Accumulation of bosons between fermions due to the Pauli exclusion principle

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We examine the field theoretical impact of the Pauli exclusion principle on the formation of the ground state of two fermions that are coupled with each other through the interaction with bosons. As expected, in case where the two fermions are indistinguishable, their binding strength due to the force-mediating bosons is reduced and their spatial distribution in the ground state is wider compared to the corresponding state for the distinguishable particles. Surprisingly, the spatial distribution of the bosons in the ground states is even fundamentally different for both systems. In fact, the Pauli exclusion principle leads to a strong accumulation of the bosons between the two fermions.

Quantum field theory is the most accurate and the best confirmed theory in modern physics. In recent decades, it was pivotal for reliable predictions of few-electron systems in the presence of nuclear fields such as the energy levels of positronium and muonium. The bound states (and resonances, which are metastable bound states) correspond to poles in the scattering matrix for the interacting quanta [1]. In principle, the appropriate tool to study bound states is the Bethe-Salpeter formalism [2,3]. However, for various practical reasons its applications to both quantum electrodynamics and chromodynamics is limited, as the Bethe-Salpeter equation can only be solved perturbatively within the so-called ladder approximation. The accurate computation of the fermionic and especially the bosonic properties of bound states within the framework of quantum field theory remains a challenging task.

In order to have a more universal approach for general interactions with arbitrary coupling strength, a computational method was recently proposed that is based on the construction of the Hamiltonian from the quantum field theoretical Lagrangian density [4, 5]. By choosing a suitable set of discretized basis states [6], the energy eigenvalues and eigenfunctions can be calculated by diagonalizing the matrix representation for the Hamiltonian numerically.

In this work, this numerical approach is applied to examining the effect of the indistinguishability of two interacting fermions on their quantum field theoretical bound state as well as on the properties of the force-intermediating bosons. It is well-known that for two free indistinguishable particles (such as protons) the antisymmetry of the wave function under particle exchange and the resulting Pauli exclusion principle [7] prohibit the double occupation of the same position or momentum state. While two protons are not allowed to share exactly the same location and momentum and therefore effectively repell each other (at least locally), there is no principle that would prohibit them from becoming arbitrarily close to each other. However, in the presence of interactions this principle has significant energetic and also spatially long-ranged implications for the fermions. Their binding energies are reduced as the exchange interaction increases the average distance between two identical particles. The Pauli repulsion mechanism is therefore in competition with the binding mechanism due to the interaction with the bosons. While all of these phenomena are fundamental to atomic and molecular physics, to the best of our knowledge, the impact of this fermionic principle on the force-intermediating bosons (such as mesons for nuclear forces or photons for electromagnetic forces) has not received a lot of attention.

In order to be able to focus solely on the effect of the Pauli mechanism, we compare two simple models of distinguishable and indistinguishable particles, where all parameters as well as the chosen interaction with the bosons are kept identical for both systems. We will first confirm the expected impact on the energy and the spatial distribution of the fermions in the ground state and then apply this model to obtain some new insight on the role of the bosons.

Let us first discuss some technical details of the two model systems and then proceed to the results. The (1+1)-dimensional Yukawa-like interaction [8,9] of the fermions with the bosons is given by the energy $V = \lambda \int dx\, [\, \Psi_b^\dagger(x)\, \gamma^0\, \Psi_b(x) + \Psi_d^\dagger(x)\, \gamma^0\, \Psi_d(x)]\, \phi(x)$, where the parameter λ is the coupling strength, Ψ_b and Ψ_d are the two-component Dirac field operators for the protons (b) and neutrons (d) and ϕ denotes the scalar boson operator. For the special case of massless bosons this system could also be viewed as a simplified model to explore QED interactions, where the "photon" has spin zero [10]. The three field operators can be expanded in terms of annihilation and creation operators that fulfill the usual anti-commutator and commutator relationships $[b(p), b^\dagger(p')]_+ = [d(p), d^\dagger(p')]_+ = [a(p), a^\dagger(p')]_- = \delta(p-p')$ and $[b(p), d(p')]_- = [b(p), d^\dagger(p')]_- = 0$. For coupling strengths λ that are not exceedingly large, such that anti-fermions can be neglected, the corresponding Hamiltonian for the distinguishable particles (called below loosely "proton-neutron") takes the form $H = H_0 + V$ with

$$H_0 = \int dp\, e(p)\, [b^\dagger(p)b(p) + d^\dagger(p)d(p)] + \int dk\, \omega(k)\, a^\dagger(k)a(k) \qquad (1a)$$

$$V = \lambda \int dp \int dk\, \Gamma(p,k)\, [b^\dagger(p+k)b(p) + d^\dagger(p+k)d(p)]\, [a(k) + a^\dagger(-k)] \qquad (1b)$$

The coupling function $\Gamma(p,k) \equiv [e(p+k)e(p)+M^2c^4-p(p+k)c^2]^{1/2}\, [8\pi\omega(k)e(p+k)e(p)]^{-1/2}$ is the result of the scalar product among the Dirac spinors and acts as a natural cut-off function as it decreases with increasing fermion and boson momenta p and k. Here M and m denote the the fermions' and bosons' masses. For the indistinguishable fermions (called loosely "proton-proton"), we omit the operator d(p) and the model Hamiltonian can be written as

$$H_0 = \int dp\, e(p)\, b^\dagger(p)b(p) + \int dk\, \omega(k)\, a^\dagger(k)a(k) \qquad (1c)$$

$$V = \lambda \int dp \int dk\, \Gamma(p,k)\, b^\dagger(p+k)b(p)\, [a(k) + a^\dagger(-k)] \qquad (1d)$$

Note that in atomic units (c=137.036 a.u.) the free energies of the fermions and bosons are given by

$e(p) \equiv (M^2c^4+c^2p^2)^{1/2}$ and $\omega(k) \equiv (m^2c^4+c^2k^2)^{1/2}$, respectively.

The system becomes computationally accessible if we represent the states on a discretized spatial grid of total length L such that all creation and annihilation operators and the Hamiltonian H can then be represented by a matrix. In order to preserve the operator algebra, we have defined the dimensionless discretized operators $b_p \equiv (2\pi/L)^{1/2}\, b(p\, \Delta p)$, which satisfy $[b_p, b_{p'}^{\dagger}]_+ = [d_p, d_{p'}^{\dagger}]_+ = [a_p,a_{p'}^{\dagger}]_- = \delta_{p,p'}$ based on the Kronecker symbol. The same parameter $\Delta p \equiv (2\pi/L)$ corresponds to the spacing between the momentum modes of the bosons as well as the fermions. The matrix elements for the Hamiltonian related to the distinguishable particle system in the chosen basis are given by

$$\langle p,q \mid H \mid p',q'\rangle = (e_p + e_q)\, \delta_{p,p'}\, \delta_{q,q'} \qquad (2a)$$

$$\langle p,q;k \mid H \mid p',q';k'\rangle = (e_p + e_q + \omega_k)\, \delta_{p,p'}\, \delta_{q,q'}\, \delta_{k,k'} \qquad (2b)$$

$$\langle p,q \mid H \mid p',q';k'\rangle = \kappa\, \Gamma(p',k')\, [\delta_{p,p'+k'}\, \delta_{q,q'} + \delta_{q,q'+k'}\, \delta_{p,p'}] \qquad (2c)$$

where the $\kappa \equiv \lambda\, (2\pi/L)^{1/2}$ appears as an effective coupling constant and p, q and k denote integers.

For the proton-proton case, the Hilbert space is different as $| p,q\rangle = -| q,p\rangle$ and the Pauli principle forbids the two particles to occupy the same state. To avoid overcounting, we have to restrict the basis states $|p,q\rangle$ and $|p,q; k\rangle$ to fulfill $p<q$. The matrix elements for the Hamiltonian take the form

$$\langle p,q \mid H \mid p',q'\rangle = (e_p + e_q)\, \delta_{p,p'}\delta_{q,q'} \qquad (2d)$$

$$\langle p,q;k \mid H \mid p',q';k'\rangle = (e_p + e_q + \omega_k)\, \delta_{p,p'}\, \delta_{q,q'}\, \delta_{k,k'} \qquad (2e)$$

$$\langle p,q \mid H \mid p',q';k'\rangle = \kappa\, \Gamma(p',k')\, [\delta_{p,p'+k'}\, \delta_{q,q'} + \delta_{p,p'}\, \delta_{q,q'+k'} + \delta_{p,q'}\, \delta_{q,\, p'+k'} + \delta_{p,\, q'+k'}\, \delta_{q,p'}] \qquad (2f)$$

The states are dimensionless, i.e. $\langle p,q;k| p',q';k'\rangle = \delta_{p,p'}\, \delta_{q,q'}\, \delta_{k,k'}$ and the scalar products correspond to summations. The size of the Hilbert space can be controlled by the number of permitted states and by the largest possible momentum (denoted by P_{max}) on our grid. Both numbers were chosen sufficiently large in each simulation to have fully converged results. Due to the translation invariance of the interaction V, states with different total momentum P_{tot} are not coupled with each other and the operator ∫ dp p [$b^\dagger(p)b(p) + d^\dagger(p)d(p) + a^\dagger(p)a(p)$] is conserved in time.

Let us now proceed to our results. As a first step we have to calculate the energy $E_g(2)$ of the lowest energetic state for the two fermions for both systems. In order to remove the effect of the unavoidable single-fermion dressing due to the bosons (renormalization), we subtract from $E_g(2)$ twice the lowest energy of the corresponding one-fermion sector, denoted by $E_g(1)$. The binding energy is therefore defined here [11] by the energy difference as $E_b \equiv E_g(2) - 2\ E_g(1)$. If the interaction with the bosons lowers the energy of the two-fermion ground state from $2Mc^2$ by a larger amount than that of the single-fermion ground state, then E_b is negative and the two (boson-dressed) fermions effectively attract each other.

The calculation of the numerical values for $E_g(1)$ and $E_g(2)$ is actually non-trivial. By using a momentum mode spacing of $\Delta p = 2\pi/40$ and the largest momentum P_{max} = 3500 a.u. (corresponding to a Hilbert space of dimension 40,002) we obtained for a coupling strength of λ=7000 a.u. the energy $E_g(1)$ = 18736.5267 a.u. This means that the interaction lowers the unperturbed single fermion energy by $Mc^2 - E_g(1)$ = 42.3386 a.u., which is 0.225% of Mc^2. The coresponding gigantic size of the Hilbert space for the two-fermion sector (about 3,893,087 states) would make the calculation for $E_g(2)$ not feasible. However, fortunately, it turns out that while bosons of large momentum are required to describe the boson-dressing of the single and two-fermion system accurately, the impact on the energy shifts due to the bosons with large momentum is essentially identical. Therefore only bosons with smaller momentum contribute to the energy difference $E_g(2) - 2E_g(1)$. It is therefore possible to calculate E_b for a (numerically feasible) Hilbert space based on only small momentum bosons. We have systematically varied the two numerical parameters Δp as well as P_{max} and found that the binding energies are converged within an uncertainty of less than 3%. This required the diagonalization of a non-sparse 196,412×196,412 dimensional matrix, which takes a CPU time of about 90 hours on a super computer cluster with 400 processors. We obtained E_b= -15.6484 a.u. for the proton-neutron system, while the Pauli exclusion principle decreases the binding strength $|E_b|$ for the proton-proton system to E_b = -12.0597 a.u.

This reduction confirms that the Pauli principle can be interpreted (at least locally) as an effective repulsive force [7]. This "Pauli-force" would be in competition with the attractive binding mechanism due to the interaction with the bosons. This also suggests that the force intermediating bosons play a dual role. In the absence of any coupling (λ=0) the ground state energy of the two-fermion sector is $2Mc^2$ for both the proton-proton and proton-neutron system. Therefore the Pauli exclusion principle has no direct energetic implication. Only the interaction with the bosons uncovers any energetic signature of the indistinguishability of the fermions.

Next we analyze the ground states also from a spatially resolved perspective. In Figure 1 we show the spatial distribution $\rho(r)$ of the fermions as a function of the relative position r between the two fermions. Due to the translational invariance of the state with $P_{tot} = 0$, it is sufficient to freeze the location of one particle at z_1=0 and define the relative position r as $r \equiv z_2 - z_1$. Therefore, $\rho(r)$ is determined from the expectation value of the spatial creation and annihilation operators

$$\rho_{p\text{-}n}(r) \equiv \langle b^\dagger(r)\, d^\dagger(0)\, d(0)\, b(r)\rangle = |\Sigma_p\, \phi_1(p)\, e^{ipr}\,|^2 + \Sigma_k\, |\, \Sigma_p\, \phi_2(p;k)\, e^{ipr}|^2 \qquad (3a)$$

for the proton-neutron system. The spatial operators b(r) and d(r) are computed as the Fourier transform of b(p) and d(p). Here $\phi_1(p)$ and $\phi_2(p;k)$ denote the real ground state momentum amplitudes in the expansion $|gs\rangle = \Sigma_p\, \phi_1(p)\, |\text{-}p,p\rangle + \Sigma_p\, \Sigma_k\, \phi_2(p;k)\, |\text{-}p\text{-}k,p;k\rangle$ for the proton-neutron system.

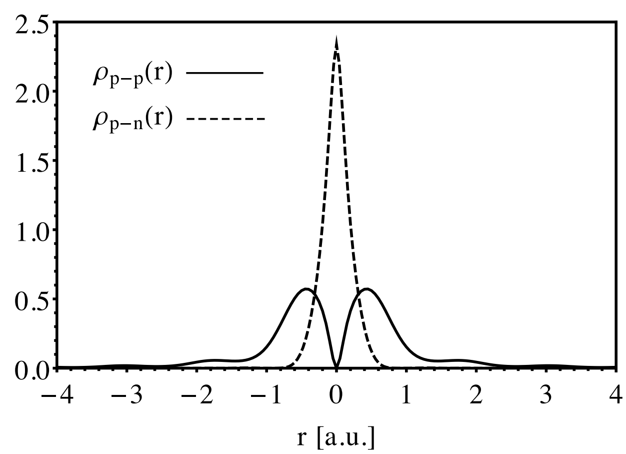

Figure 1 The distribution of the two fermions $\rho(r)$ as a function of their separation $r \equiv z_2\text{-}z_1$ in the lowest bound state in the two fermion sector. The other parameters are λ=7000 a.u., $\Delta p=2\pi/L$ with L=40 a.u. and $P_{max} = 600\Delta p$. The masses of the particles are M=1.0 a.u. and m=0.1 a.u.

For the indistinguishable particles (proton-proton), the corresponding distribution is given by

$$\rho_{p\text{-}p}(r) \equiv \langle\, b^\dagger(r)\, b^\dagger(0)\, b(0)\, b(r)\,\rangle$$
$$= |\Sigma_{p>0}\, \psi_1(p)\, (e^{ipr} - e^{-ipr})|^2 + \Sigma_k\, |\Sigma_{p>-k/2}\, \psi_2(p;k)\, (e^{ipr} - e^{-i(p+k)r})|^2 \qquad (3b)$$

Here $\psi_1(p)$ and $\psi_2(p;k)$ denote the real ground state momentum amplitudes in the expansion $|gs\rangle = \Sigma_{p>0}\, \psi_1(p)\, |-p,p\rangle + \Sigma_k\, \Sigma_{p>-k/2}\, \psi_2(p;k)\, |-p-k,p;k\rangle$ for the proton-proton system.

One could expect that due to the locality of the Pauli exclusion principle the difference between the ground states for distinguishable and indistinguishable particle systems might occur only for those positions that are identical to each other, i.e. for r equal to zero. However, we see a significant differences even in the overall spatial structures of the proton-proton and proton-neutron systems. In fact, the density for the proton-proton system is significantly lowered in an entire *region* around r=0. This is a clear indication that due to the bosonic interaction the Pauli principle can be indeed interpreted as an effectively repulsive force with a finite range whose action is not solely constrained to those locations where the particles are exactly on top of each other. For larger coupling strengths the separation between the two maxima reduces, but the likelihood of finding two protons at the same location remains zero, i.e. $\rho_{p\text{-}p}(r=0) = 0$.

In direct contrast, the Yukawa interaction makes the simultaneous occupation of the same position state most likely for the proton-neutron system, i.e., the density $\rho_{p\text{-}n}(r)$ takes its maximum at r=0. The difference between the zero and maximum density at r=0 can be tracked back to different terms in the analytical expressions for $\rho_{p\text{-}p}(r)$ and $\rho_{p\text{-}n}(r)$ in Eqs. (3).

As one might expect, the proton-proton bound state is less binding and has indeed a significantly wider spatial distribution reflecting a larger average separation of the two protons than the one for the proton-neutron case.

While the Pauli exclusion principle induced widening of the ground state is qualitatively expected, the model permits us also to enter a new territory: to examine the properties of the bosons in the ground state. While the interaction term with the bosons in the two Hamiltonians leads to an identical single-fermion dressing, the resulting impact of the bosons on two fermions in the ground state is apparently different. We will now show that this has also significant implications for the spatial distribution $\chi(z)$ of the force-mediating bosons. We examine the distributions of the bosons in the ground state and fix the positions of the two fermions z_1 and z_2. For the proton-neutron system, the density $\chi_{p\text{-}n}(z)$ can be calculated as

$$\chi_{p\text{-}n}(z) = \langle b^{\dagger}(z_1)\, d^{\dagger}(z_2)\, d(z_2)\, b(z_1)\, a^{\dagger}(z)\, a(z)\rangle$$
$$= |\Sigma_{k}\text{-}\Sigma_p\, e^{ipz_1}\, e^{-i(p+k)z_2}\, e^{ikz}\, \phi_2(p;k)|^2 \qquad (4a)$$

while the corresponding distribution for proton-proton system is given by

$$\chi_{p\text{-}p}(z) = \langle\, b^{\dagger}(z_1)\, b^{\dagger}(z_2)\, b(z_2)\, b(z_1)\, a^{\dagger}(z)\, a(z)\,\rangle$$
$$= |\Sigma_{k}\text{-}\Sigma_{p>-k/2}\, (e^{-i(p+k)z_1}\, e^{ipz_2} - e^{-i(p+k)z_2}\, e^{ipz_1})\, e^{ikz}\, \psi_2(p;k)|^2 \qquad (4b)$$

For the data displayed in Figure 2, we have assumed that the two fermions are at locations z_1=–0.75 a.u and z_2=0.75 a.u., respectively.

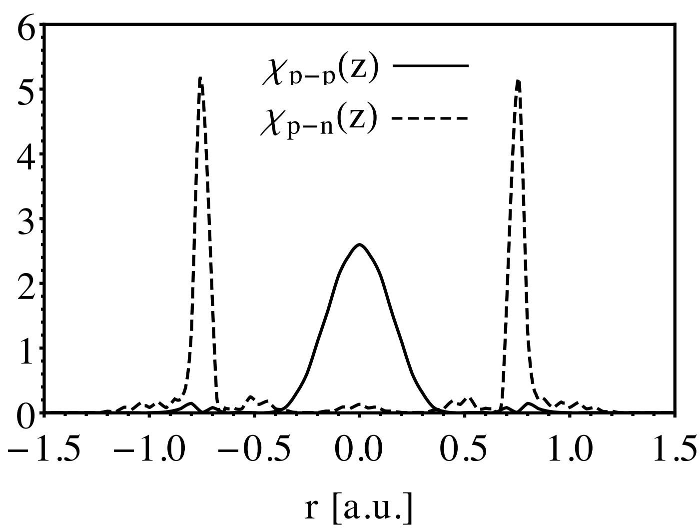

Figure 2 The bosons' spatial distribution $\chi(z)$ in the ground state. The two fermions assumed to be at locations z_1=–0.75 a.u. and z_2 =+0.75 a.u. corresponding to r = 1.5 a.u. in Figure 1. The other parameters are the same as in Figure 1.

We can see that the bosonic distributions for the distinguishable and indistinguishable-particle systems are fundamentally different. The proton-neutron system, $\chi_{p\text{-}n}(z)$ has two symmetric peaks at z=±0.75 a.u., which means that the bosons are mainly accumulated around the two fermions. The rather symmetric structure of $\chi_{p\text{-}n}(z)$ around z=±0.75 a.u., suggests that the presence of the one fermion does not affect the boson-dressing of the other particle. In fact, the distribution is very similar to the single-particle dressing [12]. In contrast, the bosonic distribution $\chi_{p\text{-}p}(z)$ for proton-proton interaction reveals a large likelihood between the two fermions.

Last, we will consider if the different spatial structures of the binding bosons have also implications for their momentum distributions S(k), which can be computed from the expectation value of the bosonic particle number operator $a^{\dagger}(k)a(k)$ in the ground state.

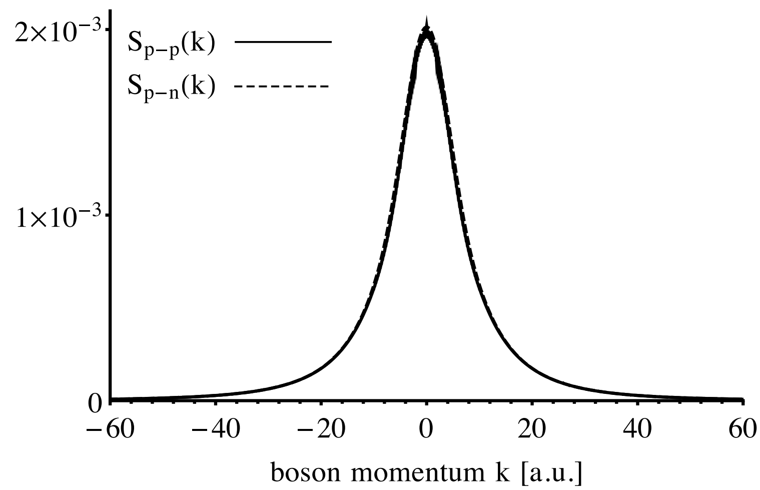

Figure 3 The momentum spectrum of the bosons in the ground state of the two different model systems. The other parameters are the same as in Figure 1.

For the ground state of the proton-neutron and proton-proton system we obtain

$$S_{p\text{-}n}(k) = \langle\, a^{\dagger}(k)\, a(k)\, \rangle = \Sigma_p |\, \phi_2(p;\, k)|^2 \tag{5a}$$

$$S_{p\text{-}p}(k) = \langle a^{\dagger}(k)\, a(k)\rangle = \Sigma_{p>-k/2}\, |\psi_2(p;\, k)|^2 \tag{5b}$$

Note that while the final expressions for $S_{p\text{-}p}(k)$ and $S_{p\text{-}n}(k)$ are functionally similar, they still reflect the different properties of the systems as the Hilbert spaces and the amplitudes ϕ_2 and ψ_2 are different.

The momentum distributions of the bosons graphed in Figure 3 are remarkably similar, with an area of about 0.037. In contrast to their entirely different spatial distributions, the momentum distributions for the distinguishable and indistinguishable particle systems both take a single maximum at the center k=0. Furthermore, only bosons with relatively small momentum (<45 a.u.)

are required for the binding. This is consistent with the monotonically decreasing coupling function Γ(p,k), which favors the fermion-boson interaction for lower energetic bosons and confirms that only bosons with small momentum contribute to the binding energy for both systems.

In summary, we have proposed a numerical approach to calculate bound states in the framework of quantum field theory. As expected, this method confirms that the binding energy $|E_b|$ of the distinguishable particle system is larger than the one for indistinguishable particle system as the Pauli exclusion principle acts as an effective repulsion force. This indistinguishability can not only reduce the binding of the system but also leads to a significant widening of the spatial distribution of the fermions in the ground state. Most remarkably, the fermionic Pauli-principle leads to fundamentally different spatial distributions of the force-intermediating bosons.

In contrast to the boson-induced binding mechanism whose strength depends on the coupling λ, the magnitude of the symmetry-based Pauli repulsion might be independent of λ. One could therefore conjecture that there might be a certain threshold coupling strength, below which the Pauli repulsion dominates and the two fermions cannot even form a discrete bound state, manifest by an E_b that is positive. Preliminary data suggest that for small λ, E_b can become positive for the proton-proton system, while E_b for the proton-neutron system remains negative. However, in this limit the physical extension of the bound state is very large and can become comparable to the size of the finite numerical box, which makes the binding energy also depend on our numerical box length [13].

On the more macroscopic (and non-quantum) level the action of the dynamical force intermediating bosons is usually approximated by classical force-fields, given by the Yukawa or Coulomb law. However, here these inter-particle forces are assumed to have exactly the same position-dependence, independent of whether the two fermions are indistinguishable or not. This is certainly quite different from our quantum field theoretical description where we have seen that the position dependence of the binding bosons depends crucially on the exchange symmetries of the fermions. In our opinion, it remains a future challenge to better understand how the bosonic distributions are related to the traditional force fields in the classical limit. It suggests that the observed transfer of the fermionic Pauli exclusion principle onto the bosons is likely an intrinsically quantum field theoretical effect without any classical mechanical counterpart.

Acknowledgements

QZL would like to thank ILP for the nice hospitality during his visit to Illinois State. We acknowledge helpful discusions with S. Dong. This work has been supported by the NSF and the NSFC (#11529402).

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