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Phys. Rev. Lett. **106**, 023601 — Published 10 January 2011

DOI: [10.1103/PhysRevLett.106.023601](https://doi.org/10.1103/PhysRevLett.106.023601)

A space-time resolved approach for interacting quantum field theories

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We present an alternative approach to the usual perturbative S-matrix evaluation of quantum field theories which is non-perturbative and provides full space-time resolution. This method is used to study the dynamical development of the force between two fermion wave packets for a one-dimensional Yukawa system. The spatial distribution of the virtual bosons that act as mediators of the force can be analyzed along with the fermionic densities. The fermion-fermion interaction can be approximated by a potential function, which is used to develop classical and quantum models. It is shown that these models are good approximations to the exact field theoretical calculations when the Fock space is restricted to only one boson, but in the full quantum field theory the fermion-fermion force is enhanced by higher-order multi-boson processes. Furthermore, the normally attractive fermion-fermion Yukawa force can in principle be manipulated to even be repulsive if the momentum modes available to the virtual bosons are restricted.

Quantum electrodynamics is one of the most successful and well-tested theories in physics. Its typical treatment is based on a perturbative S-matrix approach [1]. While this approach has proven to have incredible predictive power in beam experiments and the measurement of the electron's anomalous magnetic moment, it has two disadvantages; first, only the perturbative approximation to the theory can be calculated, and second, only the asymptotic in- and out-states are relevant and therefore there is no knowledge of the underlying space- and time-resolved dynamics of the system. This theory relates the origin of all forces to the emission and absorption of virtual bosons as essential mediators of force. The dynamical aspects of how the exchange of intermediary bosons can lead to repulsive or attractive forces between two fermions of equal or opposite charge is presently not fully understood. For example, how is the state of the bosons modified during this exchange, or are there measurable time delays between emission and absorption?

In this work we examine a model fermion-boson Yukawa system using a numerical approach [2] that is non-perturbative and also allows for the visualization of the space-time dynamics of both fermionic and bosonic densities. Our initial goal is not to make quantitative predictions for a specific experimental realization, but to introduce a theoretical framework to better understand the role virtual and dressing bosons play in the fermion-fermion interaction. If the dynamical states of the bosons can be manipulated externally, the resulting fundamental forces can be controlled.

In order to focus on the fermion-boson dynamics, antifermions are neglected in this model. This not only reduces the size of the Hilbert space, thus making computations more feasible, but also removes ultraviolet divergences in the boson propagator, thereby eliminating the need for renormalization of the theory. We denote the quantum field operators for the fermions (modeling electrons) and neutral scalar bosons (modeling photons) with $\hat{\Psi}(z)$ and $\hat{\phi}(z)$, where z denotes the (one-dimensional) spatial coordinate. We can expand these operators in momentum states

$$\hat{\Psi}(z) \equiv \int dp \hat{b}(p) (2\pi)^{-1/2} u(p) \exp(ipz/\hbar) \quad (1a)$$

$$\hat{\phi}(z) \equiv \int dk c \hbar^{1/2} (4\pi\omega(k))^{-1/2} \hat{a}(k) \exp(ikz/\hbar) + \text{h.c.} \quad (1b)$$

where the fermionic and bosonic creation and annihilation operators fulfill the anticommutator and

commutator relationships $[\hat{b}(p), \hat{b}(p')^\dagger]_+ = \delta(p-p')$ and $[\hat{a}(k), \hat{a}(k')^\dagger]_- = \delta(k-k')$. As is customary in atomic physics and quantum optics, from now on we will use units where the speed of light $c=137$ a.u., the electron's mass and charge $m=e=1$ a.u., and $\hbar=1$ a.u. The two-component spinor coefficient is defined as $u(p) \equiv [1 + (pc/(Mc^2 + E(p)))^2]^{-1/2} [1, pc/(Mc^2 + E(p))]^T$, where we use Dirac matrices represented here in terms of the Pauli matrices, $\gamma^0 = \sigma_3$ and $\gamma^1 = \sigma_1$. We denote the free energies by $E(p) \equiv \sqrt{M^2 c^4 + c^2 p^2}$ and $\omega(k) \equiv \sqrt{m^2 c^4 + c^2 k^2}$, where the bare masses of the fermion and boson are M and m , respectively. The Hamiltonian of this system is then given by:

$$H = \int dp E(p) \hat{b}(p)^\dagger \hat{b}(p) + \int dk \omega(k) \hat{a}(k)^\dagger \hat{a}(k) + V \quad (2a)$$

$$V = \gamma c^{5/2} \int dp \int dk \Gamma(p, k) \hat{b}(p+k)^\dagger \hat{b}(p) [\hat{a}(k) + \hat{a}(-k)^\dagger] \quad (2b)$$

The coupling function $\Gamma(p, k) \equiv [E(p+k)E(p) + M^2 c^4 - p(p+k)c^2]^{1/2} [8\pi\omega(k)E(p+k)E(p)]^{-1/2}$ is the result of the scalar product among the Dirac spinors and acts as a natural cut-off function as it decreases with increasing momenta p and k .

In order to examine the dynamics, we have to compute the time evolution of the quantum field theoretical state $|\Phi(t)\rangle\rangle$ as a solution to the equation of motion, $i \partial |\Phi(t)\rangle\rangle / \partial t = H |\Phi(t)\rangle\rangle$ for a given initial state $|\Phi(0)\rangle\rangle$. Solving this equation is aided by the existence of two conserved quantum numbers, the fermion number $\int dp \hat{b}(p)^\dagger \hat{b}(p)$ and the total momentum $\int dp p \hat{b}(p)^\dagger \hat{b}(p) + \int dk k \hat{a}(k)^\dagger \hat{a}(k)$. The system is discretized by placing it in a box with periodic boundary conditions, and then the still infinite-dimensional Fock space is further restricted to only the dynamically relevant bosonic states. We have verified that other boson modes have only very low occupation and the results are only minimally affected by restricting the maximum occupation number. Due to momentum conservation, each momentum block can be diagonalized separately, permitting us to diagonalize numerically a $10^5 \times 10^5$ Hamiltonian matrix. The eigenvalues and eigenvectors are used to construct the time evolution of the state, which is used to calculate the spatial probability density of the (bare) fermions via $\rho_f(z, t) \equiv \langle\langle \Phi(t) | \hat{\Psi}(z)^\dagger \hat{\Psi}(z) | \Phi(t) \rangle\rangle$ and similarly for the bosons.

In order to compare the quantum field theoretical dynamics based on the annihilation and

creation of particles with quantum and classical mechanical descriptions, we need to approximate the interaction Eq. (2.b) by a potential. Such an effective fermion-fermion potential can be obtained in the non-relativistic limit if the momenta are small. Under the Greenberg-Schweber approximation [3], the energy of the fermion is assumed to be independent of momentum and is approximated by the rest energy, $E(p) \approx Mc^2$. The factor $\Gamma(p,k)$ appearing in Eq. (2b) becomes independent of p . The bare annihilation operators $\hat{b}(p)$ and $\hat{a}(k)$ can then be transformed into dressed operators $\hat{B}(p)$ and $\hat{A}(k)$ by a unitary transformation

$$U_{GS} = \exp \{ \gamma c^{3/2} \int dp \int dk (4\pi \omega(k)^3)^{-1/2} \hat{b}(p)^\dagger \hat{b}(p+k) [\hat{a}(k)^\dagger - \hat{a}(-k)] \} \quad (3)$$

This transformation is very similar to the interaction picture transformation $U(-\infty, \infty)$ but with the integration beginning from $t=0$ instead, $U(0, \infty)$. When the Hamiltonian is rewritten in the new dressed operator variables \hat{B} and \hat{B}^\dagger , it is found to contain a term

$$V_{GS} = \int dz \int dz' \hat{B}(z)^\dagger \hat{B}(z) V(z-z') \hat{B}(z')^\dagger \hat{B}(z') \quad (4)$$

where the non-local interaction potential is

$$V(z-z') = -(\gamma^2 c^2 / 2m) \exp[-c m |z-z'|] \quad (5)$$

We note that the same expression for the Yukawa potential can also be obtained by starting with the first term in the perturbative expansion of the fermion-fermion and antifermion-fermion elastic scattering S-matrix element and comparing the resulting differential cross section with what one would obtain by using the Born approximation with the above potential [4].

In Figure 1a we show the fully space- and time-resolved dynamics for two initially Gaussian distributed fermions. In contrast to the construction of a single physical fermion wave packet and its bosonic component [5], the required dressed two-fermion state is more complicated. If the associated bosonic clouds do not spatially overlap, the state can be obtained from antisymmetrized products of the dressed (single-fermion) creation operators applied to the vacuum. The spatial distribution under the influence of interactions is the curve labeled $t=T$, while the spreading

behavior that would occur in the absence of any interaction ($\gamma=0$) is shown for comparison as the dashed curve. In the region around $z=0$, we see that the fermionic density is much higher when interactions are turned on, indicating that the two fermions are attracted to each other. Furthermore, we see that the fermion density on the wings of the distribution with and without interactions are in close agreement; in this region the two fermions are too far away from each other, such that the force is nearly zero.

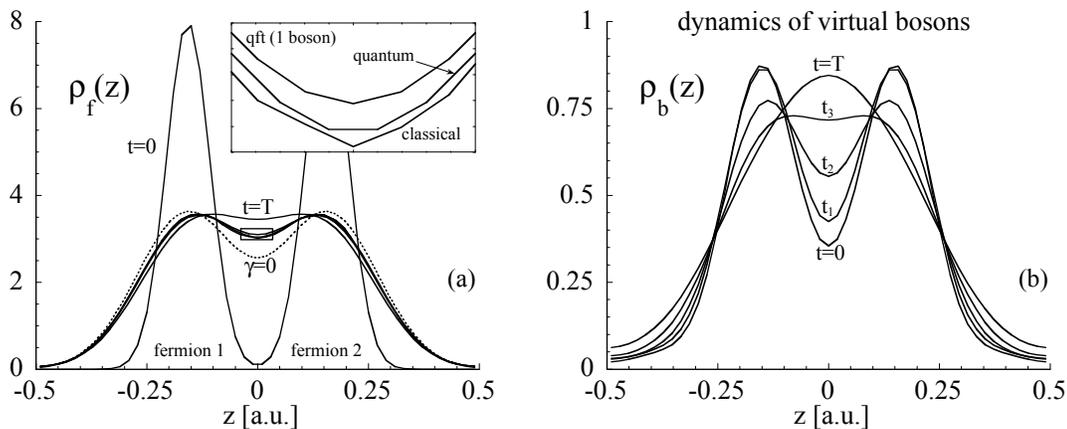


Figure 1.

(a) The fermions' spatial probability density $\rho_f(z)$ at the initial and final time T . To measure the impact of the virtual bosons, the dashed curve (denoted by $\gamma=0$) is the fermions' final density without any interaction. The inset shows the corresponding densities obtained from a classical mechanical ensemble of 10^7 two-particle pairs and a quantum mechanical wave function solution to the relativistic two-particle Schrödinger equation based on the attractive Yukawa force, enlarged for the small central region between both fermions $-0.05 \text{ a.u.} < z < 0.05 \text{ a.u.}$. The top curve in the inset is quantum field theoretical density where the Fock space has been restricted to only 1 boson.

(b) Five snapshots of the spatial density of the corresponding virtual bosons $\rho_b(z)$ at times $t=n \times 2.5 \times 10^{-3} \text{ a.u.}$ ($n=0,1,2,3,4$). [Parameters: fermion and boson masses $M=1 \text{ a.u.}$ and $m=0.05 \text{ a.u.}$ respectively, box length $L=1 \text{ a.u.}$, coupling $\gamma=0.05 \text{ a.u.}$, Fock space restricted to a maximum of 3 bosons, and the initial state is two Gaussians located at $z_0=\pm 0.16 \text{ a.u.}$ with width $\Delta z=0.05 \text{ a.u.}$. Both Gaussians have zero average momentum].

The attraction between the dressed fermions shown in the Figure was due to the virtual bosons. A pair of initially bare fermions would produce a rapidly oscillating bosonic field at short times [6]. The associated virtual bosonic cloud surrounding each fermion is shown in Fig. 1b. These dressing bosons attached to a fermion can be regarded as the "electric field" produced by the "charge". In contrast to the fermions' initial densities, which do not overlap initially, the virtual boson cloud associated with one fermion overlaps with the other fermion, leading to an immediate attraction. Also note that at the final time, the virtual bosons, acting now as force-mediators, have moved to the region between the two fermions.

The quantum field theoretical system can be modeled by classical and quantum mechanical approximations based on the Yukawa potential $V(z-z')$. For the classical mechanical model, the Bakamjian-Thomas construction [7] can be used. This technique allows for the introduction of an instantaneous action-at-a-distance potential energy function while still preserving the relativistic Poisson bracket algebra [8-10] for the boost k , the total momentum p and the Hamilton function h , $\{h,k\}=p$, $\{p,k\}=h/c^2$, and $\{h,p\}=0$. The fact that action-at-a-distance can be combined with a relativistic algebra is highly non-trivial [11]. In this formalism the two-particle Hamiltonian h is written as $h = [(M_r+V(r)/c^2)^2 c^4 + (p_1+p_2)^2 c^2]^{1/2}$, where $V(r)$ is the Yukawa potential Eq. (5). The variable $r \equiv z_1 - z_2 + (z_1 - z_2)(p_1 + p_2)^2 / M_r [(h_1 + h_2 + M_r c^2)^{-1} - 4p^2 (h_1 + h_2)^{-1} M_r^{-2} c^{-2}]$ is the relativistic equivalent of the non-relativistic relative position $(z_1 - z_2)$, $h_{1,2} \equiv [M^2 c^4 + c^2 p_{1,2}^2]^{1/2}$ is the single-particle free Hamiltonian, and z_1, z_2, p_1 , and p_2 are the positions and momenta of the two particles. The mass function $M_r \equiv [(h_1 + h_2)^2 - c^2 (p_1 + p_2)^2]^{1/2} / c^2$ plays the role of the total effective relativistic mass of the system. The Gaussian distributed 2-fermion initial state is simulated in classical mechanics by an ensemble of 2×10^7 point particles with appropriate position and momentum distributions corresponding to the quantum field theory densities. The results of the classical model are shown in Fig. 1a and its inset.

The quantum mechanical model is obtained by the numerical solution to the two-particle Schrödinger equation $i \partial \Psi(z_1, z_2, t) / \partial t = [h_1 + h_2 + V(z_1 - z_2)] \Psi(z_1, z_2, t)$, where $h_{1,2} \equiv [M^2 c^4 - c^2 \partial^2 / \partial z_{1,2}^2]^{1/2}$, and $V(z_1 - z_2)$ is again the Yukawa potential. Because the system consists of two identical fermions, the initial wave function was chosen to be anti-symmetric, $\Psi(z_1, z_2, t=0) = \phi_1(z_1)\phi_2(z_2) - \phi_1(z_2)\phi_2(z_1)$, where ϕ_1 and ϕ_2 are single particle wave functions. A corresponding symmetrized two-electron state would lead to a different time evolution but these differences are negligible for our parameters. The effective single-particle quantum mechanical density $\int dz_2 |\Psi(z, z_2, t)|^2$ is also shown in Figure 1a.

As seen in the Figure, the classical and quantum mechanical models are in remarkably close agreement with each other, and as expected both show an attraction between the two fermions when compared with the non-interacting spreading (dashed curve). However, the quantum field theory result shows a substantially greater attraction. Although the classical and quantum models are evaluated non-perturbatively, they are both based on the Yukawa potential, which was derived

perturbatively by assuming the exchange of only a single boson between the fermions. We might therefore speculate that the difference between the field theory result and the two models is due to higher-order multi-boson processes. To test this hypothesis, the quantum field theory calculation was performed, but with the Fock space restricted to only those states containing at most one boson. As seen in the inset of Fig. 1, the one-boson result is now almost in perfect agreement with the classical and quantum models suggesting that the excess attraction seen in the unrestricted quantum field theory is indeed a result of such multi-boson processes.

In order to gain greater insight into the nature of the interactions and the resulting effective force, we now turn to an analysis of the effects of the individual momentum modes of the bosonic field. In Figure 2, the results of a field theoretical calculation are shown where the Fock space was restricted to a maximum of one boson, and only a single bosonic momentum mode was allowed, as indicated in the Figure. The initial state was chosen again to represent two Gaussian distributed fermions with centers located at a distance of 0.5 a.u. from each other and with a narrow spatial width. For $k=1\Delta k$ (where $\Delta k=2\pi/L$, with L the box length), we again see that the force between the two fermions is attractive as there is an excess density of fermions in the region between the two initial locations, $z\approx 0$. It is also evident that there is a slight overall translation of the distribution to the left. This can most easily be seen by comparing it with the graph for no interactions (dashed line), since the non-interacting graph is perfectly symmetric with respect to the origin. This shift occurs because the only active boson mode has positive momentum ($k=+1\Delta k$), so by conservation of momentum the fermion distribution must pick up a negative momentum and move slightly to the left.

For $k=2\Delta k$, the situation is more complicated. There is an excess of bosons in the central region, again indicating an attractive force between the two fermions. However, there is also an excess density over the non-interacting curve in the outer wings of the distribution. Such an excess in this region indicates that here the force must be repulsive. Therefore, the $k=2\Delta k$ portion of the interaction appears to be attractive at short distances and repulsive at long range. For $k=3\Delta k$, there is a deficit in the density distribution in the central region and an excess on the outermost wings, showing that the force is repulsive across the entire range. Finally, for $k=4\Delta k$, when including the effects of the overall translation of the system to the left, there is a very slight deficit in fermionic density in the central region, indicating a repulsive force at these short distances, and there is also a deficit on the wings, which indicates an attractive force at longer ranges.

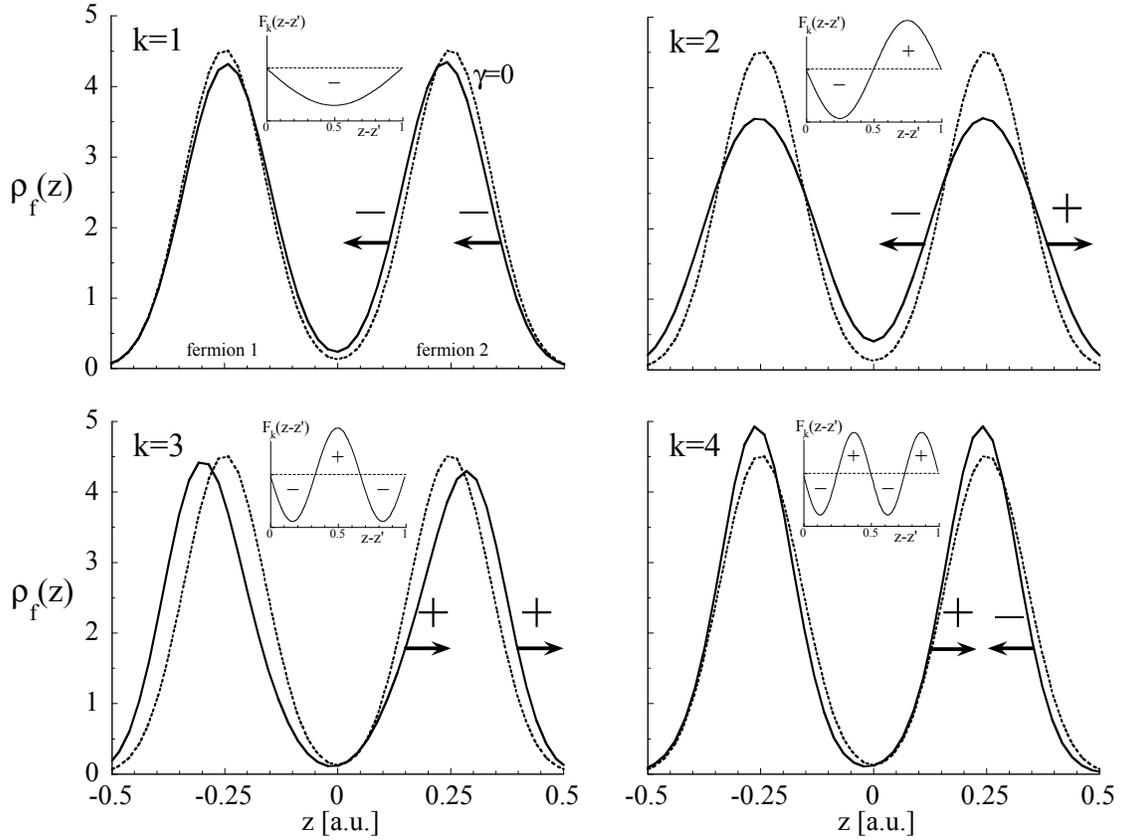


Figure 2. Fermion densities after time $T=0.01$ a.u. where the interaction is associated with only a single bosonic momentum mode $k=1, 2, 3$, or $4 \Delta k$. For comparison, the dashed line is the density without any interaction between the dressed fermions. The inset of each Figure shows the force $F_k(z-z')$ associated with the specific mode of the virtual bosons as a function of the relative coordinate $z-z'$. The plus (minus) sign indicates a region of mutual repulsion (attraction). Note that 0.5 a.u. is the average distance between the fermions. [Parameters: fermion and boson masses $M=1$ a.u. and $m=0.05$ a.u. respectively, box length $L=2$ a.u. (full box length not shown in figure), coupling $\gamma=0.3$ a.u., and the initial state is two Gaussians located at $z_0=\pm 0.25$ a.u. with width $\Delta z=0.03$ a.u. Both Gaussians have zero average momentum].

These results can be understood by examining the contributions of each boson mode to the potential $V(z-z')$. When confined to a box with periodic boundary conditions, the potential becomes the discrete sum $V(z-z') = -(\gamma^2 c^5 / 2\pi) \Delta k \sum_k \omega_k^{-2} \exp[i(z-z')k \Delta k]$, where Δk is again the spacing between modes and k is now an integer. If we consider only a pair of modes $\pm k'$, then we may write an effective potential for these two modes $V_k(z-z') = -(\gamma^2 c^5 / \pi) \Delta k \omega_k^{-2} \cos[(z-z') k' \Delta k]$. Each potential leads to a characteristic force $F_k(z-z') = -dV_k(z-z')/dz$ associated with each mode of the virtual bosons. The effective forces created by these virtual bosons are shown in the insets on

top of each figure.

We see that the force caused by the virtual bosons of low momentum $k=1$ is negative and therefore attractive over the entire box length. Other bosons can be either attractive or repulsive in different spatial regions. For example, virtual bosons with momentum $k=2$ lead to an attraction for fermions that are close to each other $|z-z'|<0.5$, while those that are further apart repel. For the parameters used in Figure 2, the distance between the centers of the two Gaussian wave packets was 0.5 a.u. Therefore the force $F_{k=2}(z-z')$ predicts that the inside wings of the two Gaussians should move towards each other, while the outside wings move apart. This is exactly the behavior that is observed in the Figure. Furthermore, the $k=3$ mode is purely repulsive around 0.5 a.u. There are two trends that make virtual bosons with larger momentum less important; first the regions of attraction and repulsion become shorter and therefore their dynamical impact self-averages out to zero as the two fermions evolve, and, second, the amplitude of the force decreases.

An important question concerns the applicability of these results to the case of a boson of mass zero and spin 1. While the massive bosons of spin zero modeled by the Yukawa Hamiltonian are much easier to be treated computationally, the ultimate goal would be to use the exact QED Hamiltonian to study the full three-dimensional time-evolution of Coulombic electron-electron and electron-positron interactions through a photon field. While the simplified model presented here yielded finite results, quantum electrodynamics would not converge without a further analysis of the issue of renormalization.

Acknowledgements

We have enjoyed several discussions with Drs. S. Bowen, C.C. Gerry, S. Hassani and E.V. Stefanovich. This work has been supported by the NSF and Research Corporation.

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