Paired states of interacting electrons in a two-dimensional lattice

D. Souza and F. Claro

Facultad de Física, Pontificia Universidad Católica de Chile, Casilla 306, Santiago 22, Chile

(Received 8 May 2010; revised manuscript received 28 October 2010; published 30 November 2010)

We show that two tight-binding electrons that repel may form a bounded pair in two dimensions. The paired states form a band with energies that scale like the strength of the interaction potential. By applying an electric field we show that the dynamics of such states is that of a composite particle of charge 2*e*. The system still sustains Bloch-type states so that if the two bands overlap single and paired states might coexist allowing for a bosonic fluid component that, if condensed, would decrease the resistance at low temperatures. The presence of two bands allows for new oscillations whose experimental detection would permit a direct measurement of the interaction potential strength.

I. INTRODUCTION

Bound states are normally associated with basins of attraction, and it is always surprising to find them in the presence of a repulsive interaction. The most remarkable case is the pairing of electrons in normal superconductors, mediated by lattice distortions. A new kind was recently observed for ultracold rubidium atoms in an optical lattice,[1] where the binding arises from pure quantum interference. The pairs were shown to be stable, thus suggesting that they might form a superfluid phase if the composite is a boson.

The effect was originally predicted for a one-dimensional string.[2–5] The eigenstates decay exponentially in the relative coordinate while in the center-of-mass coordinate they are extended over the whole lattice. In higher dimensions one can argue that paired states may exist as well. To see this, consider two particles that repel moving in a two-dimensional (2D) lattice. Together, the pair combine four spatial degrees of freedom, thus allowing that it be formally described as a single particle moving in a four-dimensional (4D) lattice. A particle-particle interaction appears then as an interface potential in four dimensions, which decays to both sides of the hyperplane $x_1 = x_2$ and $y_1 = y_2$, where (x_1, y_1) and (x_2, y_2) are Cartesian coordinates for the particles position in real 2D space. Surface states bounded to the interface are then expected even if the potential locally rises, as would occur under particle-particle repulsion. Since the interface represents matching coordinates for the two particles in 2D such surface states are paired states in the lattice. A similar argument applies in three dimensions.

We find the 2D case particularly interesting since the onset of pairing could be relevant to high-temperature superconductors where transport is related to conducting sheets, and to certain 2D experimental probes for which the physics is still controversial.[6–16] It is believed that in the latter case localization due to disorder on the conducting sheet should produce a divergent resistivity as the temperature is lowered but this behavior was not observed at all electron densities in metal-oxide-semiconductor field-effect transistors. In fact, a metal-insulator transition was found in low-density 2D samples as the density is slightly increased.[8] An early prediction invoked the strongly interacting nature of a low-density electron fluid[9,10] while more recent theories study the effect of formation of a Wigner solid[13] or a superconducting phase,[14] a strong spin-orbit interaction,[15] and a few classical effects,[16] none of which has received consensus for describing the physics at the root of the transition.[17]

As we shall show, paired singlet states are predicted to exist in 2D for repelling particles in a lattice. In Sec. II we define the model and show that the density of states reveals the presence of two bands of different character, one corresponding to a Bloch particle in 4D and one describing a 2D surface state. In Sec. III we show that the dynamics of such surface state is that of a composite boson of charge 2*e*, our main finding, and in Sec. IV we discuss our results.

II. MODEL

Consider for definiteness two interacting tight-binding electrons in 2D in a uniform external field. The associated Hamilton operator for such system reads,

$$
\begin{aligned}
H = \lambda \sum_{x,y} \sum_s \, & (c^\dagger_{x,y+1,s} c_{x,y,s} + c^\dagger_{x,y,s} c_{x,y+1,s} + c^\dagger_{x+1,y,s} c_{x,y,s} \\
& + c^\dagger_{x,y,s} c_{x+1,y,s}) + eEa \frac{\hat{n} \cdot \vec{R}}{\sqrt{2}} \sum_{x,y} \sum_s c^\dagger_{x,y,s} c_{x,y,s} \\
& + U \sum_{x,y} c^\dagger_{x,y,\uparrow} c_{x,y,\uparrow} c^\dagger_{x,y,\downarrow} c_{x,y,\downarrow},
\end{aligned}
\tag{1}
$$

where $c^\dagger_{x,y,s}$ and $c_{x,y,s}$ are the creation and annihilation operators for one electron located at the site (x, y) with spin $s = \uparrow, \downarrow$, λ the usual hopping energy parameter, $\vec{R}$ the sum of position vectors, e the charge of the electron, E and $\hat{n}$ the electric field magnitude and direction, respectively, and a the lattice parameter. The last term represents a two-body Hubbard contact-interaction potential U. We assume that the interaction is strongly screened and may be ignored for particle-particle separations beyond a lattice constant and discuss only the singlet state.[3]

In the Wannier representation, the time-dependent wave function for the pair in a singlet state may be expanded as

$$|\phi(t)\rangle = \sum_{x_1,y_1} \sum_{x_2,y_2} f_{x_1,y_1;x_2,y_2}(t)|x_1,y_1,s_1;x_2,y_2,s_2\rangle, \qquad (2)$$

where the sum runs over all lattice sites, $f_{x_1,y_1;x_2,y_2}(t)$ is the amplitude for an electron with spin s_1 to be at (x_1,y_1), and another with spin $s_2 \neq s_1$ to be at (x_2,y_2), while the ket $|x_1,y_1,s_1;x_2,y_2,s_2\rangle$ represents such state. The amplitude obeys the Schrödinger equation of motion,

$$i\hbar \frac{d}{dt} f_{x_1,y_1;x_2,y_2}$$

$$= -\lambda \tilde{f}_{x_1,y_1;x_2,y_2} + (eEaX + U\delta_{x_1,x_2}\delta_{y_1,y_2})f_{x_1,y_1;x_2,y_2}, \qquad (3)$$

where $\tilde{f}$ is the sum of amplitudes of all nearest neighbors to the site (x_1,y_1,x_2,y_2) in the lattice and $X = (x_1 + y_1 + x_2 + y_2)/\sqrt{2}$ in units of the lattice constant. We have assumed that the electric field is along the diagonal $x_1 = y_1$ and $x_2 = y_2$.

By making the replacement,

$$f_{x_1,y_1;x_2,y_2} = e^{ik_x(x_1+x_2)} e^{ik_y(y_1+y_2)} g(x_2-x_1, y_2-y_1),$$

the associated eigenvalue equation in the absence of an external field becomes

$$\begin{aligned} Eg(u,v) = &-2\lambda\{\cos k_x a[g(u-1,v)+g(u+1,v)] \\ &+\cos k_y a[g(u,v-1)+g(u,v+1)]\} \\ &+\delta_{u,0}\delta_{v,0}Ug(u,v), \end{aligned} \qquad (4)$$

where now $u = x_2 - x_1$ and $v = y_2 - y_1$. One can easily check that $g(u,v) = \delta_{u,0}\delta_{v,0}$ is an eigenvalue of this equation at the lowest band edge $k_x = 0 = k_y$, of eigenvalue $E = U$. This solution represents extreme pairing, when one particle is precisely on top of the other.

In the absence of interaction solutions of Eq. (4) are plane waves in a Bloch band, with eigenvalues $E = -4\lambda(\cos k_x a + \cos k_y a)$, where $\vec{k} = (k_x, k_y)$ is the center-of-mass wave number. The band remains when the repulsive interaction is turned on while additional states appear at positive energy. This is seen in Fig. 1, where the density of states obtained by numerical diagonalization of the eigenvalue equation for several positive values of the parameter U is shown. Data correspond to a finite lattice with $N = 49$ plaquettes using periodic boundary conditions. The bell shaped curve represents the density of states of a single particle in 4D, the analog problem in this case, while a 2D-like density-of-states profile representing surface states in 4D moves away as U grows. Note that the lower edge of this band is at $E = U$ as expected.

III. EVIDENCE FOR BOUNDED PAIRS

To confirm the presence of two different kinds of states, we have calculated the average distance between particles

$$d_j = a \sum_{x_1,x_2} \sum_{y_1,y_2} \sqrt{(x_1-x_2)^2 + (y_1-y_2)^2} |f^j_{x_1,y_1;x_2,y_2}|^2 \qquad (5)$$

on a finite 2D sample of N plaquettes using periodic boundary conditions. Here j labels the eigenstate considered. The results are shown in Fig. 2, where the quantity d_j is shown as
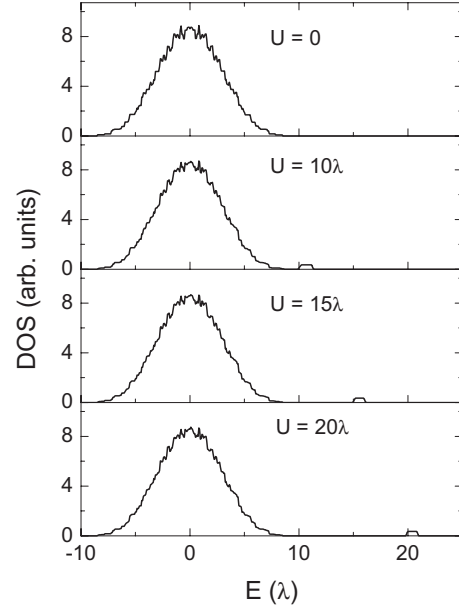

FIG. 1. Density of states of two interacting electrons in a 2D lattice of 49 sites. For $U = 0$, it is that of a single tight-binding particle in 4D. When $U \neq 0$ a new subband emerges, moving to higher energies as U is increased.

a function of sample size both for states in the B band as well as states in the U band. We see that the average separation of the particles is essentially null for states in the U band for all cell sizes, as is expected for a bounded pair. For states in the Bloch band the separation is finite with a value that grows linearly with $N^{1/2}$ as expected for extended states in two dimensions.

A more dramatic confirmation that repelling electrons in a lattice form bounded pairs is found when the electric field is turned on and the time evolution of a given initial state is followed by solving Eq. (3). It is well known that charged particles in a lattice experience Bloch oscillations in the presence of the field with a frequency proportional to the particle charge.[18] To find out if such oscillations are present we stud-
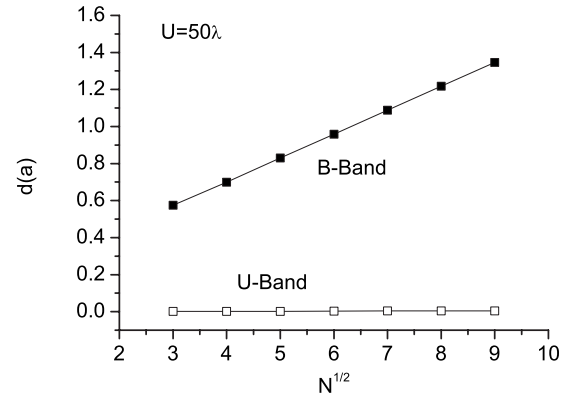

FIG. 2. Average mean distance of Bloch and U states plotted for different lattice sizes and a contact potential $U = 50\lambda$. The mean separation in a Bloch state (B band) grows linearly with the edge size while for the U band it stays near zero as expected for paired states.
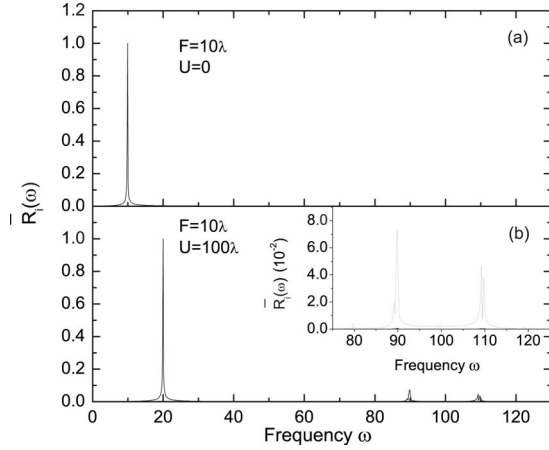
FIG. 3. Frequency spectrum of the average position of each particle in a 2D lattice of 81 sites and an external field of strength $F=10\lambda$. (a) is in the absence of interactions and (b) is for a Hubbard interaction strength $U=100\lambda$. The inset shows details near the Hubbard frequency. Frequencies are in units of λ.

ied the time evolution of the average position along the x axis of each particle,

$$R_i^x(t) = a \sum_{x_1,y_1} \sum_{x_2,y_2} |f_{x_1,y_1;x_2,y_2}(t)|^2 x_i, \qquad (6)$$

where $i=1,2$ is the particle index and a similar equation for the coordinate y. The numerical work was done using a half implicit numerical method which is second-order accurate and unitary.[19] The positions were indeed found to oscillate, not simply performing Bloch-type oscillations but a more complex pattern depending on initial conditions. Figure 3 shows the power spectrum for a 2D lattice of $N=81$ sites and an electric field energy $F=eEa=10\lambda$, set rather large in order to avoid reflections from the edges in our reduced numerical sample. In the absence of interactions only the Bloch frequency $\omega=F$ ($\hbar=1$) has any weight, as seen in Fig. 3(a). We next set the interaction strength at $U=100\lambda$, a large value appropriate to have a U band well separated from the extended states. For an initial condition with zero amplitude save for points far from the interaction region $x_1=x_2$, $y_1=y_2$, the situation is unchanged. But for an initial condition with unit amplitude in sites over the interaction hyperplane in the 4D space of coordinates $(x_1,y_1,x_2,y_2)=(r,s,r,s)$, $r,s=4,5,6$, and either r or $s=5$ when $r\neq s$, representing a portion of the hyperplane and a few nearby points, we see a Bloch oscillation with twice the Bloch frequency, with a power spectrum as shown in Fig. 3(b). We interpret this new frequency as arising from motion of a composite particle of charge $2e$ in an electric field, thus confirming that the pair behaves dynamically as a stable composite in the absence of dissipation. Additional interaction-induced oscillations appear near $U+F$ and $U-F$, shown in more detail in the inset. These latter oscillations, seen also in 1D systems, are the

result of pure correlated electron transport.[20] We note that our numerical results show that the features just described persist as the interaction strength enters the region $U\sim\lambda$, only that hybridization of bounded and independent states makes the power spectrum more complex.

IV. DISCUSSION

In summary, we have shown that two interacting electrons moving in a lattice in 2D have singlet paired states grouped in a band, with the dynamics of a composite particle of charge $2e$. Our results were obtained for a highly screened contact repulsive potential, yet studies in 1D show that a Coulomb tail does not destroy the pairing[2] in the singlet state. Although the specific treatment refers to electrons in a lattice, the main results may be extended to other systems such as atoms in an optical lattice.[1]

In order to understand the origin of the paired states we recall that ordinary Bloch states may be thought of as atomic states that hybridize with lattice neighbors, forming a tunneling network capable of sustaining extended states that are grouped in bands. Similarly, the paired eigenstates may be described as a high-energy two-electron single well state that forms a band of extended states owing to pair tunneling throughout the lattice. The Hubbard model captures the essence of this picture but details such as possible molecular two-electron extended states may arise if a finite range interaction is included.

The energy of the paired states scales like the interaction strength U. If this latter quantity is on the order of the bandwidth, such states may lie partly or wholly within the band of extended states, allowing pairs to form in the ground state if there are enough electrons in the sample. The paired states equal in number the extended states since they correspond to single-particle surface states over a 2D planar interface in a 4D lattice. We thus speculate that if condensation of such pairs indeed occurs then a transition to low resistance should take place as the density is increased, as is actually observed in experiment.[11]

Our model yields a pair whose dynamics is that of a stable composite of charge $2e$. Such stability may be reduced by dissipation mechanisms such as phonon excitation. In a static periodic potential such as that generated by an optical lattice phonons are not present, and a pair of energy $\sim U>8\lambda$ above the band center is expected to be stable since its decay into a band state is forbidden by energy conservation. Under an external field F, transitions between extended and localized states give rise to oscillations. If the associated frequencies $\omega_+=U+F$ and $\omega_-=U-F$ were accessible to experiment, then the sum $\omega_++\omega_-=2U$ would yield a direct measure of the interaction strength in the 2D sample.

[1] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. Hecker Denschlag, A. J. Daley, A. Kantian, H. P. Büchler, and P. Zoller, Nature (London) **441**, 853 (2006).

[2] F. Claro, J. F. Weisz, and S. Curilef, Phys. Rev. B **67**, 193101 (2003).

[3] J. F. Weisz and F. Claro, J. Phys.: Condens. Matter **15**, 3213 (2003).

[4] L. Jin, B. Chen, and Z. Song, Phys. Rev. A **79**, 032108 (2009).

[5] S. M. Mahajan and A. Thyagaraja, J. Phys. A **39**, L667 (2006).

[6] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

[7] B. L. Altshuler, A. G. Aronov, and P. A. Lee, Phys. Rev. Lett. **44**, 1288 (1980).

[8] S. V. Kravchenko, G. V. Kravchenko, J. E. Furneaux, and V. M. Pudalov, and M. DIorio, Phys. Rev. B **50**, 8039 (1994); S. V. Kravchenko, W. E. Mason, G. E. Bowker, J. E. Furneaux, and V. M. Pudalov, and M. DIorio, *ibid.* **51**, 7038 (1995); S. V. Kravchenko, D. Simonian, M. P. Sarachik, W. Mason, and J. E. Furneaux, Phys. Rev. Lett. **77**, 4938 (1996).

[9] A. M. Finkel'stein, Z. Phys. B: Condens. Matter **56**, 189 (1984); C. Castellani, C. Di Castro, P. A. Lee, and M. Ma, Phys. Rev. B **30**, 527 (1984); C. Castellani, C. D. DiCastro, and P. A. Lee, *ibid.* **57**, R9381 (1998).

[10] Q. Si and C. M. Varma, Phys. Rev. Lett. **81**, 4951 (1998).

[11] V. Dobrosavljevic, E. Abrahams, E. Miranda, and S. Chakravarty, Phys. Rev. Lett. **79**, 455 (1997).

[12] S. Chakravarty, L. Yin, and E. Abrahams, Phys. Rev. B **58**, R559 (1998).

[13] S. Chakravarty, S. Kivelson, C. Nayak, and K. Voelker, Philos. Mag. B **79**, 859 (1999).

[14] P. Phillips, Y. Wan, I. Martin, S. Knysh, and D. Dalidovich, Nature (London) **395**, 253 (1998); D. Belitz and T. R. Kirkpatrick, Phys. Rev. B **58**, 8214 (1998); J. S. Thakur and D. Neilson, *ibid.* **58**, 13717 (1998).

[15] Y. Lyanda-Geller, Phys. Rev. Lett. **80**, 4273 (1998).

[16] S. He and X. C. Xie, Phys. Rev. Lett. **80**, 3324 (1998); B. L. Altshuler and D. L. Maslov, *ibid.* **82**, 145 (1999); S. Das Sarma and E. H. Hwang, Phys. Rev. Lett. **83**, 164 (1999).

[17] For a review see S. V. Kravchenko and M. P. Sarachik, Rep. Prog. Phys. **67**, 1 (2004).

[18] E. E. Mendez, F. Agulló-Rueda, and J. M. Hong, Phys. Rev. Lett. **60**, 2426 (1988).

[19] A. Goldberg, H. M. Schey, and J. L. Schwartz, Am. J. Phys. **35**, 177 (1967).

[20] See Ref. 2, Eq. (6). A Fourier expansion of this expression yields oscillations at frequencies $U+F$ and $U-F$.