A Tonks Giradeau Gas in the Presence of a Local Potential

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(Dated: Jan 08 2006)

Abstract

The physics of a Tonks-Giradeau Gas in the presence of a local potential is studied. In order to evaluate the single particle density matrix (SPDM) of the many-body ground state, the Wiger-Jordan transformation is used. The eigenvector with the largest eigenvalue of the SPDM corresponds to the ”Bose-Einstein Condensate” (BEC) State. We find that the ”BEC” state density at the position of the local potential decreases, as expected, in the case of a repulsive potential. For an attractive potential, it decreases or increases depending on the strength of the potential. The superfluidity of this system is investigated both numerically and perturbatively. An experimental method for detecting the effect of an impurity in a Tonks-Giradueau gas is discussed.
I. INTRODUCTION

The effect of impurity and disorder on many body system has been one of the main themes of condensed matter physics[1]. It plays an important role in our understanding of phenomena such as superconductivity, superfluidity, and Kondo physics. The rapid progress in ultra-cold atom experiments provides a unique platform for the study of such many-body systems. In these experiments, the external potential, the dimensionality, and the interaction can be tuned using external fields. Fascinating many body phenomena have already been realized in experiments [2], including recent realization of a Tonks-Girardeau Gas [3].

A natural extension of this line of research is the study of the effect of impurities in these many body systems, both theoretically [7], and experimentally [8]. Here we study the Tonks-Girardeau gas in the presence of a local potential. A Tonks-Giradeau gas is a quantum gas consisting of hard core bosons. This system can be mapped to a free fermion system, allowing for an exact solution. The study of the effect of an impurity on such an exactly solvable system serves two purposes: first, it shows, in its simplest form, the interplay between interaction, superfluidity, and impurity. Second, the theoretical predictions can be compared readily with experimental observables.

II. MODEL OF THE TONKS-GIRARDEAU GAS WITH AN IMPURITY

The Hamiltonian we use to describe such a system is of the tight binding type

$$H = t \sum_i \left( a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \right) + u a_0^\dagger a_0$$

(1)

where $a_i^\dagger$ and $a_i$ are the bosonic operators that create and annihilate a particle at site $i$, respectively. They obey the commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$. The particle interaction is included by imposing $a_i^2 = (a_i^\dagger)^2 = 0$. The quantity $t$, which is generally negative, is the hopping amplitude between nearest neighbors and $u$ characterizes the local potential strength at site zero. The behavior of the many body system is determined by the ratio of $u/t$. When $|u/t| < 1$, the kinetic parts dominate and the particles distribute uniformly to lower the kinetic energy. On the other hand, when $|u/t| > 1$, the local potential becomes important. In this regime, local charge fluctuations are suppressed and the coherence among particles is degraded. This degradation is a main interest of this paper. We numerically
evaluate the SPDM of the many-body ground state, and compute the effect of a local potential (impurity) on the spectrum of the sSPDM, on the ”BEC” wavefunction, and on the superfluidity of the many-body ground state.

In order to solve for the ground state of the system, the Hamiltonian (1) can be mapped to an non-interacting fermion Hamiltonian via the Wigner-Jordan Transformation

\[ a_i = \prod_{\alpha=1}^{i-1} e^{i\pi c_\alpha^\dagger c_\alpha} c_i, \quad a_i^\dagger = \prod_{\alpha=1}^{i-1} e^{-i\pi c_\alpha^\dagger c_\alpha} \]

Here the \( c_i^\dagger \) and \( c_i \) are fermionic operators, which satisfy the anticommunication relation \( \{c_i, c_j^\dagger\} = \delta_{ij} \). Under this transformation, it is straightforward to show that the Hamiltonian[1] can be written in the following form

\[ H = t \sum_i \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + uc_0^\dagger c_0 \]

The ground state \(|G_F\rangle\) of this Hamiltonian corresponds to the well-known Fermi sea, in which fermions fill the single particle levels up to the Fermi surface. The corresponding ground state \(|G_B\rangle\) of the boson Hamiltonian (1) can be obtained from \(|G_F\rangle\) by symmetrizing the corresponding many body fermionic wave function.

III. CONDENSATE FRACTION AND CONDENSATE WAVEFUNCTION

We seek the one particle density matrix [9], which is the expectation value of \( a_i^\dagger a_j \) in the ground state.

\[ \rho_{ij} = \langle G_B | a_i^\dagger a_j | G_B \rangle = \langle G_F | c_i^\dagger \prod_{\alpha=1}^{i-1} e^{-i\pi c_\alpha^\dagger c_\alpha} \prod_{\alpha=1}^{j-1} e^{i\pi c_\alpha^\dagger c_\alpha} c_j | G_F \rangle \]

The diagonal part of the density matrix, \( \rho_{ii} \), gives the density \( \langle n_i \rangle = \langle G_B | a_i^\dagger a_i | G_B \rangle \) at site \( i \), while the off diagonal part gives the coherence in the many body ground state for different sites. In the uniform case, the coherence \( \rho_{ij} \) depends only on the difference, \(|i - j|\). In the presence of a local potential, however, the coherence depends on both \( i \) and \( j \) separately. In addition to that, \( \rho_{ij} \) is much smaller than its uniform counterpart when \( i \) and \( j \) are on different sides of the local potential. Diagonalizing the density matrix gives a set of eigenvectors corresponding to the reduced one-particle states. The corresponding
eigenvalues represent the occupation probability for the corresponding reduced one particle states. The one with a significant large eigenvalue is the "BEC" State [9] (Note that in 1D, there should be no Bose Einstein Condensation in the thermodynamical limit. In the particular case of the Tonks-Girardeau case, the particles that condense into a single state are calculated to be order of $\sqrt{N}$ [4]. However, this state, compared with other states, is the only state that is significantly occupied. With this clarification, we will call that state the BEC state and the corresponding occupation the condensate fraction).

The evaluation of this density matrix is not simple even when the ground state is known. Here we adopt the technique developed by M. Rigol and A. Muramatsu [6]. This method allows us to calculate a system with up to a thousand lattice sites. We focus on the low occupation limit only, which corresponds to a continuum case. We have verified that 9 particles in 100 lattice sites already converges very well to the continuum case. In the following calculation, unless otherwise stated, all the calculations are based on a system of 9 particles in one dimensional lattice of 100 sites, with an impurity located at site zero. Periodic boundary condition is imposed on this one dimensional chain.

Since all the physics is determined by the ratio $u/t$, in the following numerical calculations, we fix $t = -1$ and vary $u$. Fig [1a] shows single particle density matrix spectrum for different $u$’s. The significant peak corresponds to the BEC state occupation or condensate fraction. The introduction of an impurity lowers the condensate fraction, as shown in Fig [1b]. The attractive and repulsive potentials almost equally deplete the condensate fraction for small impurity potential $u$, with the attractive potential having a slightly larger effect. The physics that gives rise to this behavior, as is shown in the following, is that an attractive local potential has a stronger effect on decreasing the coherence between particles.

Since only the BEC state is significantly occupied, the BEC state determines the most important features of the many-body system. It would be useful to look at the BEC wavefunction itself (see figure [2a]). For a repulsive local potential, we find that the BEC density decreases near the impurity. In the case of an attractive potential, for $u > -1$, there is an increase in the probability of the BEC density at the impurity site. For the case of $u < -1$, in contrast to what one might expect, there is a decrease of the BEC density at the impurity site. This feature actually arises from the competition between two effects: the single particle effect, i.e. the potential attracts particles, and the many body effect, i.e. the imp-
FIG. 1: (a) shows the SPDM spectrum at different local potential strength $u$. Here we have normalized the population to be one. One of the reduced one-particle states is overwhelmingly occupied comparing with all the others, and it is identified as the BEC state. We show only part of spectrum and omitting parts which are negligibly small. (b) shows the condensate fraction as a function of the local potential strength. The attractive potential is seen to have a slightly larger effect in decrease the condensate fraction.

Purity decreases the coherence among particles. We have also included the particle density plot in Fig [2b]. It shows an increase of particle density for any attractive potential. For the BEC density, we see that, for each attractive potential, there is a peak at the impurity site corresponding to the local bound state. However, due to the lack of coherence between bound and extended states, the bound state is less likely to participate the BEC state, which
results in a overall decrease of the BEC density at site zero compared with the uniform case. This is the main observation of this paper. To be more specific on how the impurity decreases the coherence among particles, we plot some of the relevant off-diagonal elements of the single particle density matrix (see Fig [3]) In particular, we take the coherence between an arbitrary site and the fifth site next to the local potential site zero as an example. We find that, given the same distance, the coherence between particles on different sides of the impurity is much smaller than that of the particles located on the same side of the impurity. For the same magnitude of the attractive and repulsive potential, we find that the effect of the attractive and repulsive potential are roughly the same, with the attractive one having a stronger effect in decreasing the overall coherence among particles. This actually explains the fact the attractive potential has a stronger effect on decreasing the condensate fraction. The only place that the attractive potential resulting in a large coherence than the repulsive one with the same magnitude is near the impurity site. This is due to the presence of a local bound state, which effectively increase the probability of finding particles at the impurity site. This bound state is well known [10] in the tight binding Hamiltonian. Its eigenenergy is $E = -\sqrt{u^2 + 4t^2}$ and its wavefunction localizes in space as $\exp[-\alpha(E)|n|]$ with $n$ being the site number and

$$\alpha(E) = -\ln \left[ \frac{E}{2t} - \sqrt{\frac{E^2}{4t^2} - 1} \right]$$

corresponds to the inverse of the characteristic length. The nice overlap of the coherence peak and the bound state wavefunction verifies our argument for the increase of coherence in the vicinity of impurity. The small peak in the impurity site is purely a single particle effect.

With the picture of the impurity introducing decoherence, one would suggest that in higher dimensions, since the impurity has a weaker effect in decreasing coherence among particles, a smaller effect of the impurity should be found. We have verified this point numerically by extending our calculation to two dimensions The condensate fraction is shown in Fig[4]. At dimensions greater than one, there is no simple mapping from bosons to fermions. An exact diagonalization has been done for this case which limits the calculation to a system of five particles in a three by three lattice.
FIG. 2: (a) The BEC wavefunctions for different strengths of the local potential are shown. In the special case of $u=0$, the BEC wavefunction is constant all over the lattice. Note that the BEC wavefunction corresponding to $u = -1$ has a lower value at the impurity site comparing with the $u = 0$ uniform case. (b) The particle density is shown with respect to lattice sites for different $u$’s. Here we see for attractive $u$, the particle density at the impurity site is always larger than that of the uniform case.

IV. SUPERFLUIDITY

It is well known that BEC is neither necessary nor sufficient for the existence of a superfluid. As mentioned by Lieb and Sieringer[5], a particular example is the Tonks-Girardeau gas. Even it does not Bose condense, the system without impurity actually exhibits super-
FIG. 3: The off diagonal SPDM elements that measure the coherence between lattice sites \(-5\) and any arbitrary lattice sites is plotted for \(u=-1\) and \(u=1\), respectively. The coherence with the negative sites are relatively larger than the coherence with the positive sites. The smaller peak of the coherence for the attractive potential between any sites and the sites zero can be explained by the increase of the density at impurity site, due to the presence of a bound state. The bound state wavefunction is plotted and it coincides well with the peak of the coherence in the impurity site.

fluidity. It is interesting to investigate how the superfluidity is decreased in the presence of an impurity. We emphasize that we use the word superfluidity strictly in the sense of the following phenomenological definition

\[
\frac{E(v)}{N} - \frac{E(0)}{N} = \frac{1}{2} f_s m v^2 + O(v^4)
\]
FIG. 4: This figure shows the condensate fraction in a three by three lattice with an impurity located in the center. The impurity is characterized by a local potential strength $u$. The total single particle density spectrum is normalized to one. We see that in two dimensions, the condensate fraction is larger than its one-dimensional counterpart. Moreover, the relative change of the condensate fraction due to the presence of the local potential is much smaller than the one-dimensional case.

where $E(v)$ is the ground state energy of the many-body system in the presence of a perturbative velocity field $v$, $f_s$ is the superfluid fraction, and $m$ is the mass of the particle. The velocity field is introduced by imposing a twisted boundary condition [5], which amounts to a phase jump $e^{i\varphi}$, $\varphi = \frac{vLm}{\hbar}$ whenever the wave function passes through the boundary. We restrict $\varphi < \pi$ to yield a single valued function. Note that since the definition is based only on the static properties of the many-body system, it can tell us only whether the ground
state has the property of superfluidity, and it cannot predict the stability of the superfluidity.

The result of numerical calculations is shown in Fig [5]. We see that without impurity, the system exhibits superfluidity with superfluid fraction close to unity. The degree of degradation on the superfluid fraction produced by impurity depends on both the local impurity strength and the size of the system. In a large system, the superfluidity drops sharply with the presence of the local impurity. Note that as far as the spectrum is concerned, the fermi ground state is equivalent to the boson ground state. This allows an understanding of the superfluidity in a single particle picture. As the lattice size increase, the particle kinetic energy goes like $\frac{1}{L^2}$ while the local potential energy goes like $\frac{1}{L}$. Therefore, in the limiting case of large $L$, the local potential always dominates the kinetic energy. For a repulsive potential, the particle has to hop through the barrier. For an attractive potential, since the local bound state is always occupied, for hard core bosons, in order to get through this potential, a potential barrier of order $\frac{1}{L}$ is also present, which gives rise to the sharp drop of superfluidity in the presence of a local potential.

This problem can be understood quantitatively by considering the following single particle model $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + g\delta(x)$, with $x$ defined in the regime $[-L, L]$ with the twisted boundary condition. As an example, we consider only two states with energy close to $\frac{\hbar^2}{2mL}$ and $\frac{\hbar^2}{2mL^2}$. To calculate the eigenenergy with different boundary condition is elementary. It is just the one dimensional piecewise potential problem. The modification of eigenenergy due to the presence of the velocity field is $[E(v) - E(0)]/2 = \frac{1}{2}mv^2 (1 - 0.008g^2L^2)$ [11] in the perturbative limit that $gL$ is small. This result shows that the superfluid fraction is $f_s = 1 - 0.008g^2L^2$. There is no modification to first order in $gL$, which is consistent with discussions concerning repulsive and attractive potentials.

V. DISCUSSION AND CONCLUSION

The effect of an impurity on the Tonks-Girardeau Gas can be studied in an experiment using an optical lattice. The local potential we model here may be realized in an experiment by introducing a laser beam, an impurity atom, or an ion at a particular lattice site. The real space density distribution will be the same as the free fermion in the presence of a local potential, which contains only information on the diagonal part of the density matrix. The non-trivial part of the density matrix, the off diagonal coherence, can be detected by
FIG. 5: Superfluid fraction is plotted as a function of different local potential strength $u$. The case of nine particle occupying 100 and 200 lattice sites are shown. The larger the system, the sharper the superfluid peak is found.

measuring the momentum distribution, defined as

$$n(k) = \frac{1}{N} \sum_{m,n=-N/2}^{N/2} \rho_{mn} e^{i(m-n)k}$$

We have ignored the localized Wannier function profile.

In figure [6] we show peak value density in momentum space for different impurity strengths. The highest momentum density peak corresponds to the case with no impurity. The attractive potential has a larger effect on the broadening compared with the repulsive one. The superfluidity of the system can be measured by imposing a velocity field on the
FIG. 6: The peak value of the density distribution in the momentum space is shown. The maximum of zero momentum occupation is reached in the uniform case.

many-body system. This can be realized in the experiment by changing of the external potential with time. The measurement can be done by looking at the damping motion of the particles.

In summary, we have presented a numerical calculation of a Tonks-Girardeau Gas in the presence of a local potential. It is shown that the impurity decreases the occupation of condensate fraction. The BEC density at the local potential decreases in a strong attractive potential, as oppose to particle density, which always increases for attractive potentials. The superfluidity is also degraded by the impurity, the degradation scales like $g^2L^2$ in the small $gL$ limit. This effect of impurity on a many-body system can be measured by looking at the momentum distribution and the system response an external velocity field.
Acknowledgments

We would like to thank P. R. Berman for useful discussions and careful readings of the manuscript. HF would like to thank supports from NSF and FOCUS Grant. AR would like to thank supports from NSF and from the Research Corporation, Cotrell College Science Award.

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Note that in order to solve for the eigenenergy we come up with the following equation
\[ k \cos \varphi - k \cos(2kL) - \frac{2m \sin(2kL)}{\hbar^2} = 0 \]
with \( k = \sqrt{2mE/\hbar} \). We are looking for solution \( k \sim \frac{\pi}{L} \), this allows a expand in order of \( k - \frac{\pi}{L} \). This parameter converges slowly and it is found that one have to expand to \( (k - \frac{\pi}{L})^4 \) to yield reasonable result.