Efficient and robust initialization of a qubit register with fermionic atoms

L. Viverit\textsuperscript{1,2}, C. Menotti\textsuperscript{1}, T. Calarco\textsuperscript{3,4}, and A. Smerzi\textsuperscript{1}

\textsuperscript{1}CRS BEC-INFM and Dipartimento di Fisica, Università di Trento, I-38050 Povo, Italy
\textsuperscript{2}Dipartimento di Fisica, Università di Milano, via Celoria 16, I-20126 Milan, Italy
\textsuperscript{3}European Centre for Theoretical Studies in Nuclear Physics and Related Areas, I-38050 Villazzano (TN, Italy)
\textsuperscript{4}Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck (Austria)

We show that fermionic atoms have crucial advantages over bosonic atoms in terms of loading in optical lattices for use as a possible quantum computation device. After analyzing the change in the level structure of a non-uniform confining potential as a periodic potential is superimposed to it, we show how this structure combined with the Pauli principle and fermion degeneracy can be exploited to create unit occupancy of the lattice sites with very high efficiency.

Ultra-cold neutral atoms list among the most promising candidates for quantum computing (QC) applications\textsuperscript{1}. Several possible QC schemes using cold atoms have recently been proposed\textsuperscript{2}, and various groups are presently working for their experimental realization\textsuperscript{3}. The common starting point is the creation of a quantum register, i.e. a scalable array of well-characterized qubits\textsuperscript{4}. The qubits are usually identified with two internal states, typically hyperfine states, of a single atom. The atom-qubits need to be spatially well separated, and yet to be at a distance which allows to efficiently activate their interaction. These requirements are nearly ideally fulfilled by a periodic potential with exactly one atom localized at each lattice site. Such a periodic potential can be generated, for instance, by counter-propagating laser beams or with microscopic magnetic surface traps (atom chips). As a natural consequence of the vast knowledge developed in the last decade in the field of Bose-Einstein condensation\textsuperscript{5}, until now most efforts towards atomic QC implementations have been directed at the use of bosonic atoms. Only recently an increasing interest has been devoted to the cooling and manipulation of fermionic atoms in confining potentials\textsuperscript{6,7} and optical lattices\textsuperscript{8}. In particular the possibility to create a quantum register with fermionic atoms in a homogeneous optical lattice via coherent filtering has been proposed in\textsuperscript{9}.

In a uniform system, a lattice with a single atom per site can be created by confining $N$ atoms in a one-dimensional box of length $L$, and by subsequently superimposing a periodic potential of spatial period $d$, so that the number of lattice sites in the box is $L/d = N$. If the periodic potential is raised sufficiently slowly and if the effective atom-atom interaction is repulsive, the system ends up in its ground state which has an average occupation of one atom per site. One could equivalently use bosons with a positive scattering length or polarized fermions, in which case the Pauli principle provides a strong effective repulsion. In either case, however, this simple scheme has significant problems. To avoid the creation of defects like holes or multiply occupied wells, it requires equal number of particles and lattice wells besides a long adiabaticity time.

In this Letter we show that, in the presence of a non-uniform external confinement instead, fermionic atoms have crucial advantages over bosonic atoms and we propose a simple protocol to create a quantum register which directly exploits the peculiar properties of the Pauli principle.

Before discussing our proposal, it is useful to further consider the case of non-interacting fermions confined by a homogeneous box. In the absence of the periodic potential, the $N$ fermions occupy the $N$ lowest single-particle levels up to the Fermi energy $E_F = \pi^2 \hbar^2 N^2 / 2 m L^2$, with $m$ being the atomic mass. When the periodic potential is raised, in order for the number of lattice sites to be equal to the number of particles we should have $E_r = E_F$, where $E_r = \pi^2 \hbar^2 / 2 m d^2$ is the recoil energy of the lattice. Increasing the depth of the optical lattice slowly enough to avoid excitations, the lowest $N$ levels gradually cluster to form the first Bloch band, yet conserving their initial unit occupancy due to the Pauli principle. Eventually, in the limit $s \to \infty$ the $N$ levels become degenerate and the Wannier wavefunctions, which are $N$ linear combinations of the Bloch states localized one in each well, are exact eigenstates of the system. Under realistic conditions this procedure has the following drawbacks:

1. For finite $s$, the Wannier states are only approximate eigenstates and delocalize on a time scale of the order of the inverse of the bandwidth $\delta$. This limits the time over which one can perform QC operations.

2. Randomly distributed defects appear in the register
   (i) if $\epsilon_F \neq E_r$ — the condition $\epsilon_F < E_r$ results in empty sites, while $\epsilon_F > E_r$ results in multiply occupied sites;
   (ii) if the initial temperature is not much smaller than the energy level spacing;
   (iii) if the adiabaticity condition is not perfectly fulfilled, i.e. if the raising time of the lattice is not large as compared to the inverse level spacing.

The conditions required to create a lattice with unit filling along the lines specified above are unrealistically strict, and more complex schemes (see e.g.\textsuperscript{10}) are needed in order to eliminate the defects produced in the register.

When the Pauli principle is combined with a non-uniform confinement, the scenario changes completely. We first consider a one-dimensional geometry, which can be realized in practice with a tight radial confinement, so as to freeze excitations of the radial degrees of freedom. The extension to higher dimensions will be briefly dis-
cussed later. In the presence of an external confinement, \( V_{ext} \), the total trapping potential is

\[
V(z) = V_{ext}(z) + sE_r \sin^2(\pi z/d),
\]

where \( sE_r \) is the lattice height. In order to present the corresponding loading procedure, we need to analyze the behavior of the energy eigenvalues and the corresponding eigenstates as a function of the optical potential depth. In Fig. 1 we consider the specific case of a harmonic external confinement \( V_{ext}(z) = m\omega^2(z-z_0)^2/2 \), where \( z_0 \) is an arbitrary offset between the center of the confining potential and the optical lattice. As the periodic potential is raised, the eigenstates change from the well known oscillator states at \( s=0 \), to states localized at the lattice sites for large \( s \).

![FIG. 1: Energy levels relative to the ground state \( E_0 \) as a function of the optical potential depth \( s \), for a harmonic confinement with \( \hbar\omega = E_r/(2\pi^2) \) and \( z_0 = d/3 \).](image)

It is a general feature that the eigenvalues of the initial external confinement \( (s=0) \) can be grouped into two sets:

(I) The states with energy smaller than the recoil energy change smoothly as \( s \) increases;

(II) The levels with energy larger than the recoil energy show a more complicated behavior characterized by several avoided crossings.

The reason for this distinction, and the mentioned localization of the eigenstates, can be understood by looking at the behavior of the eigenvalues and the eigenfunctions, illustrated in Fig. 2. The figure shows the spatial position and the extension of the eigenfunctions versus the corresponding eigenvalues for two values of \( s \). When \( s \) increases the eigenfunctions become more and more localized in space and a band-like structures appear. The gaps between pseudobands open at the center of the trap, and the one between the first and the second band separates the initial eigenstates with energy smaller and larger than \( E_r \), i.e. the states in sets (I) and (II) above. The eigenfunctions with initial energy smaller than \( E_r \) gradually localize, each one in a different well. The energy of the eigenfunction in the well at position \( \ell d \) (with \( \ell = 0, \pm 1, \pm 2, \ldots \)) is approximately given by

\[
E_\ell \simeq \frac{1}{2} \hbar\omega + V_{ext}(\ell d),
\]

where \( \hbar\omega = \sqrt{\varepsilon E_r} \) is the energy of the lowest level of the lattice well. The first important observation is that, contrary to the uniform system case, the localized states are here exact eigenstates of the system for finite values of \( s \). The amount of localization of the eigenfunctions depends on \( s \) and the external potential. The second crucial point is that, by increasing \( s \), states with higher initial energy evolve into states localized farther away from the origin as compared to those with lower initial energy. For the register loading procedure, this implies that the constraint \( \varepsilon_F = E_r \) of the homogeneous system is relaxed to \( \varepsilon_F \leq E_r \), since the missing particles result in empty holes localized at the wings, and not randomly distributed as before. These facts change dramatically the loading conditions and are the major results of the present work.

For large \( s \), the energy spectrum is characteristic of all states in the first pseudoband, while the states in the second pseudoband have energy approximately given by \( 3\hbar\omega/2 + V_{ext}(\ell d) \). One could have hoped that the condition \( E_r \geq \varepsilon_F \) could be further relaxed, since the energy of the states in the second pseudoband progressively increases for increasing \( s \), leaving more and more

![FIG. 2: Spatial position and extension of the eigenfunctions versus the corresponding eigenvalues for \( s = 1.2 \) (a), and \( s = 12 \) (b); Density profiles calculated for a number of atoms such that \( \varepsilon_F = E_r \) at \( s = 0 \), for \( s = 1.2 \) (c), and \( s = 12 \) (d). The confining potential is the same as in Fig. 1](image)
localized states of the first pseudoband energetically allowed. This is, in fact, not the case as can be seen by looking at the behaviour of the levels of set (II). These initially correspond to states in different pseudobands. Due to the localization effect, as soon as a gap opens, there is very little spatial overlap between eigenfunctions with similar energy belonging to different pseudobands. The small spatial overlap corresponds to a very small tunnelling between almost degenerate states. This fact is also clearly reflected in the structure of levels in Fig. 1 where for increasing $s$ the gaps at the avoided crossings very quickly tend to disappear. For our loading purposes this means that over the time scales of interest, the atoms will remain trapped in their pseudoband even if, by increasing $s$, states in lower pseudobands have much lower energy. Thus if initially $\epsilon_F > E_r$, the ground state of the final potential cannot be reached in realistic time scales and one will be left with more than one particle in the central wells.

The level structure of the combined potential and the Pauli principle have crucial consequences also on the effects of a finite temperature, $T$, and on the adiabaticity time condition. We here summarize all the properties in a detailed comparison with the uniform system case:

1. For large but finite $s$ the eigenstates of the Hamiltonian can be well localized, depending on the particular shape of the external confinement.

2. An inner part of the register virtually free of defects can be generated since:
   
   (i) The strict requirement $\epsilon_F = E_r$, fixing the initial number of atoms, is relaxed to $\epsilon_F < E_r$;
   
   (ii) In an adiabatic process at finite $T$, the occupation number of the final localized states is equal to that of the corresponding level of the confining potential. For the states at lower energy in current experiments this can differ from unity by as little as one part in $10^8$.

As long as $T \ll T_F$ and $f(E > E_r) \ll 1$ (with $f$ being the Fermi thermal distribution), the states with occupancy significantly different from one are localized in a region $\sim k_BT$ around the Fermi level.

(iii) Strict adiabaticity is not required. Since the excitations induced by a potential varying in a time of the order of $\tau$ are only created around the Fermi level in a shell of the order of $h/\tau$, one just has to enforce that the raising process be slow compared to the inverse of the Fermi energy. For instance in the case of a 1D harmonic oscillator, the condition becomes $\tau \gg h/\epsilon_F = 1/(N\omega)$, allowing a factor of $N$ faster initialization than in the bosonic case.

We remark that the points (ii) and (iii) are direct consequences of the fermionic nature of the atoms, and do not have a direct analogue in the Mott insulator phase of trapped bosons.

To complete our analysis of the loading it is necessary to discuss more in detail the localization of the eigenstates. In Fig. 2 we plot the density profiles at $T = 0$ for two values of $s$, with a number of atoms such that $\epsilon_F = E_r$. We see that the density becomes flat in the presence of a deep periodic potential. A uniform density distribution, however, does not imply the perfect initialization of the quantum register. Comparing Fig. 2 (d) and Fig. 3 (a) (corresponding to the same parameters), we see that even if the density distribution is flat, the lowest eigenfunctions are not yet localized.

The degree of localization of the eigenfunctions at site $\ell$ arises from the interplay between the tunneling $\delta$ and the energy difference between neighboring wells at position $\ell d$, given by $\Delta E_\ell \approx d(\partial V_{ext}(z)/\partial z)_{z=\ell d}$. In the large $s$ limit, the eigenstates will be localized in the single wells, apart from a small contamination with first neighbors. The probability amplitude for the atom localized at site $\ell$ to find itself in the site $\ell \pm 1$ is given by $\alpha \approx \delta/(2\Delta E_\ell)$. This simple relation, whose validity was also checked numerically, implies that it is the first derivative of the potential to be important for localization. In the case of a harmonic potential then, the atoms are very well localized in the outer wells, while the central wells always suffer some tunnelling, even if small, due to the vanishing derivative. In a V-shaped potential $V_{ext}(z) = \mu_{B}B|z-z_0|/(2\pi^2 d)$ (b). The V-shaped potential is chosen to have the same slope as the harmonic one at $z = 4d$.

Consequently, while on the one hand in a shallow confining potential a larger number of atoms can be loaded following the above scheme, since more levels are found below the recoil energy, on the other hand, once the lattice is raised, a steep potential is required to get a good localization of the eigenstates. A convenient procedure to obtain both a large number of particles and a good localization is, thus, to first raise the optical lattice up to its maximum depth in the shallow trap (determined e.g. by $\omega_{in}$ or $\nabla B_{in}$), and then to make the external confine-
mment steeper (determined by \(\omega_{\text{fin}}\) or \(\nabla B_{\text{fin}}\)) in order to ensure good localization of all populated levels.

With a very steep final confinement, it might happen that states localized in sites away from the center of the trap become higher in energy than states in the second or higher pseudobands localized in the center of the trap. This happens if \(V_{\text{ext}}(\ell d) > 3\sqrt{s}E_r\). This is not a problem as long as states in different pseudobands are localized in different regions of space and the tunneling between those states is negligible. The outermost atom in the register localized at \(\ell_{\text{max}} = N/2\) is degenerate with the state in the second pseudoband localized around site \(\ell'\), given by \(V_{\text{ext}}(\ell'd) + \hbar \omega = V_{\text{ext}}(\ell_{\text{max}}d)\). The condition for negligible tunneling is \(\ell_{\text{max}} - \ell' \gg 1\). The explicit expressions for harmonic and V-shaped confinement are respectively \(\ell_{\text{max}} - \ell' = (8/\pi^2)^{1/3}\sqrt{s}N(\omega_{\text{in}}/\omega_{\text{fin}})^2\) and \(\ell_{\text{max}} - \ell' = (8/3)^{1/3}\sqrt{s}N(\nabla B_{\text{in}}/\nabla B_{\text{fin}})^2\).

We now consider, as specific examples, \(^{40}\text{K}\) atoms in a lattice with periodicity \(d = \lambda/2 = 335.5\) nm and \(^{6}\text{Li}\) atoms in a lattice with periodicity \(d = \lambda/2 = 335.5\) nm. For both species, we take the magnetic moment equal to the Bohr magneton \(\mu_{B}\). The first step of our procedure consists in raising the optical lattice to its final depth. The next step is to make the external confinement tighter. The conditions fixing the strength of the final confinement are a good localization of the eigenstates (\(\alpha < 10^{-2}\)) and a negligible tunneling to higher bands (\(\ell_{\text{max}} - \ell' \gg 1\)). In Table I, we show the parameters required to trap a maximum number of atoms \(N = E_r/\epsilon_F = 10^3\). The final optical lattice depth is \(s = 30\), corresponding to a tunneling parameter \(\delta = 10^{-3}E_r\). Lighter atoms require stronger confinements in order to be well localized. Moreover, as already discussed in Fig. 3 the V-shaped potential is more efficient than the harmonic confinement, since the eigenstates are localized to the same degree throughout the register.

| Harmonic confinement | V-shaped confinement |
|---------------------|---------------------|
| \(^{40}\text{K}\) | \(^{6}\text{Li}\) |
| \(\omega_{\text{in}}\) | \(\omega_{\text{fin}}\) | \(\alpha_{N/20}\) | \(\alpha_{N/2}\) | \(\ell_{\text{max}} - \ell'\) | \(\nabla B_{\text{in}}\) | \(\nabla B_{\text{fin}}\) | \(\alpha\) | \(\ell_{\text{max}} - \ell'\) |
| 2\(\pi\times 6.7\) Hz | 2\(\pi\times 170\) Hz | 3 \(\times 10^{-2}\) | 3 \(\times 10^{-2}\) | 7 | 0.8 G/cm | 10 G/cm | 5 \(\times 10^{-3}\) | 120 |
| 2\(\pi\times 74\) Hz | 2\(\pi\times 1.9\) KHz | 3 \(\times 10^{-2}\) | 3 \(\times 10^{-4}\) | 7 | 1.2 G/cm | 140 G/cm | 5 \(\times 10^{-3}\) | 120 |

TABLE I: Experimental parameters for the realization of a quantum register with \(^{40}\text{K}\) and \(^{6}\text{Li}\) atoms, where we fix \(N = 10^3\) and \(s = 30\). The parameter \(\alpha\) describes the localization around site \(\ell\) (which is site-dependent in the harmonic case).

The extension of our proposal to 2D and 3D lattices is straightforward, as far as the relation \(\epsilon_F < E_r\) fixing the maximum achievable number of atoms, the adiabaticity condition and the effect of finite temperature are concerned. However, the localization properties of the eigenstates have to be investigated carefully. A higher dimensional register can contain a larger number of atoms. For instance, in the case of cubic lattice and harmonic confinement, the problem scales in a simple way with dimensions. In 3D, defining \(\bar{a}_{\text{ho}} = \sqrt{\hbar/m\omega}\) and \(\bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}\), we have \(N \approx (\pi^2\bar{a}_{\text{ho}}^3/2d^3)\), which can be easily of the order of \(10^6\).

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