle$. The time dependent coefficients are obtained from Schrödinger's equation: $i\hbar \frac{\partial \Psi(t)}{\partial t} = H\Psi(t)$.

3. Solution for a single site on the screen

The scattering of a matter field from a double slit and the "wave - particle duality" observed in these experiments is in our theory interpreted as follows. If there is a site on the screen which is energetically degenerate with the initial wave $|\Psi(t=0)\rangle$, the configuration $|\mathcal{K}_{\kappa_{proj}}\rangle$ with the gas particle field having significant strength on this site will get strongly entangled with the degenerate gravonon configurations on this site. As the excitations of the gravonons in the hidden dimensions depend on the matter field being extremely localized near the chosen site the matter field strength cannot drift away as long as the excited gravonons are moving around in the large hidden dimensions. If this takes time long enough for other physical-chemical processes to be initiated, it will result in an experimentally detectable event. Such an event would be called "collapse" in the framework of Copenhagen quantum mechanics.

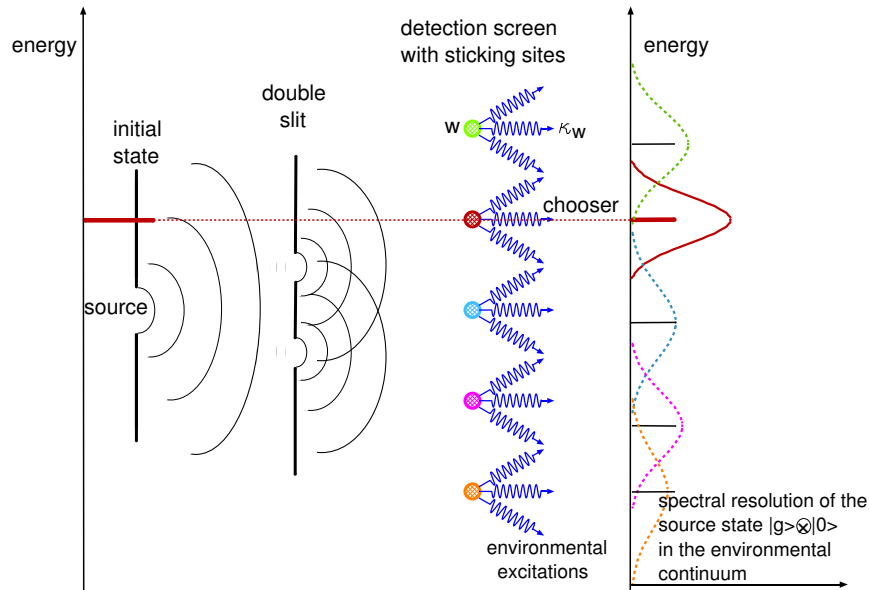


Figure 1. Model of adsorbate sticking in a double-slit diffraction experiment: a matter wave incident from a source interferes with itself between the slits and the screen. Hitting the detection screen allows entanglement with the gravonons. The initial matter wave determines the energy shell and, since the interaction with the gravonons is very weak, only on-shell coupling with a selected site on the screen, named chooser in the drawing, is effective, leading to particle sticking. Many experiments with different initial matter waves lead to the interference pattern due to adsorbed particles on the detection screen.

This situation has been treated theoretically in a simplified manner in ref. [25]. The Green function $G_{K\kappa_{proj}}^+$ has the form

$$G_{K\kappa_{proj}}^+(\epsilon_\kappa) = \frac{1}{\epsilon_\kappa - \alpha(\epsilon_\kappa) + i\Gamma(\epsilon_\kappa)} \quad (2)$$

where α and Γ are the real and imaginary parts of the self-energy, respectively, with

$$\Gamma(\epsilon_k) = \pi \sum_{\kappa_w} |V_{0,\kappa_w}|^2 \delta(E - \epsilon_\kappa) = \pi \frac{U^2}{\Delta} \text{ if } |\epsilon_k| < \Delta \quad (3)$$

which defines U . The last equation implies an approximation where the matter wave - gravonon interaction $V_{0,\kappa_w} = \frac{U}{\sqrt{N}}$ is non-zero and energy independent over an energy range of width Δ and zero otherwise. N is the number of gravonons in the energy interval Δ . Defining the density ρ_ϵ of gravonon levels at $\epsilon_\kappa = 0$

$$\frac{\rho_\epsilon}{N} = -\frac{1}{\pi} \text{Im} G_{K\kappa_{proj}}^+ = \frac{1}{\Delta} = \frac{1}{\pi\Gamma}, \quad (4)$$

yields $\Delta = \pi\Gamma$. In order to study the time dependence due to the coupling to the gravonons we start from the formal solution of the time dependent Schrödinger equation

$$|\Psi(t)\rangle = e^{-iHt} |00\rangle = \sum_{\kappa_w} e^{-i\epsilon_\kappa t} |K\kappa_w+\rangle \frac{V_{0,\kappa_w}}{\epsilon_\kappa - \alpha(\epsilon_\kappa) - i\Gamma(\epsilon_\kappa)} \quad (5)$$

where we assumed V_{0,κ_w} to be real. $\{|K\kappa_w+\rangle\}$ describe gravonons modified by the incoming gas matter wave. For the projection of $|\Psi(t)\rangle$ on these configurations we obtain:

$$\sum_{\lambda_w} |\langle K\lambda_w+ | \Psi(t)\rangle|^2 \approx 1 - e^{-2\Gamma t}, \quad (6)$$

where from eq. (3) $\frac{U^2}{\Delta} = \Gamma/\pi$ and $\Delta = \pi\Gamma$ from eq. (4).

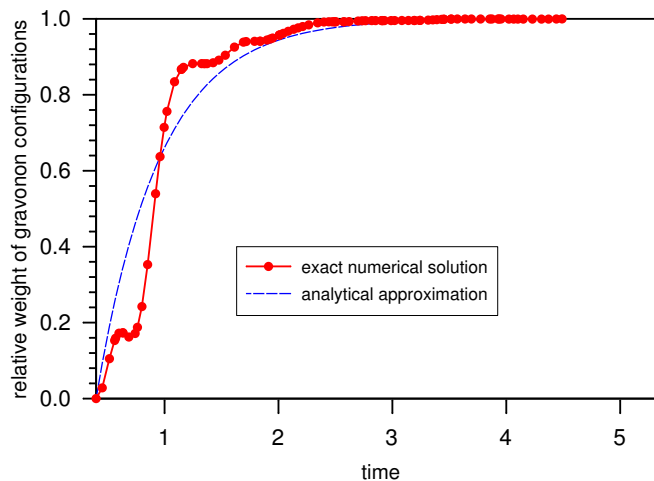


Figure 2. The chooser at work: the numerical solution (full curve) in comparison to the analytical approximation eq. (6) (dashed curve). The time is in units of $\hbar/2\Gamma$.

Equation (6) and fig. 2 show that we have an exponential increase with time of the weight of the incident wave packet in the warp resonance due to entanglement with the gravonon continuum, i.e. the incident wave becomes localized on the adsorption site.

4. The sticking time problem

The time of flight between the nano lattice and the screen can be reduced arbitrarily by reducing the distance between them. At one point the gravonon coupling becomes too weak to capture the particle during the short time of flight. The particle then moves back to the nano lattice where it is diffracted again or reflected. At some reduced distance the experimentally observed diffraction pattern should change and/or display a reduced intensity. If this does not occur, the coupling gravonon modes need to have a sufficiently large frequency.

This would be understandable within the framework of the $\gamma - \eta$ model [26]. In the limit where the frequency of the softest gravonon mode tends to zero one has for the coupling strength $\gamma = \frac{\omega_A^2}{\omega_S^2} \approx \frac{1}{1-\eta}$ where ω_A characterizes the motion of the gravonon image of the gas particle, i.e. the spacetime deformation of the gas particle, relative to the gravonon images of the atoms in the screen surface. ω_S is the unperturbed gravonon frequency. η is the parameter specifying the importance of forces between the local spacetime deformations in the gravonon space. If $\eta \rightarrow 1$ these forces are of little importance, γ becomes large and the softest gravonon mode which dominates the gravonon coupling can have a relatively large frequency ω_{soft} , provided it remains softer than any of the modes in the four dimensional environment.

In this way the sticking times might differ by eight orders of magnitude, explaining eight orders of magnitude different diffusion rates of hydrogen on Cu(001) and Ni(001) [27, 28]. In

the experiment on the diffraction of phthalocyanine waves [13] we do not know the coupling strength, however, knowing the sticking time of approximately 10^{-4} seconds allows us to make an estimate of the coupling strengths V_{gp} and V_{wp} of the order of 10^{-11} eV, which is also the order of magnitude of ω_S and ω_A .

If the time of flight between the nano lattice and screen becomes smaller than $1/\omega_{soft}$, a standing wave between lattice and screen will develop. The change of the matter wave will change the diffraction pattern and this might offer a possibility for experimentally determining the sticking time. In this way it might be possible to demonstrate experimentally that collapse (which is equal to sticking in this case) is not infinitely fast but needs a finite time. This would give a clue, whether decoherence is at work (which is predicted to be extremely fast) or the process displayed in fig. 2.

5. Time dependent solution of the model Hamiltonian neglecting the coupling to the gravonons

The treatment of the problem with a "hopping hamiltonian" (also called tight binding hamiltonian in solid state physics) requires many empty lattice points to simulate plane wave motion. To understand the problem consider in the following a one dimensional situation. If for a distance L between source and screen there are N empty lattice points separated by a lattice constant a , then the largest k -vector is $k_{max} = \frac{\pi}{a} = N\pi/L$. As an example take $L = 10^{10}$ bohr (roughly 50 cm), the mass of the diffracting particle $M = 10^5$ (roughly 50 proton masses) and the velocity $k/M = 10^{-5}$ (roughly 50 m/sec). The k -vector is then $k \approx 1$. Then we need at least $N = kL/\pi \approx 3 \times 10^9$ empty lattice points. This is much too large for our numerical simulations because of lack of symmetry in the system source - slits - screen and because of the high dimensionality of the gravonon fields.

If we would have only two empty lattice points between the source and the warp resonances in the screen, then choosing the highest energy of such a hopping model equal to the kinetic energy of the diffracting particle (≈ 1 meV) would yield a "transfer time" (now this is the time for half a Rabi-like oscillation) of $t = 10^5$ a.u. = 10^{-12} seconds, which differs by 10 orders of magnitude from the experimental transfer time $ML/k \approx 10^{15}$ a.u. $\approx 10^{-2}$ seconds. Because reasonable time scales are essential for our investigation, we choose the hopping parameter in such a way that the Rabi-oscillation time agrees with the experimental transport time. This means that for the discussed example the hopping matrix element should be of the order of 10^{-12} eV.

Figure 3 shows snapshots of the time development of a wave packet created in the source and interacting with the two slits and several sites on the screen. The area of the spots scales linearly with the amplitude squared of the wave packet at different places in the source, the slits and on five sites on the screen, as a function of time. At short time a big spot in the source, nothing in the slits and on the screen corresponds to the initial situation with the wave packet in the source. Gradually with time the wave packet is distributed everywhere, in the slits and on different sites on the screen. An interference pattern starts evolving at the position of the screen. The time dependent Schrödinger equation of the wave packet in interaction with the source, the slits and the screen shows the tendency to build the interference pattern. However, Rabi-like oscillations bring back the system to the initial situation and the cycle is repeated. This is not shown in fig. 3. Using the first two lines of the Hamiltonian eq. (1) leads to the interference pattern on the right hand side of fig. 3. However, this is not what is observed experimentally. The first two lines of the Hamiltonian do not lead to sticking of the particle on one site on the screen. There is no definite choice, but a distribution over many sites with different intensity. Furthermore permanent Rabi-like oscillations from the source to the screen and back occur.

The theoretical interference pattern is the same as in experiment. Within the Copenhagen interpretation of quantum mechanics solving the time dependent Schrödinger equation, using

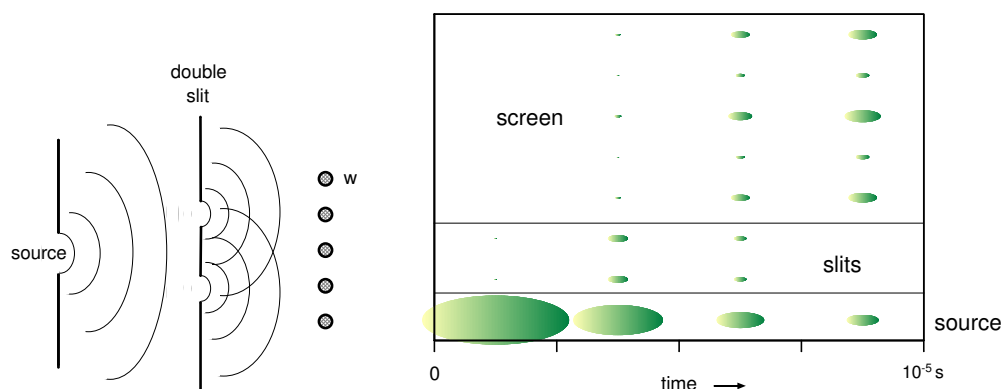


Figure 3. Left: geometric model of a double slit experiment with matter wave, without accounting for the interaction of the gas particle with the gravonons. Right: interference pattern created after 10^{-5} seconds.

the collapse and probabilistic concepts, the experimental interference pattern is reproduced and interpreted. However, the time dependent Schrödinger equation in four dimensional spacetime cannot explain the experiment: the collapse of the wave packet on a definite point on the screen cannot be predicted, with Copenhagen quantum mechanics we have no chooser, we have only the possible choices if we know what the final states are, however, there is no mechanism to select a single definite choice at a time.

6. Time dependent solution of the model Hamiltonian including the coupling to the gravonons

With the entanglement to the gravonons included (the last line in eq. 1) the result is displayed in fig. 4 for a single particle wave. In experiment the interference pattern on the screen develops as one particle after the other in successive emission of wave packets from the source sticks on the screen. The enhancement of the spot on the screen with time means that the incident wave becomes localized on a selected site transforming in a localized particle. This mechanism of sticking on a definite site on the screen we call the chooser. In each sticking event we have a definite site on the screen where the incident wave localizes. So instead of "God playing dice" we have the chooser mechanism defining the final site for sticking. There are no Rabi-like oscillations which bring the particle back to the source, the particle stays on this site on the screen for a long time, enabling the building up of the interference pattern in many successive sticking events, before it diffuses to a different site.

Then how does the chooser work? The condition to come to this result is a local and very weak interaction with the gravonons. Experimentally one can prepare a flat and ideal surface, however, the sites on the surface are never identical. Tiny differences between the sites matter because the interaction with the gravonons is very weak. The choice depends on the weakness of the interaction. If the interaction is zero we have the result with no chooser mechanism, hence no definite outcome. Turning on a very weak interaction with the gravonons means involving just those environmental configurations which are resonant or near-resonant with the initial configuration. (Perturbation theory shows that their involvement is inversely proportional to the energy difference with the initial configuration.) And, since the sites on the screen differ in energy, only those sites, whose energy differs from that of the initial configuration on the order of their interaction energy, will be involved. For a very weak interaction this can be just one site.

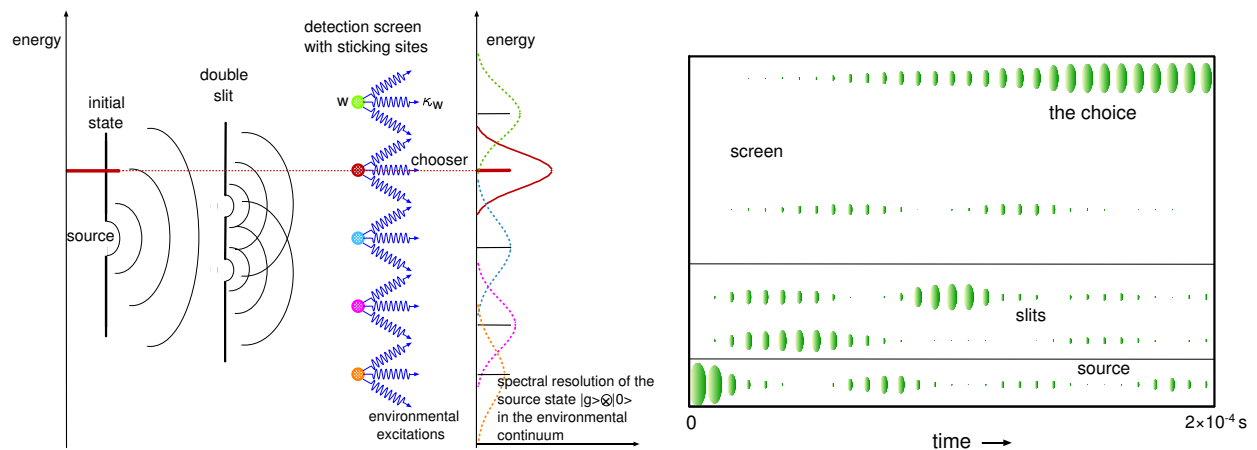


Figure 4. Left: geometric model of a double slit experiment with matter wave, taking into account the entanglement of the gas particle with the gravonons. Right: solving the time dependent Schrödinger equation a point in the diffraction pattern is created by a single sticking particle.

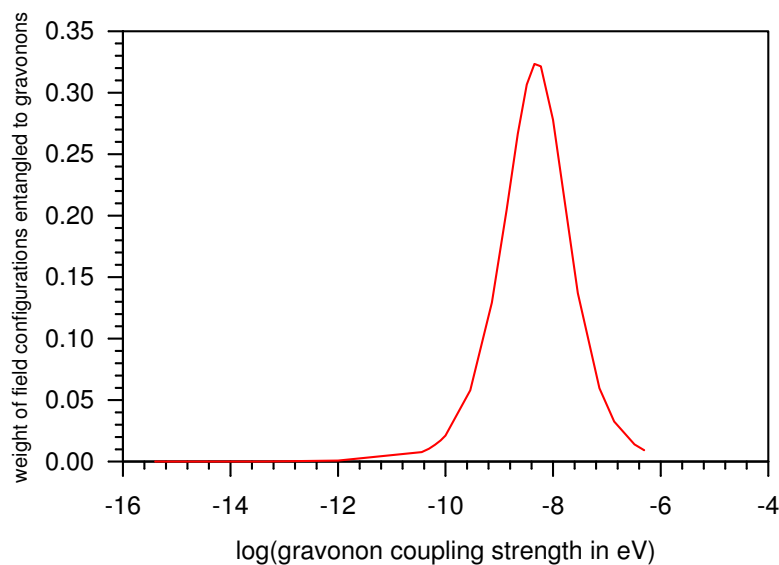


Figure 5. Summed weight of all field configurations entangled to gravonons versus the logarithm of the gravonon coupling strength $\sqrt{\sum_{\kappa_w} |V_{0,\kappa_w}|^2}$ in eV.

With the next incident wave packet prepared, the condition for degeneracy coupling will be satisfied on a different site on the screen. The interaction is so weak that it is weaker than the energy differences between the sites, hence just one site will satisfy the resonance condition.

Is this behaviour dependent on the coupling strength V_{0,κ_w} ? If the interaction with the gravonons is localized and strong then environmental excitations of different nature over a broad energy interval will be involved, states describing particle reflection back into the vacuum included. So the particle wave will be preferentially reflected from the screen rather than to accommodate and stick as an adsorbate. The reflected state is the preferred final state rather than sticking because with sticking there is the need to excite many highly energetic modes

(phonon modes, tomonagons) to dissipate the energy. However, particle wave reflection is not seen in experiment.

Very local and weak interaction V_{0,κ_w} with the gravonons warrants coupling of the initial wave packet with degenerate gravonons as shown in fig. 1 by the dashed horizontal line and the spectral distribution of the initial configuration $|g\rangle \otimes |0\rangle$ in the continuum of environmental configurations $\{|w\rangle \otimes |\kappa_w\rangle\}$ shows. Since the entangled gravonons are degenerate the density of environmental configurations is high, the energy differences are small, hence the time for particle localization is long.

Even if the warp resonances are exactly on the energy shell, the coupling to the gravonons must not become arbitrarily small, if sticking is required to occur. The reason is that the gravonons represent a local spacetime structure exhibiting few modes of extremely small but non-zero frequency. If the matrix elements for gravonon coupling become smaller than the softest gravonon mode, gravonons will no longer entangle with the particle motion. We have studied this by calculating the degree of entanglement as a function of gravonon coupling strength. In fig. 5 the summed weight of all field configurations entangled to gravonons is plotted versus the logarithm of the gravonon coupling strength in eV. Entanglement to gravonons is effective over two orders of magnitude and becomes unimportant for weaker and stronger interaction. A variation of this interaction strength by 10^{-6} eV or even less from site to site can decide, whether the particle sticks here or somewhere else. The results of fig. 5 are, of course, only valid for the model structure and the parameters applied here. They depend on the nature of the particle (shape, mass, electronic structure) and on the nature of the screen.

7. Conclusions

A particle incident as a delocalized wave sticks at one point on the screen. A delocalized matter wave is transformed in a particle stuck on a selected site on the detection screen. Adsorbate sticking is thus the result of solving Schrödinger's time dependent equation, taking into account the entanglement with gravonons in high dimensional spacetime. The wave-to-particle transition is due to the local and weak interaction with gravonons. The interference pattern develops in the matter wave between the slits and the screen. Transition from wave to particle occurs where the amplitude of the interference wave is high because of enhanced entanglement with the gravonons. Minima in the amplitude of the interference wave mean attenuated entanglement with gravonons. Particle localization and sticking in the developed theory are apparently statistical. It has been demonstrate here, however, that they are deterministic. In this sense the problem of definite outcome has been solved. The apparent statistical behaviour is due to different initial conditions. (This is in contrast to refs. [29, 30, 31].) The incoming state, as prepared in experiment, is degenerate with warp resonances at a small number of sites on the screen. In the limiting situation just a single on-shell site is the only one where entanglement with gravonons can be efficient because the interaction energy with gravonons is weaker than the energy differences of the sites for adsorbate sticking. The theory is nonlocal, non-locality is implicit as it is implicit in the Schrödinger equation. The theory is quantum realistic. Whereas in the Copenhagen interpretation of quantum mechanics the wave function serves just to provide the probability for different outcomes of a measurement, in our theory the world wave function is the real system itself.

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