Hubbard-like Hamiltonian for ultracold atoms in a 1D optical lattice

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Abstract

Based on the standard many-fermion field theory, we construct models describing ultracold fermions in a 1D optical lattice by implementing a mode expansion of the fermionic field operator where modes, in addition to space localisation, take into account the quantum numbers inherent in local fermion interactions. The resulting models are generalised Hubbard Hamiltonians whose interaction parameters are derived by a fully-analytical calculation. The special interest for this derivation resides in its model-generating capability and in the flexibility of the trapping techniques that allow the tuning of the Hamiltonian interaction parameters over a wide range of values. While the Hubbard Hamiltonian is recovered in a very low-density regime, in general, far more complicated Hamiltonians characterise high-density regimes, revealing a rich scenario for both the phenomenology of interacting trapped fermions and the experimental realization of devices for quantum information processing. As a first example of the different situations that may arise beyond the models well known in the literature (the unpolarised-spin fermion model and the noninteracting spin-polarised fermion model), we derive a Rotational Hubbard Hamiltonian describing the local rotational activity of spin-polarised fermions. Based on a standard techniques we obtain the mean-field version of our model Hamiltonian and show how different dynamical algebras characterize the case of attractive and repulsive two-body potentials.

PACS numbers: 71.10.Fd, 05.30.Fk, 03.75.Ss
I. INTRODUCTION

Since the Bose-Einstein condensation of alkali atoms in magnetic traps \cite{1, 2}, a massive experimental and theoretical effort has been dedicated to the investigation of confined atoms in the extremely low-temperature regime (for a review see \cite{3, 4, 5, 6}).

The flexibility of optical trapping techniques has suggested the devise of different configurations (lattices \cite{5, 7, 8, 9, 10}, superlattices, etc. \cite{11, 12, 13, 14, 15, 16}), opening a vast scenario of research. The ability to tune atomic interactions via a magnetic field (Feshbach resonance \cite{17}), along with the proposal of single atom trap loading techniques \cite{18}, has proven to be of capital importance for ultracold fermions physics, yielding the possibility to study fundamental aspects of superfluidity (BCS-BEC crossover, see e.g. \cite{19, 20, 21, 22}) and envisaging new perspectives in quantum information processing \cite{23, 24}.

The present work focuses on the theoretical investigation of the properties of (few) fermionic ultracold atoms loaded into a 1D optical lattice, where global confinement is ensured by a magnetic trap. The description of such a physical system can be naturally performed in terms of a generalised Hubbard Hamiltonian (gHH) which is deduced from a general field-theoretic Hamiltonian with two body interaction \cite{25}. At this stage, particular care must be taken in the choice of the function basis for the field operator expansion. Although the symmetries of the system can provide selection rules that reduce the involvement of the gHH, the resulting coefficient structure is very rich and, as a direct consequence, the Hamiltonian hardly tractable. Nevertheless, the generality of the model gives rise to a wealth of sub-models, depending upon different approximations and regimes. The guideline to find simplified Hamiltonians is given by the thorough analysis of the gHH coefficient structure.

From this perspective the analytical knowledge of the coefficients is a powerful tool to establish the physical relevance of different sub-models in the various situations that may be conceived in the framework of the trapped ultracold atoms physics. Moreover, the nontrivial dependence of the coefficient from controllable external parameters provides the possibility to use these parameters to control the dynamics of the atoms trapped in the optical lattice. Thus the key aspect of this paper is the analytical determination of the hopping and interaction coefficients as a function of experimental parameters such as magnetic trap frequency, laser intensity, wavelength, angle between laser sources, $s$-wave scattering length etc.

We would like to stress that the procedure followed here for the determination of the
coefficients is statistics-independent: the bosonic or fermionic nature of the atoms loaded into the trap is completely taken into account by the commutators of raising and lowering operators that will be described in the paper. For example with the calculations performed here it seems feasible to go beyond the approximations that lead to the Bose-Hubbard model in the description of the BEC dynamics in optical lattices, taking into account the specific nature of the interaction between alkali atoms in a low density regime. Even for a ground-state calculation it can be shown that it is necessary to include levels beyond the single particle ground state (see [26]).

The confinement model considered here has a direct experimental relevance (see e.g. [27, 28]). However, while in [27, 28] a number of atoms of the order of $10^4$ is considered, allowing thus the adoption of a semiclassical model, we focus on a low occupation-number regime similarly to what is done in [29] and [30], yet extending to a multi-band model whose correctness is limited by the validity limit of the space-mode approximation.

Challenging tasks for the future will include the determination of tractable yet interesting models for different aspects for theoretical condensed matter physics and quantum mechanics. On the other hand the experimental realisation of systems that exhibit a behaviour which can be described in the framework of the various models here proposed, would represent an important achievement for both condensed matter experimentalist and theoreticians: the main difficulties seem to arise from the nearly-single atom trap loading and, quite naturally, from the coupling with the external environment.

Throughout the paper we have tried to emphasise the generality of the procedure followed. However we have decided to write down and plot few numerical values of the coefficients to stress the fact that this calculation is a direct and relatively simple tool to shape out simplified and approximate Hamiltonians for different physical situations.

In section II we depict the potential configuration of the system, moving then to the description of our field-theoretical approach. The field operators are written in terms of mode raising and lowering operators. Each mode corresponds to a set of quantum numbers, one of them identifies the lattice site (hence space-mode approximation) while the others describe on-site quantum numbers (local-mode) [31]. As previously stated this choice is not unique, but symmetry constraints suggest expansions that emphasise conservation laws and selection rules.

In section III we evaluate the expression of the Hamiltonian hopping and interaction
coefficients and we try to describe the interaction coefficient symmetry properties into some detail.

The purpose of section IV is twofold. One the one hand we show how, with suitable approximations, the Hamiltonian of the system reduces to known cases, such as the Hubbard Hamiltonian or a trivial non-interacting Hamiltonian. On the other we introduce a novel Rotational Hubbard Hamiltonian, as a first instance of the involvement of higher order approximations. For this case, by means of established mean-field approaches [32, 33], we suggest a possible path of research involving general group-theoretical procedures [33]. It will be shown that these procedures, even if the explicit solution for the ground state is not given, allow to grasp interesting aspects of the physics of the model here discussed.

We have included two Appendices where the relatively simple but lengthy calculations of the tunnelling and interaction coefficients are provided explicitly. In Appendix A there are various plots of multilevel hopping parameters that supply a good example of the scenario that we are moving in and may constitute a good starting point for further investigation.

II. FERMIONS TRAPPED IN 1D OPTICAL LATTICES

A. General features

The general field-theoretic Hamiltonian (see e.g. [25]) with 2-body interaction can be written as

\[ \hat{H} = \int dr \hat{\Psi}^\dagger(r) H_{1b}(r) \hat{\Psi}(r) + \int dr dr' \hat{\Psi}^\dagger(r) \hat{\Psi}^\dagger(r') H_{2b}(r, r') \hat{\Psi}(r') \hat{\Psi}(r) \]  

where \( H_{1b}(r) \) represents the 1-body term of the Hamiltonian (kinetic + external potential term) while \( H_{2b}(r, r') \) the 2-body interaction potential term, \( \hat{\Psi}(r) \) is the field operator and \( \hat{\Psi}^\dagger(r) \) its adjoint.

As previously mentioned we will stick to neutral fermionic atoms loaded into a 1D optical lattice. The lattice is generated by two lasers counter-propagating along the \( x \)-axis, with wavenumber \( K \). The depth – or height, depending if red or blue detuning of the laser is considered – in each point \( x \) the potential is proportional to the intensity of the laser and thus, according to the considered setup, to \( \sin^2(2Kx) \), for the evaluation of the multiplicative constant see e.g. [3]. Here we set the multiplicative constant equal to \( m\omega^2/(2K^2) \) where \( \omega \) represents the harmonic oscillator frequency in the second order expansion of the term \( V_{ext} \).
Global confinement is ensured by a cigar-shaped magnetic trap with principal axis along the \(x\)-direction (see e.g. [34]). This trap can be modelled by a 3D harmonic an isotropic trap of axial and radial frequencies equal to \(\Omega_x\) and \(\Omega_{\perp}\) respectively (\(\Omega_x \ll \Omega_{\perp}\)).

The magneto-optical trap can be thought as if the constituents of the system were trapped in the cigar shaped potential with a “slicing” effect of the laser, giving rise to a linear array of 3D prolate harmonic oscillators. Besides, the radial trapping frequency has a deep influence on the interaction among the constituents of the system, allowing to control the volume of each “disk”. With the previous assumptions \(H_{1b}\) becomes

\[
H_{1b} = E_{\text{kin}} + V_{\text{ext}}
\]

where

\[
E_{\text{kin}} = -\frac{\hbar^2 \nabla^2}{2m}
\]

\[
V_{\text{ext}} = \frac{m}{2} \left[ \Omega_x^2 x^2 + \Omega_{\perp}^2 \rho^2 \right] + \frac{m\omega_x^2}{2K^2} \sin^2(Kx),
\]

(2)

and the second term of \(V_{\text{ext}}\) represents the harmonic confinement of the magnetic trap, while the third one corresponds to the optical potential and \(\rho^2 = y^2 + z^2\). For future convenience, we write equation (2) as

\[
H_{1b} = E_{\text{kin}} + \sum_j V_j + \left( V_{\text{ext}} - \sum_j V_j \right)
\]

(3)

with

\[
V_j = \Pi_j(x) \frac{m}{2} \left[ \Omega_x^2 x_j^2 + \Omega_{\perp}^2 \rho_j^2 \right]
\]

(4)

\(\Pi_j(x) = \Pi(\frac{Kx}{\pi} - j)\) where \(\Pi(x)\) is the rectangle function (\(\Pi(x) = 1\) for \(-1 \leq x < 1\), \(\Pi(x) = 0\) elsewhere), \(k = l_{\perp} K\) (with \(l_{\perp} = \sqrt{\hbar/(m\omega_{\perp})}\)) and \(x_j = (x - j\frac{\pi}{K})\). Here the harmonic axial confinement of the magnetic field has been considered as a site-dependent – with \(j\) site index – constant additive term, merely shifting the local minima of the optical potential. From Eq. (3) with the properties of the rectangle function we obtain

\[
H_{1b} = \sum_j \Pi_j(x) \left[ (E_{\text{kin}} + V_j) + (V_{\text{ext}} - V_j) \right]
\]

(5)

Hereafter the axial confinement of the magnetic trap will be neglected (small \(\Omega_x\)).
We are now led to consider two different terms in Eq. (5). The first represents a local harmonic-oscillator Hamiltonian

\[ H_{h.o.}^{j} = \Pi_{j}(x)(E_{kin} + V_{j}) \]

\[ = \Pi_{j}(x) \left[ \frac{\hbar^{2} \nabla^{2}}{2m} + \frac{m\omega^{2}}{2} x_{j}^{2} + \frac{m\Omega_{j}^{2}}{2} \rho^{2} \right] \]

(6)

and a hopping one

\[ H_{\text{tunn}}^{j} = \Pi_{j}(x)(V_{\text{ext}} - V_{j}) \]

\[ = \Pi_{j}(x) \left[ \frac{m\omega^{2}}{2K^{2}} \sin^{2}(Kx) - \frac{m\omega^{2}}{2} x_{j}^{2} \right]. \]

(7)

The term \( V_{j} \) is the local second-order expansion of the optical potential, thus equation (7) represents the discrepancy between an harmonic potential and the true optical potential, describing hopping of atoms between neighbouring sites.

Neutrality of the atoms, ensuring a finite-range interaction allows us to introduce a pseudo-potential approximation (see e.g. [35])

\[ U(r) = \sum_{j} \Pi_{j}(x)\tilde{a}_{s}(r) \frac{\partial}{\partial r} r, \quad \tilde{a}_{s} := \frac{4\pi\hbar^{2}a_{s}}{m}, \]

(8)

where \( r \) is the interatomic distance and \( a_{s} \) the \( s \)–wave scattering length (\( a_{s} \) in our approximation is considered constant). The validity of this model is ensured by the low energies involved in these interactions, direct consequence of both low temperature limit (virtually zero) and diluteness (low Fermi energy). Besides, the form of Eq. (8) shows that on-site terms only will contribute to the interaction Hamiltonian. Thus Eq. (1) can be rewritten in the form

\[ \hat{H} = \sum_{j} \left[ \int d\mathbf{r}\hat{\Psi}^{\dagger}(\mathbf{r}) \left( H_{h.o.}^{j}(\mathbf{r}) + H_{\text{tunn}}^{j}(\mathbf{r}) \right) \hat{\Psi}(\mathbf{r}) + \right. \]

\[ + \tilde{a}_{s} \int d\mathbf{r} d\mathbf{r}'\hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}^{\dagger}(\mathbf{r}')\delta(\mathbf{r} - \mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}). \]

(9)

B. The (space+local)-modes expansion

The choice of the basis for the expansion of the field operators is crucial. As already suggested by the grouping of terms in Eq. (6), we will choose a basis constituted by local harmonic oscillator eigenfunctions. In addition, because of the symmetry of the system we
have chosen central-symmetric 2D h.o. eigenfunctions for the 2D isotropic radial h.o. [36], instead of decomposing it in 1D h.o. eigenfunctions, this will give us deeper insight into conservation laws and selection rules imposed by the symmetries of the system. We then have

$$\hat{\Psi}(x) = \sum_{i,n_x,J,m,\sigma} u_{n_x}(x-x_i) \mathcal{L}_{J,m}(\rho, \phi) \xi(\sigma) \hat{c}_{n_x,J,m,i,\sigma}$$

with

$$u_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi l_x}}} H_n(x/l_x) e^{-x^2/2l_x^2},$$

$$\mathcal{L}_{J,m}(\rho, \phi) = \frac{e^{2im\phi}}{\sqrt{\pi l_\perp}} C_{Jm} \left(\frac{\rho}{l_\perp}\right)^{2m} L_{2J-m}^2 \left(\frac{\rho}{l_\perp}\right),$$

$$C_{Jm} = \sqrt{(J+m)!/(J-m)!},$$

$$\xi(\sigma)$$ is a spin function and $l_x = \sqrt{\hbar/(m\omega_x)}$. In this decomposition $u_n(x)$ is a 1D harmonic-oscillator eigenfunction ($H_n$ represent the $n$th Hermite polynomial) and $\mathcal{L}_{J,m}$ a 2D harmonic-oscillator eigenfunction [36] with $L_{2J-m}^2(x)$ a generalised Laguerre polynomial.

Fermionic operators will thus have 5 indexes: 3 of them ($n_x, J, m$) identify (2+1)D local harmonic oscillator states, while $i$ identifies the site and $\sigma$ the spin. While $n_x$ has its usual interpretation of 1D harmonic oscillator number operator eigenvalue, $J$ and $m$ can be construed as angular momentum and $x-$axis component of the angular momentum, respectively.

This decomposition can be thought as a generalised space-mode approximation, with additional local modes that, in the present case, correspond to the local (2+1)D harmonic-oscillators quantum numbers. If not explicitly required, we will use $\phi_\alpha = u_{\alpha}(x-x_{i_\alpha}) \mathcal{L}_{J_\alpha,m_\alpha}(\rho, \phi) \xi(\sigma_\alpha)$, with $\alpha = \{n_\alpha, J_\alpha, m_\alpha, i_\alpha, \sigma_\alpha\}$ to simplify the index notation. We wish to stress that decomposition (10) is an approximation of field $\hat{\Psi}(x)$: there is a non-nil overlapping between wavefunctions belonging to different sites, thus orthogonality is not fulfilled. Nevertheless these overlapping integrals are supposed to be small, ensuring the consistency of this choice [10].

In the forthcoming calculation of the interaction term, Eq. (11) allows us to easily recognise that $m$ is a conserved quantity. If we come back to (10), with the decomposition
we obtain
\[
\hat{H} = \sum_j \sum_{\alpha, \beta} \left[ \int dr \phi^*_\alpha(r) H^j_{ho} \phi_\beta(r) \hat{c}_\alpha \hat{c}_\beta + \int dr \phi^*_\alpha(r) H^j_{tunn} \phi_\beta(r) \hat{c}_\alpha \hat{c}_\beta + \right]
\]
\[\tilde{a}_\gamma \sum_{\gamma, \delta} \int dr' dr' \phi^*_\alpha(r) \phi^*_\gamma(r') \times \delta(r - r') \phi_\delta(r) \hat{c}_\alpha \hat{c}_\beta \hat{c}_\gamma \hat{c}_\gamma \right] \quad (13)

III. HAMILTONIAN COEFFICIENTS

We are now in the position to calculate all the coefficients in Hamiltonian (13). The first term becomes
\[
\hat{H}^j_{ho} = \sum_{j, \alpha, \beta} \lambda_\beta \int_{-\infty}^{\infty} dr \Pi_j(x) \phi^*_\alpha(r) \phi_\beta(r) \hat{c}_\alpha \hat{c}_\beta ,
\]
where \(\lambda_\beta\) is the (2+1)D harmonic-oscillator eigenvalue
\[
\lambda_{n_\beta, j_\beta, m_\beta, i_\beta, \sigma_\beta} = \left[ \hbar \omega_x \left( n_\beta + \frac{1}{2} \right) + \hbar (2J_\beta + 1) \right].
\]
Eq. (14) can be written as
\[
\sum_{j, \alpha, \beta} \lambda_\beta \delta_{\alpha, \beta} \delta_{i_\alpha, j} \hat{c}_\alpha \hat{c}_\beta = \sum_{\alpha} \lambda_\alpha \hat{n}_\alpha \quad (15)
\]
where the second Kronecker delta is a consequence of the space-mode approximation, i.e. we consider only superposition of wavefunctions among which at least one is a local harmonic-oscillator eigenfunction, while the first one stems from the orthogonality of the \(\phi_\gamma(x)\) functions.

We move now to the evaluation of the integral in the second term of equation (13). Namely
\[
\hat{H}^j_{tunn} = \sum_{j, \alpha, \beta} \int dr \phi^*_\alpha(r) \Pi_j(x) H^j_{tunn}(x) \phi_\beta(r)
\]
being \(H^j_{tunn}(x)\) independent of radial and spin degrees of freedom, we can rewrite equation (17) as
\[
\hat{H}^j_{tunn} = \sum_{j, \alpha, \beta} \delta_{j_\alpha, j_\beta} \delta_{n_\alpha, n_\beta} \delta_{\sigma_\alpha, \sigma_\beta} \delta_{i_\alpha, i_\beta} \int dx u^*_\alpha(i_\alpha)(x) H^j_{tunn}(x) u_{n_\beta, i_\beta}(x) \hat{c}_\alpha \hat{c}_\beta .
\]
(18)

With the same assumptions of the local harmonic-oscillator case the integral in equation (18) becomes
\[
K_{n_\alpha, n_\beta} \hbar \omega_x \int dy e^{-\frac{(y - \tau)^2}{4}} H_{n_\alpha}(y - \tau) H^j_{tunn}(y) e^{-\frac{y^2}{2}} H_{n_\beta}(y) ,
\]
(19)
where $K_{n_{\alpha},n_{\beta}} = [2^{n_{\alpha}+n_{\beta}}n_{\alpha}!n_{\beta}!\pi]^{-1/2}$ and we have put $y = (x - i_{\beta}d)/l_x$ (where $d = \pi/k$), $\tau = (i_{\beta} - i_{\alpha})$ and $\Omega = K l_x$. By substituting the expression of $H_{tunn}^{j}(y)$ from equation Eq. (7) we obtain
\[
K_{n_{\alpha},n_{\beta}} \hbar \omega x \int dy \, e^{-\frac{(y-x)^2+y^2}{2}} H_{n_{\alpha}}(y-\tau) H_{n_{\beta}}(y) \left[ 1 - \frac{\cos(2\Omega y)}{4\Omega^2} - \frac{y^2}{2} \right] \hat{c}_\alpha^\dagger \hat{c}_\beta. \tag{20}
\]
If we define
\[
T_{\alpha,\beta} = \frac{K_{n_{\alpha},n_{\beta}}}{2} \delta_{J_{\alpha},J_{\beta}} \delta_{m_{\alpha},m_{\beta}} \delta_{\sigma_{\alpha},\sigma_{\beta}} \hbar \omega_x \int dy \, e^{\frac{(y-x)^2+y^2}{2}} \times H_{n_{\beta}}(y) H_{n_{\alpha}}(y-\tau) \left[ \frac{y^2}{2} - \frac{1 - \cos(2\Omega y)}{4\Omega^2} \right] \tag{21}
\]
equation (14) becomes
\[
\hat{H}_{tunn} = -\sum_{\alpha,\beta} T_{\alpha,\beta} \hat{c}_\alpha^\dagger \hat{c}_\beta. \tag{22}
\]
Then the term $T_{\alpha,\alpha} \hat{c}_\alpha^\dagger \hat{c}_\alpha$ can be incorporated into the $\hat{H}^{h.o.}$ term, giving
\[
\mu_\alpha = \lambda_\alpha - T_{\alpha,\alpha}. \tag{23}
\]
We will here skip the explicit solution of the integral in Eq. (21), along with the analytic expression of $T$, which can be found in Appendix A. These calculations allow us to write
\[
T_{\alpha,\beta} = \delta_{J_{\alpha},J_{\beta}} \delta_{m_{\alpha},m_{\beta}} \delta_{\sigma_{\alpha},\sigma_{\beta}} T_{n_{\alpha},n_{\beta},i_{\alpha},i_{\beta}}. \tag{24}
\]
In Fig. 1 we have the plot the coefficient $T_{n_{\alpha},n_{\beta},i_{\alpha},i_{\beta}}$ as a function of the ratio between distance and the period of the optical lattice, for $n_{\alpha}, n_{\beta} = 0, 1$. In boldface we have marked the points corresponding to discrete values of the ratio $x/d$, i.e. the points with a relevant physical meaning. The values of $T$ plotted here are in arbitrary units. Even if the correctness of the above procedure seems undoubted, it must be remembered that it is entirely based on the space-mode approximation, whose validity depends on the overlapping of wavefunctions belonging to different sites and thus might be violated.

These plots show how the tunnelling amplitude varies with the distance. In particular it is clear how, for long-distance tunnelling, there is a negative exponential dependence. Nevertheless, if the experimental conditions are properly chosen (i.e. angle between counterpropagating laser beams and their power), it is possible to obtain conditions where, for instance nearest-neighbour and next-to-nearest neighbour tunnelling coefficients have opposite signs (see e.g. Fig. 2 $T_{0,0,i_{\alpha},i_{\beta}}$), and thus the model, in that case, might exhibit frustration.
We will now move to the determination of the interaction term, namely the last term of equation (13). As a first step, we can write the integral in cylindrical coordinates

$$\tilde{a}_s \int d\mathbf{r} d\mathbf{r}' \phi^*_\alpha(r)\phi^*_\gamma(r')\delta(\mathbf{r} - \mathbf{r}')\phi_\beta(r)\phi_\delta(r') =$$

$$\tilde{a}_s \int dx dx' u^*_{n_\alpha}(x - x_{i_\alpha})u^*_{n_\gamma}(x' - x_{i_\gamma})\delta(x - x')u_{n_\beta}(x - x_{i_\beta})u_{n_\delta}(x' - x_{i_\delta})$$

$$\times \int d\tilde{\rho} d\tilde{\rho}' \frac{\tilde{\rho}}{\pi} \int d\phi d\phi' \mathcal{L}^*_{J_{\alpha,m_{\alpha}}}(\tilde{\rho}, \phi)\mathcal{L}^*_{J_{\gamma,m_{\gamma}}}(\tilde{\rho}', \phi')\delta(\rho - \rho')$$

$$\delta(\phi - \phi') \mathcal{L}_{J_{\beta,m_{\beta}}}(\tilde{\rho}, \phi)\mathcal{L}_{J_{\delta,m_{\delta}}}(\tilde{\rho}', \phi')$$

(25)

with $\tilde{\rho} = \rho/\ell_\rho$ and the identity

$$\delta(\mathbf{r}) = \frac{\delta(\rho)\delta(\phi)}{\pi \rho}.$$

As we are dealing with a short range interaction modelled by a $\delta(\mathbf{r} - \mathbf{r}')$ function, we will consider on-site interaction only ($\tilde{x}_{i_\alpha} = \tilde{x}_{i_\beta} = \tilde{x}_{i_\delta} = \tilde{x}_{i_\gamma}$).

This choice is completely justified because the interaction term is modelled by a pseudopotential term for which nearest-neighbours interactions become negligible. In this case
the first integral on the left-hand side of Eq. (25) becomes

\[ U_x = \frac{1}{\pi l_x} \sqrt{\frac{2 - (n_x + n_y + n_z + n_d)}{n_x! n_y! n_z! n_d!}} \int d\bar{x} H_{n_x}(\bar{x}) H_{n_y}(\bar{x}) H_{n_z}(\bar{x}) e^{-2\bar{x}^2} \]  

(26)

with \( \bar{x} = x/l_x \), whose explicit calculation is given in Appendix B. Here we just give the final result

\[ U_x = \frac{\delta_{||\bar{n}||, 2N}}{\pi l_x} \sum_{\bar{s}} \frac{\Xi(\bar{s})}{\sqrt{2^{||\bar{s}||} + 3}} \Gamma \left( \left( ||\bar{n}|| \right) - \left( \bar{s} \right) \right) + 1 \]  

(27)

with

\[ \Xi(\bar{s}) = \begin{cases} 0 & \text{if } s_\theta \text{ odd} \\ \prod_{\theta} \frac{1}{n_\theta!} H_{s_\theta}(0) & \text{if } s_\theta \text{ even} \end{cases} \]  

(28)

The summation is to be intended as 4 separate summations over the components of a vector \( \bar{s} = \{ s_\alpha, s_\beta, s_\gamma, s_\delta \} \) from \( \{ 0, 0, 0, 0 \} \) to \( \bar{n} = \{ n_\alpha, n_\beta, n_\gamma, n_\delta \} \). The norm \( ||\bar{x}|| \) is a 1-norm \((||\bar{x}|| = \sum_\theta |x_\theta|, \theta = \alpha, \beta, \gamma, \delta) \) and the \( \delta \) in Eq. (26) represents the parity selection rule, obtained from the explicit calculation of the integral.

For the radial part of the integral we have

\[ U_\rho = \int \int d\rho d\phi \frac{\rho}{\pi} L_{J_\alpha, m_\alpha}(\rho, \phi) L_{J_\gamma, m_\gamma}(\rho, \phi) L_{J_\beta, m_\beta}(\rho, \phi) L_{J_\delta, m_\delta}(\rho, \phi) \]  

(29)

with the definition given by Eq. (11), we can easily perform the angular integration and we obtain

\[ U_\rho = \frac{2\delta_{m_\alpha + m_\beta + m_\gamma + m_\delta}}{\pi^2} \int_0^\infty d\rho \rho R_{J_\alpha, m_\alpha}(\rho) R_{J_\gamma, m_\gamma}(\rho) R_{J_\beta, m_\beta}(\rho) R_{J_\delta, m_\delta}(\rho). \]  

(30)

The reader is again addressed to Appendix B for the explicit evaluation of the integral in Eq. (30). The result is given by

\[ U_\rho = \frac{\delta_{m_\alpha + m_\beta + m_\gamma + m_\delta}}{\pi^2 l^2} \sum_{\bar{q} = |\bar{m}|} \Lambda(\bar{J}, \bar{m}, \bar{q}) \frac{\Gamma(||\bar{q}|| + 3/2)}{2^{||\bar{q}||+3/2}} \]  

(31)

with

\[ \Lambda(\bar{J}, \bar{m}, \bar{q}) = \prod_{\theta = \alpha, \beta, \gamma, \delta} (-1)^{J_\theta - q_\theta} \frac{\sqrt{(J_\theta + m_\theta)! (J_\theta - m_\theta)!}}{(J_\theta - q_\theta)! (q_\theta + m_\theta)! (q_\theta - m_\theta)!} \]  

(32)

and, following previous notation, we obtain \( \bar{q} = \{ q_\alpha, q_\beta, q_\gamma, q_\delta \} \), \( \bar{J} = \{ J_\alpha, J_\beta, J_\gamma, J_\delta \} \) and \( |\bar{m}| = \{|m_\alpha|, |m_\beta|, |m_\gamma|, |m_\delta|\} \). The overall interaction coefficient can then be written as the
product of Eqs. (31) and (27)

\[
U_{\alpha,\beta,\gamma,\delta} = \delta \|\bar{n}\| \, 2\sqrt{N} \sum_{\alpha,\beta,\gamma,\delta} \sum_{q=|m|}^{\bar{n}} \frac{\Lambda (\bar{J}, \bar{m}, \bar{q}) \Xi (\bar{s})}{\sqrt{2^{\|\bar{s}\|+2|q|}}} \times \Gamma \left( \|\bar{q}\| + \frac{3}{2} \right) \Gamma \left( \frac{(\|\bar{n}\| - \|\bar{s}\| + 1)}{2} \right).
\]  

(33)

We are thus enabled to rewrite Hamiltonian (13) in terms of the calculated coefficients obtaining

\[
\hat{H} = \sum_{j} \left[ \sum_{\alpha,\beta} \lambda_{\alpha,\beta} \hat{n}_{\alpha} + \sum_{\alpha,\beta} T_{\alpha,\beta} \hat{c}_{\alpha} \hat{c}_{\beta} + \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\gamma,\delta} \hat{c}_{\alpha} \hat{c}_{\beta} \hat{c}_{\delta} \hat{c}_{\gamma} \right].
\]  

(34)

We will refer to (34) as the generalised Hubbard Hamiltonian. For sake of simplicity, in Eq. (34) we have not written down explicitly the selection rules imposed by symmetry constraints (see below).

A. Symmetry properties of the interaction term

In addition to global symmetry properties, such as 1) rotational symmetry along the \( x \)-axis and 2) left-right symmetry, reflected by momentum \( x \)-component conservation and parity conservation for the 1D harmonic oscillators along the \( x \)-axis, it is clear from equation (33) that the coefficient \( U_{\alpha,\beta,\gamma,\delta} \) has some symmetry properties: a) \( U \) does not depend on the sign of \( m_\chi \) with \( \chi = \alpha, \beta, \gamma, \delta \), provided the conservation \( m \) during the interaction \( (m_\alpha + m_\beta = m_\gamma + m_\delta) \); b) \( U \) possesses a permutational symmetry, namely

\[
U_{\alpha,\beta,\gamma,\delta} = U_{\beta,\alpha,\gamma,\delta} = U_{\alpha,\beta,\delta,\gamma} = U_{\beta,\alpha,\delta,\gamma}.
\]  

(35)

We would like to draw reader’s attention to the two \( \delta \) functions in equation (33) which make explicit the conservation laws that might have been expected by simply considering the symmetry of the problem. The first one represents parity conservation, while the second conservation of the \( x \) component of the angular momentum. In table II, we give the analytical value of \( U \) for interaction between particles belonging to the first three shells of the 2D radial harmonic oscillator and to the first level for the axial harmonic oscillator. These symmetry constraints allow to class the possible quantum numbers of the interacting particles according to the value of the corresponding \( U \). For example for

\[
\alpha = \{0, 1, 0, i, \sigma\}, \quad \beta = \{0, 0, 0, i, \sigma'\},
\]
\[ \delta = \{0, 0, 0, i, \sigma\}, \quad \gamma = \{0, 0, 0, i, \sigma'\}, \]

and

\[ \alpha = \{0, 0, 0, i, \sigma\}, \quad \beta = \{0, 0, 0, i, \sigma'\}, \]
\[ \delta = \{0, 1, 0, i, \sigma\}, \quad \gamma = \{0, 0, 0, i, \sigma'\}, \]

we have the same value of \( U \), henceforth the class definition of table II. We would like to point out two aspects of this example. First of all it may be noticed that the angular momentum \( J \) is not conserved throughout the interaction: this is a general feature of the system considered, there is not global rotational symmetry but only in the plane orthogonal to the 1D optical lattice. Moreover in this particular interaction the value for the coefficient \( U \) is negative, this appears to be a rare (but not unique) situation. The implications of this condition will be pointed out in section IV.

IV. SPECIAL CASES

In this section we derive three model Hamiltonians for fermions in optical lattices. We consider, for both cases, only the lowest-state axial quantum number (i.e. \( n_\alpha = n_\beta = 0 \)). Hence \( T_{\alpha,\beta} \) can be written as

\[ T_{\alpha,\beta} = \delta_{J_\alpha,J_\beta} \delta_{n_\alpha,n_\beta} \delta_{\sigma_\alpha,\sigma_\beta} T_{0,0,i,\sigma} \]  \hspace{1cm} (36)

As far as an ultracold gas is considered, it seems feasible to restrict our analysis to the first few levels above the ground state (i.e. \( J_\alpha = 0, 1/2, \ldots \)). As a first example, we consider the case having \( J_\alpha = 0 \) as the only radial level allowed and the fermionic gas is spin unpolarised. From Eq. (33), along with the previous assumptions, we obtain

\[ \hat{H} = \sum_{i,\sigma} \mu_i \hat{n}_{i,\sigma} - T \sum_{i,\sigma} \left( \hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \hat{c}_{i+1,\sigma}^\dagger \hat{c}_{i,\sigma} \right) + U \sum_{i,\sigma,\sigma'} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma'} \]  \hspace{1cm} (37)

with \( T = T_{0,0,i_a,i_a+1} \) which is easily recognised as the Hubbard Hamiltonian, whose role in the ultracold atoms physics has been pointed out elsewhere. Note that in this example we have made the assumption that the tunnelling coefficient is significantly different from zero only for nearest-neighbouring sites. Nevertheless more involved situations may arise, suggesting interesting physical features, as it is shown in Appendix A.
TABLE I: Values of $\tilde{U}_{\alpha,\beta,\gamma,\delta} = [\hbar^2 a_s/(m_l \pi^2 l_{\perp}^2)]^{-1} U_{\alpha,\beta,\gamma,\delta}$ for $\{n_\alpha, n_\beta, n_\gamma, n_\delta\} = \{0, 0, 0, 0\}$, $i_\alpha = i_\beta$, $\sigma$ and $\sigma'$ satisfy symmetry constraints. The value $m_\chi$ represents the equivalence class described in the text.

| $J_\alpha$ | $J_\beta$ | $J_\gamma$ | $J_\delta$ | $m_\alpha^*$ | $m_\beta^*$ | $m_\gamma^*$ | $m_\delta^*$ | $\tilde{U}_{\alpha,\beta,\gamma,\delta}$ |
|----------|----------|----------|----------|-----------|-----------|-----------|-----------|-----------------|
| 0        | 0        | 0        | 0        | 0         | 0         | 0         | 0         | $\frac{\pi}{2\pi}$ |
| 1/2      | 1/2      | 1/2      | 1/2      | 1/2       | 1/2       | 1/2       | 1/2       | $\frac{15\pi}{2\pi}$ |
| 1        | 1        | 1        | 1        | 1         | 1         | 1         | 1         | $\frac{945\pi}{2\pi}$ |
| 1        | 1/2      | 1/2      | 1        | 1         | 1         | 1/2       | 1/2       | $\frac{105\pi}{2\pi}$ |
| 1        | 1        | 1        | 1        | 1         | 0         | 0         | 0         | $\frac{193\pi}{2\pi}$ |
| 1/2      | 0        | 1/2      | 0        | 1/2       | 0         | 1/2       | 0         | $\frac{3\pi}{2\pi}$ |
| 1        | 1        | 1        | 1        | 1         | 1         | 0         | 1         | $\frac{345\pi}{2\pi}$ |
| 1        | 1/2      | 1/2      | 1        | 1         | 0         | 1/2       | 1/2       | $\frac{33\pi}{2\pi}$ |
| 1        | 1/2      | 1/2      | 1        | 0         | 1/2       | -1/2      | 1         | $\frac{45\pi}{2\pi\sqrt{2}}$ |
| 1        | 0        | 1        | 0        | 1         | 0         | 1         | 0         | $\frac{15\pi}{2\pi}$ |
| 1        | 1        | 0        | 0        | 0         | 0         | 0         | 0         | $\frac{7\pi}{2\pi}$ |
| 1        | 1        | 1        | 0        | 1         | -1        | 0         | 0         | $\frac{45\pi}{2\pi}$ |
| 1        | 1/2      | 1/2      | 0        | 0         | 1         | 1/2       | 1/2       | $\frac{3\pi}{2\pi}$ |
| 1        | 0        | 0        | 0        | 0         | 0         | 0         | 0         | $-\frac{\pi}{2\pi}$ |

If we now consider a spin-polarised gas in a (radial) multi-level system we obtain

$$\hat{H} = \sum_{\bar{n},i} \mu_{\bar{n},i} \hat{n}_{\bar{n},i} - T \sum_{\bar{n},i} \left( \hat{c}^\dagger_{\bar{n},i} \hat{c}_{\bar{n},i+1} + \hat{c}^\dagger_{\bar{n},i+1} \hat{c}_{\bar{n},i} \right)$$

(38)

where the absence of the interaction term is related to the symmetry properties of the coefficient $U_{\alpha\beta\gamma\delta}$. The Hamiltonian (38) is readily diagonalised to yield

$$\hat{H} = \sum_{\bar{n}} \bar{H}_{\bar{n}} = \sum_{\bar{n},k,\sigma} \left[ \mu_{\bar{n}} - 2T \cos(k) \right] \hat{n}_{\bar{n},k,\sigma}$$

(39)
with the same procedure followed in the strong coupling limit in the Hubbard Hamiltonian.

**Rotational Hubbard Hamiltonian**

As the last example, we derive a third Hamiltonian that may give the reader a first insight on the increasing complexity if higher single-particle levels are taken into account. Here we consider a situation where we allow \( J_\alpha = 0, 1/2 \) (but always \( n_\alpha = 0 \), leading to \( T_{n_\alpha, i_\alpha, n_\beta, i_{\alpha+1}} = T \) as already pointed out)

\[
H_{2\text{-level}} = \sum_{i,\sigma} \sum_{a=-1}^{1} \left[ \lambda_a n_{i,a,\sigma} - T \left( c_{i,a,\sigma} c_{i+1,a,\sigma} + c_{i+1,a,\sigma}^\dagger c_{i,a,\sigma} \right) \right] + \\
\sum_{i} \sum_{a,b,c,d} U_{a,b,c,d} \sum_{\sigma,\sigma'} c_{i,a,\sigma}^\dagger c_{i,b,\sigma'}^\dagger c_{i,c,\sigma'} c_{i,d,\sigma} \tag{40}
\]

where \( U_{a,b,c,d} = U_{a,i_\alpha,b,i_\beta,c,i_{\alpha+1},d,i_{\alpha+2}} \). The label \( a \) (as well as \( b, c, \) and \( d \)) has been introduced to represent the triplet of harmonic-oscillator numbers \( (n_\alpha, J_\alpha, m_\alpha) \), hence \( \alpha = \{a, i_\alpha, \sigma_\alpha\} \). One should recall that originally \( \alpha = (n_\alpha, J_\alpha, m_\alpha, i_\alpha, \sigma_\alpha) \). Here, however, it is convenient to write in an explicit way both spin indices \( \sigma_\alpha \)'s and site indices \( i_\alpha \)'s.

The triplet \( a = (n_\alpha, J_\alpha, m_\alpha) \) is such that the value \( a = 0 \) corresponds to \((0, 0, 0), a = 1 \to (0, 1/2, +1/2) \) and \( a = -1 \to (0, 1/2, -1/2) \). The axial quantum number \( n_x \) has been “frozen” to 0 due to the disk-shaped potential form (i.e. \( \omega_\perp \gg \omega_\| \)) while the radial quantum number \( J \) has been limited to the values \( \{0, 1/2\} \) as a first approximation beyond the \( J = 0 \) (Hubbard Hamiltonian see (37)). The present model thus enriches the dynamical scenario by introducing modes that take into account the simplest possible rotational processes for fermions confined in a well.

The wealth of the scenario depicted in Eq. (40) arises from the level-dependence of the interaction coefficient \( U_{a,b,c,d} \). In fact \( U_{a,b,c,d} \), as a function of the energy levels may provide a useful tool to simplify Eq. (40) hinting the best strategy for both numerical and analytical analysis of this model. Two main aspects concerning these coefficients are worth repeating here: a) the \( m_\alpha \)-conserving nature of the interaction, related to the symmetry properties of the confining potential and of the interaction coefficient (see section \( \text{III.A} \)), reduces the number of possible processes; b) the symmetry properties of \( U_{\alpha,\beta,\gamma,\delta} \) (see Eq. (35)) allow the grouping of interaction terms, accordingly to what has been done in table I.

From a general point of view, in Hamiltonian (40) the hopping factor may be construed
as a multichannel tunnelling coefficient, where the radial quantum numbers identify the channel label, in the same spirit of Hamiltonian (39). Incidentally, this is true if axial degrees of freedom are “frozen” to \( n_\alpha = n_\beta = 0 \), otherwise there is tunnelling among levels with \( n_\alpha \neq n_\beta \), for some \( \alpha \) and \( \beta \).

Hamiltonian (40) can represent a situation where single traps are loaded with a small number of atoms, as to fill the first two radial levels of the local harmonic oscillator. To experimentally obtain one of the different simplified Hamiltonians – like (40) – it is necessary to have control of four experimental parameters: laser intensity, angle between counterpropagating lasers, axial magnetic trapping frequency, scattering length. With these parameters it is possible to gain full knowledge of “lattice constant”, interaction parameter, shape and depth of the 3D harmonic traps. The most critical point seems the few-atoms loading of the trap but a technique involving a 3D anisotropic array –a sort of 2D array of 1D arrays– might overcome the problem.

In this picture, the interaction coefficient \( U \) can then be used as a source of entanglement between different channels. Moreover the possibility of experimental control of the scattering length, and thus of the interaction term, via an applied magnetic field may provide an useful tool of external manipulation of the state of the system in the rich scenario here depicted.

To outline future paths of research, we will here sketch a way to set up a mean-field procedure for the Rotational Hubbard Hamiltonian. The main interest of this approach resides in the possibility of a general discussion of some features of the model which have a direct experimental relevance. For example it is possible to state that, according to what is usually affirmed in the literature [32], no BCS-like ground-state is possible for repulsive interaction, while for an attractive two-body potential a paired ground state is possible. The flexibility of experimental techniques involved in the study of ultracold atom physics allows to envisage experimental conditions where these two different regimes are attained. For example exploiting a Feshbach resonance it is possible to drive the scattering length \( a_s \) from positive to negative values leading thus the system through a quantum phase transition.

The analytic procedure adopted hereafter deeply relies on the concept of quasi-free state [32]. In our situation the following definition of quasi-free state can be adopted:

1) all correlation functions can be computed from Wick’s theorem;
II) four fermionic expectation values over a quasi-free state have the form

\[
\langle \phi | e_1 e_2 e_3 e_4 | \phi \rangle = \langle \phi | e_1 e_2 | \phi \rangle \langle \phi | e_3 e_4 | \phi \rangle - \\
\langle \phi | e_1 e_3 | \phi \rangle \langle \phi | e_2 e_4 | \phi \rangle + \langle \phi | e_1 e_4 | \phi \rangle \langle \phi | e_2 e_3 | \phi \rangle
\]

with \(e_i = c_i, c_i^\dagger\). In particular we would like point out how the three terms on the right hand-side will lead to the direct, the exchange and pairing energy term of a Hatree-Fock-Bogoliubov mean field Hamiltonian, which, for our RHH becomes

\[
\hat{H}_{2\text{-level}}^{HF B} = \hat{H}_0 + \sum_{i,a,b,c,d, \sigma \neq \sigma'} U_{a,b,c,d} \left[ \chi_{i,a,\sigma,c,\sigma'} \hat{c}_{i,b,\sigma}^\dagger \hat{c}_{i,d,\sigma'} + \chi_{i,d,\sigma',b,\sigma'} \hat{c}_{i,a,\sigma} \hat{c}_{i,c,\sigma'} - \chi_{i,c,\sigma,b,\sigma'} \hat{c}_{i,a,\sigma} \hat{c}_{i,d,\sigma'} - \chi_{i,a,\sigma',c,\sigma} \hat{c}_{i,b,\sigma} \hat{c}_{i,c,\sigma'} + \xi_{i,b,\sigma',a,\sigma} \hat{c}_{i,a,\sigma} \hat{c}_{i,d,\sigma'} + \xi_{i,d,\sigma',a,\sigma} \hat{c}_{i,a,\sigma} \hat{c}_{i,c,\sigma'} \right]
\]

with

\[
\hat{H}_0 = \sum_{i,a,\sigma} \left[ \lambda_a \hat{n}_{i,a,\sigma} + T \left( \hat{c}_{i+1,a,\sigma}^\dagger \hat{c}_{i,a,\sigma} + \text{h.c.} \right) \right]
\]

\[
\chi_{i,a,\sigma,b,\sigma'} = \langle \phi_{HF B} | \hat{c}_{i,a,\sigma}^\dagger \hat{c}_{i,b,\sigma'} | \phi_{HF B} \rangle
\]

\[
\xi_{i,a,\sigma,b,\sigma'} = \langle \phi_{HF B} | \hat{c}_{i,a,\sigma} \hat{c}_{i,b,\sigma'} | \phi_{HF B} \rangle
\]

The set of generators \(\{ \hat{c}_\alpha^\dagger \hat{c}_\beta - \frac{1}{2} \delta_{\alpha\beta} (1 \leq \alpha \neq \beta \leq r), \hat{c}_\alpha^\dagger \hat{c}_\beta, \hat{c}_\alpha, \hat{c}_\beta \} (1 \leq \alpha \neq \beta \leq r)\) obeys the following commutation relations

\[
\left[ \hat{c}_i^\dagger \hat{c}_j - \frac{1}{2} \delta_{ij}, \hat{c}_k^\dagger \hat{c}_l - \frac{1}{2} \delta_{kl} \right] = \delta_{jk}(\hat{c}_i^\dagger \hat{c}_l - \frac{1}{2} \delta_{il})
\]

\[
\left[ \hat{c}_i^\dagger \hat{c}_j - \frac{1}{2} \delta_{ij}, \hat{c}_k^\dagger \hat{c}_l \right] = \delta_{jk}(\hat{c}_i^\dagger \hat{c}_l - \frac{1}{2} \delta_{il})
\]

\[
\left[ \hat{c}_i \hat{c}_j, \hat{c}_k^\dagger \hat{c}_l^\dagger \right] = \delta_{ik}(\hat{c}_j^\dagger \hat{c}_l - \frac{1}{2} \delta_{jl}) + \delta_{jl}(\hat{c}_k^\dagger \hat{c}_j - \frac{1}{2} \delta_{kj})
\]

allowing to state that the dynamical algebra of this new Hamiltonian, which is now quadratic in terms of \(\hat{c}_i, \hat{c}_i^\dagger\) can be easily recognised to be \(so(2r)\) \(33\).
Having determined the dynamical algebra of the model Hamiltonian, enables us – at least in principle- to find the ground state of the system with a straightforward procedure. As it will be clear form the subsequent discussion, the main difficulties arise as the number the generators of the \( so(2r) \) algebra grows with \( r(2r - 1) \). For instance for the two-site, \( J = 0,1/2 \) model, the Hamiltonian dynamical algebra will have 276 generators.

In spite of the technical difficulties (both analytical and numerical), it is appropriate to apply algebraic techniques to diagonalise \( \hat{H}_{2\text{-level}}^{HF} \). As stated before, this general approach will give some insight to the ground state properties of the system. If we consider a unitary transformation \( g \in SO(2r) \) we can write

\[
\hat{H}_d = g \hat{H}_{HF} g^{-1}
\]

where \( \hat{H}_d \) is diagonal. As a direct consequence the ground state \( |\phi_{HF} > \) of \( \hat{H}_{2\text{-level}}^{HF} \) can be written as

\[
|\phi_{HF} > = g|0,0,\ldots,0,0 > = g|0 >
\]

where \( |0 > \) can be defined as the Bogoliubov particle vacuum (ground state of \( \hat{H}_d \)). Following \[33\], \( |0 > \) represents a possible choice for the extremal state for the \( SO(2r) \) group with \( U(r) \) as the corresponding maximum stability subgroup. Leading to

\[
g|0 > = \Omega h|0 > \Omega|0 > e^{i\phi(h)}
\]

where:

\[
\Omega = \exp \sum_{1 \leq \alpha \neq \beta \leq r} (\eta_{\alpha,\beta} \hat{c}_\alpha^{\dagger} \hat{c}_\beta^{\dagger} - H.c.) \in \frac{SO(2r)}{U(r)}.
\]

The phase appearing in Eq.(44) has no relevance for our purposes, as we are interested in the evaluation of observable expectation values.

The problem mentioned above about the size of the dynamical algebra, appears here with all its implications. It is necessary to exponentiate the operator \( \sum_{1 \leq \alpha \neq \beta \leq r} (\eta_{\alpha,\beta} \hat{c}_\alpha^{\dagger} \hat{c}_\beta^{\dagger} - H.c.) \) which is a \( 2r \times 2r \) matrix in the faithful matrix representation.

Nevertheless, for a repulsive two-body potential, the pairing term can be neglected \[32\], thus the dynamical algebra of the system becomes \( U(r) \). Following \[33\], we can express the Hamiltonian ground state as

\[
|\phi_{HF} >= \exp \sum_{\begin{subarray}{c} k+1 \leq \alpha \leq r \\
1 \leq j \leq k
\end{subarray}} (\eta_{\alpha,\beta} \hat{c}_\alpha^{\dagger} \hat{c}_\beta - H.c.) |0 >
\]
where
\[ |0> = \underbrace{|1, 1, \ldots, 1, 0, \ldots, 0>}_k \] (47)

which is, in fact, the ground state of the non interacting Hamiltonian. It is worth noticing that this general procedure can be greatly simplified if further constraints, related to symmetries of the problem, are imposed onto the coefficients \( \eta_{\alpha,\beta} \). For example, if we consider the two-site \((A,B)\), \( J = 0, 1/2 \) case, due to equation (36) the matrix \( \eta \) with elements \( \eta_{\alpha,\beta} \) will have the form

\[
\eta = \begin{pmatrix}
0 & \eta_{1,2} & \eta_{1,3} & \eta_{1,4} & \eta_{1,5} & \eta_{1,6} & \eta_{1,7} & 0 & 0 & 0 & 0 \\
-\eta_{1,2} & 0 & \eta_{2,3} & \eta_{2,4} & \eta_{2,5} & \eta_{2,6} & \eta_{2,8} & 0 & 0 & 0 & 0 \\
-\eta_{1,3} & -\eta_{2,3} & 0 & \eta_{3,4} & \eta_{3,5} & \eta_{3,6} & 0 & 0 & \eta_{3,9} & 0 & 0 \\
-\eta_{1,4} & -\eta_{2,4} & -\eta_{3,4} & 0 & \eta_{4,5} & \eta_{4,6} & 0 & 0 & 0 & \eta_{4,10} & 0 & 0 \\
-\eta_{1,5} & -\eta_{2,5} & -\eta_{3,5} & -\eta_{4,5} & 0 & \eta_{5,6} & 0 & 0 & 0 & 0 & \eta_{5,11} & 0 \\
-\eta_{1,6} & -\eta_{2,6} & -\eta_{3,6} & -\eta_{4,6} & -\eta_{5,6} & 0 & 0 & 0 & 0 & 0 & 0 & \eta_{6,12} \\
-\eta_{1,7} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\eta_{2,8} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\eta_{3,9} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -\eta_{4,10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\eta_{5,11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\eta_{6,12} & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix} \] (48)

thus impressively reducing the computational effort needed to evaluate the exponential in
V. CONCLUSIONS

In this paper we have investigated the complex structure of fermion interactions for a fermion gas distributed in a linear periodic array of potential wells. Based on the standard many-fermion quantum field theory endowed with a potential distribution mimicking a realistic experimental setup, we have calculated analytically the hopping and interaction coefficients that describe the interactions of fermions within a generalised multimode Hubbard Hamiltonian. Their dependence on the external controllable parameters (such as laser intensity, magnetic trap frequency, wavelength, and scattering length) has been determined.

Our analysis shows that, except for two particularly simple cases (the gas of spin unpolarised fermions and the gas of noninteracting spin polarised fermions), models with different degree of complexity can be derived depending on the interaction processes one decides to account for or to neglect [consider, e. g., that, in principle, one might introduce an unlimited number of (local) rotational levels]. In this respect, our simplest nontrivial model (40), which is able to account for the (local) rotational activity of fermions, appears to be far more complex than the Hubbard model or the spin-polarised noninteracting model derived in section IV.

Therefore, the first objective of our future work is to perform a systematic study of model (40). Based on the present analysis and exploiting the interaction-parameter scenario here depicted, the second objective is to recognise the significant regimes characterising the confined fermion gas and to derive the relevant models from Eq. (34).

We would like to stress once again how the analytical knowledge of the coefficients in
principle allows us to tailor Hamiltonians performing specific tasks.

An aspect that certainly deserves attention is the study of the zero-temperature phase diagram of model (40) (and, more in general, of sufficiently simple—and thus tractable—models derived from the gHH) and of the relevant phenomenology aimed at suggesting new possible experiments. To achieve a reliable description of these systems, several established analytical and numerical approaches (see e.g. [38, 39], and [40, 41, 42], respectively) can be implemented in analogy to what has been done for bosons [41, 42]. Moreover in the recent past several authors (see e.g. [43, 44]) have proposed to use entanglement measures as a quantum phase transition identifier. We think that our model can represent a good test-field for this new approach to quantum-phase transitions.

APPENDIX A: TUNNELLING COEFFICIENT CALCULATION

In the following calculation we will fix $n_{\beta} \geq n_{\alpha}$, without loss of generality, as it can be easily verified.

The integral in Eq. (21) can be decomposed in the sum of three terms

$$\Theta_{n_{\alpha},n_{\beta}}^{n_{\alpha},n_{\beta}} + \Theta_{n_{\alpha},n_{\beta}}^{n_{\alpha},n_{\beta}} + \Theta_{n_{\alpha},n_{\beta}}^{n_{\alpha},n_{\beta}} = \int dy e^{-\frac{(y-\tau)^2}{2}} H_{n_{\alpha}}(y-\tau) f(y) e^{-\frac{y^2}{2}} H_{n_{\beta}}(y)$$

with

$$f(y) = \left[1 - \cos(2\Omega y)\right] - \frac{y^2}{4\Omega^2},$$

integral (A1) becomes

$$\Theta_{1}^{n_{\alpha},n_{\beta}} = \int \frac{dy}{4\Omega^2} e^{-\frac{\tau^2}{2}} H_{n_{\beta}}(y-\tau) H_{n_{\alpha}}(y),$$

$$\Theta_{2}^{n_{\alpha},n_{\beta}} = \int \frac{dy}{4\Omega^2} e^{-\frac{\tau^2}{2}} \cos(2\Omega y) \times H_{n_{\alpha}}(y) H_{n_{\beta}}(y-\tau),$$

$$\Theta_{3}^{n_{\alpha},n_{\beta}} = -\frac{1}{2} \int dy y^2 e^{-\frac{(y-\tau)^2}{2}} \times H_{n_{\alpha}}(y) H_{n_{\beta}}(y-\tau),$$

The substitution $\zeta = y - \tau/2$ yields

$$\Theta_{1}^{n_{\alpha},n_{\beta}} = C_{\Omega}^{\tau} \int d\zeta e^{-\zeta^2} H_{n_{\alpha}}\left(\zeta + \frac{\tau}{2}\right) H_{n_{\beta}}\left(\zeta - \frac{\tau}{2}\right)$$
where \( C_\Omega^\tau = e^{-\tau^2/4}/(4\Omega^2) \). We then use the Hermite polynomial identity

\[
H_n(x + y) = \sum_{k=0}^{n} \binom{n}{k} H_k(x)(2y)^{n-k}
\]  
(A6)

to obtain

\[
\Theta_1^{n_\alpha,n_\beta} = \frac{e^{-\tau^2}}{4\Omega^2} \int d\zeta e^{-\zeta^2} \sum_{l,k=0}^{n_\alpha} \binom{n_\alpha}{l} \binom{n_\beta}{k} \tau^{n_\alpha+n_\beta-(l+k)} (-1)^{n_\beta-k} H_k(\zeta) H_l(\zeta)
\]  
(A7)

With the orthogonality of Hermite polynomials

\[
\int_{-\infty}^{\infty} dx H_n(x) H_m(x) e^{-x^2} = \delta_{n,m} 2^n n! \sqrt{\pi}
\]  
(A8)

we are able to perform the \( \zeta \) integration

\[
\Theta_1^{n_\alpha,n_\beta} = \frac{\sqrt{\pi} n_\alpha! 2^{n_\alpha}}{4\Omega^2(-\tau)^{n_\alpha-n_\beta}} e^{-\tau^2/4} L_{n_\alpha}^{n_\beta-n_\alpha}(\frac{\tau^2}{2})
\]  
(A9)

It is worth noting that the summation extends to \( n_\alpha \), that is \((a \, b) = 0 \) if \( a < b \). From \[36\] it can be verified that the last summation is related to generalised Laguerre polynomials, giving

\[
\Theta_1^{n_\alpha,n_\beta} = \frac{\sqrt{\pi} n_\alpha! 2^{n_\alpha}}{4\Omega^2(-\tau)^{n_\alpha-n_\beta}} e^{-\tau^2/4} L_{n_\alpha}^{n_\beta-n_\alpha}(\frac{\tau^2}{2})
\]  
(A10)

We move now to the calculation of \( \Theta_2^{n_\alpha,n_\beta} \) which is given by

\[
\Theta_2^{n_\alpha,n_\beta} = -\frac{1}{4\Omega^2} \int dy \exp \left[ -\frac{y^2}{2} \right] H_{n_\alpha}(y) \exp \left[ -\frac{(y-\tau)^2}{2} \right] H_{n_\beta}(y-\tau) \cos(\Omega y).
\]  
(A11)

Eq. (A11), with the substitution \( \zeta = y - \tau/2 \), can be written as

\[
\Theta_2^{n_\alpha,n_\beta} = -\frac{1}{4\Omega^2} \exp \left( -\tau^2/4 \right) \int d\zeta e^{-\zeta^2} H_{n_\alpha}(\zeta + \frac{\tau}{2}) H_{n_\beta}(\zeta + \frac{\tau}{2}) \cos(\Omega \zeta)
\]  
(A12)

Again, using Eq. (A6) gives

\[
\Theta_2^{n_\alpha,n_\beta} = -\frac{e^{-\tau^2/4}}{4\Omega^2} \sum_{l,k=0}^{n_\alpha} \binom{n_\alpha}{l} \binom{n_\beta}{k} \tau^{n_\beta+n_\alpha-(l+k)}
\]

\[
\times (-1)^{n_\beta-k} \int d\zeta e^{-\zeta^2} H_k(\zeta) H_l(\zeta) \cos(2\Omega \zeta)
\]  
(A13)

The integral in equation (A13) can be interpreted as the real Fourier transform of the function

\[
e^{-\zeta^2} H_k(\zeta) H_l(\zeta)
\]
Recalling that
\[ \mathcal{F}[f(x)g(x)] = \mathcal{F}[f(x)] \ast \mathcal{F}[g(x)], \]
where \( \mathcal{F}[\cdot] \) indicates Fourier transform and \( \ast \) convolution product, we obtain
\[ \Theta_{n_\alpha, n_\beta} = -\frac{e^{-\frac{\tau^2}{4}}}{4\Omega^2} \sum_{l,k=0}^{n_\alpha, n_\beta} \binom{n_\alpha}{l} \binom{n_\beta}{k} \tau^{n_\beta+n_\alpha-l-k} \]
\times (-1)^n_\beta-k \Re \left[ \mathcal{F}[e^{-\frac{\zeta^2}{2}} H_k(\zeta)] \ast \mathcal{F}[e^{-\frac{\tau^2}{2}} H_l(\zeta)] \right] \quad (A14)
giving
\[ \Theta_{n_\alpha, n_\beta} = -\frac{e^{-\tau^2/4}}{4\Omega^2} \sum_{l,k=0}^{n_\alpha, n_\beta} \binom{n_\alpha}{l} \binom{n_\beta}{k} \tau^{n_\beta+n_\alpha-(l+k)} (-1)^{n_\beta-k+l} \]
\times \Re \left[ i^{l+k} \int \epsilon e^{-\frac{2(\epsilon-2\Omega)^2}{4\Omega^2}} H_k(\epsilon) H_l(\epsilon - 2\Omega) \right]. \quad (A15)
The integral on the left-hand side of equation (A14) can be solved following the same procedure used for \( \Theta_{n_\alpha, n_\beta} \)
\[ \int \epsilon e^{-\tau^2/2} H_k(\epsilon) e^{-\frac{1}{2}(\epsilon-2\Omega)^2} H_l(\epsilon - 2\Omega) = (-1)^{k-l} \sqrt{\pi} e^{-\Omega} (2\Omega)^{k-l} l! 2^l L_{l-k}^{k-l} (4\Omega^2) \quad (A16) \]
giving
\[ \Theta_{n_\alpha, n_\beta} = -\frac{e^{-\frac{\tau^2}{4}}}{4\Omega^2} \sum_{l,k=0}^{n_\alpha, n_\beta} \binom{n_\alpha}{l} \binom{n_\beta}{k} \tau^{n_\beta+n_\alpha-(l+k)} (-1)^{n_\beta} \]
\times 2^l l! \Re \left[ i^{l+k} \frac{\sqrt{\pi}}{(2\Omega)^l-k} L_{l-k}^{k-l} (2\Omega^2) e^{-\Omega^2} \right]. \quad (A17)
The calculation of \( \Theta_{3, n_\alpha, n_\beta} \) is quite straightforward. Applying twice the identity
\[ x H_n(x) = \frac{1}{2} H_{n+1}(x) + n H_{n-1}(x) \]
we can write \( \Theta_{3, n_\alpha, n_\beta} \) as
\[ \Theta_{3, n_\alpha, n_\beta} = -\frac{e^{-\frac{\tau^2}{4}}}{2} \int d\zeta e^{-\zeta^2} \left[ \frac{1}{4} H_{n+2}(\zeta + \frac{\tau}{2}) + \frac{2n_\alpha + 1}{2} H_{n_\alpha}(\zeta + \frac{\tau}{2}) + n_\alpha(n_\alpha - 1) \right] \]
\times H_{n_\alpha-2}(\zeta + \frac{\tau}{2}) L_{n_\beta}(\zeta - \frac{\tau}{2}) \quad (A18)
With the same procedure used for \( \Theta_{1, n_\alpha, n_\beta} \), \( \Theta_{3, n_\alpha, n_\beta} \) is given by
\[ \Theta_{3, n_\alpha, n_\beta} = \frac{(-1)^{n_\beta-n_\alpha+1}}{2} \sqrt{\pi} 2^n_\alpha n_\alpha! \tau^{n_\beta-n_\alpha} e^{-\frac{\tau^2}{4}} \left[ \frac{(n_\alpha + 1)(n_\alpha + 2)}{2} \right] L_{n_\alpha+2}(\tau^2/2) + \]
\[ + \frac{\tau^2_2}{4} L_{n_\alpha-2}^{n_\beta-n_\alpha+2} \left( \frac{\tau^2}{2} \right) + \frac{2n_\alpha + 1}{2} L_{n_\alpha}^{n_\beta-n_\alpha} \left( \frac{\tau^2}{2} \right) \] \quad (A20)
Hence $T_{\alpha,\beta}$ becomes

$$T_{\alpha,\beta} = -\frac{\hbar \omega_s \delta J_{\alpha,\beta} \delta m_{\alpha,m_{\beta}} \delta \sigma_{\alpha,\sigma_{\beta}}}{\sqrt{2^{n_{\alpha}+n_{\beta}+2} n_{\alpha}! n_{\beta}!}} \left[ \Theta^{n_{\alpha},n_{\beta}}_{1} + \Theta^{n_{\alpha},n_{\beta}}_{2} + \Theta^{n_{\alpha},n_{\beta}}_{3} \right] \tag{A21}$$

with $\Theta^{n_{\alpha},n_{\beta}}_{1}$, $\Theta^{n_{\alpha},n_{\beta}}_{2}$, and $\Theta^{n_{\alpha},n_{\beta}}_{3}$ given by formulas (A10), (A17), and (A20), respectively.

We have here the plot of $T_{n_{\alpha},n_{\beta},i_{\alpha},i_{\alpha}+1}$ as a function of the difference $i_{\alpha} - i_{\beta}$ for values of $n_{\alpha}$ and $n_{\beta}$ ranging from 0 to 2.

The long distance exponential decay is common to all tunnelling coefficients, regardless of the energy level. On the other hand its detailed shape has deep relevance for nearest-neighbours and next-to-nearest-neighbours (i.e. there may be sign changes passing from $T_{n,m,i,i+1}$ and $T_{n,m,i,i+2}$) as shown in figures (2-4). Another interesting feature is that an extra-term, due to “on site” tunnelling coefficients, must be added to the harmonic-oscillator energy term.

**FIG. 2:** Plot of $T_{n_{\alpha},n_{\beta}}$ from $T_{0,0,i_{\alpha},i_{\alpha}}$ to $T_{0,2,i_{\alpha},i_{\beta}}$. The solid line represents the case of a ground-state tunnelling. In this case the hopping parameter $T_{0,0,i_{\alpha},i_{\beta}}$ is always positive. However, inter-level tunnelling already shows sign changes.

**APPENDIX B: INTERACTION COEFFICIENTS**

We provide here the detailed calculation for the interaction term matrix elements. To solve integral (26)

$$U_x = \frac{1}{\pi l_x} \sqrt{\frac{2^{-(n_{\alpha}+n_{\beta}+n_{\gamma}+n_{\delta})}}{n_{\alpha}! n_{\beta}! n_{\gamma}! n_{\delta}!}} \times \int dx H_{n_{\alpha}}(x) H_{n_{\beta}}(x) H_{n_{\gamma}}(x) H_{n_{\delta}}(x) e^{-2x^2}$$

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FIG. 3: Plot of $T_{n_\alpha,n_\beta}$ from $T_{1,0,i_\alpha,i_\beta}$ to $T_{1,2,i_\alpha,i_\beta}$. In this situation the intra-level tunnelling term $T_{1,1,i_\alpha,i_\beta}$ is always negative, but if a different external parameter choice is considered, the sign change can be placed between 1 and 2.

FIG. 4: Plot of $T_{n_\alpha,n_\beta}$ from $T_{2,0,i_\alpha,i_\beta}$ to $T_{2,2,i_\alpha,i_\beta}$. In this case the sign change for the intra-level tunnelling term occurs for the specific parameter choice performed here, but it can be removed by a different choice of the external parameters.

we exploit again Eq. (A6), obtaining

$$U_x = \frac{1}{\pi l_x} \sqrt{\frac{2^{-(n_\alpha+n_\beta+n_\gamma+n_\delta)}}{n_\alpha!n_\beta!n_\gamma!n_\delta!}} \sum \frac{(n_\alpha)}{(i_\alpha)} \left( \begin{array}{c} n_\beta \\ i_\beta \end{array} \right) \left( \begin{array}{c} n_\gamma \\ i_\gamma \end{array} \right) \left( \begin{array}{c} n_\delta \\ i_\delta \end{array} \right) H_{i_\alpha}(0)H_{i_\beta}(0)H_{i_\gamma}(0)H_{i_\delta}(0)$$

$$\times \int d\zeta (2\zeta)^{n_\alpha+n_\beta+n_\gamma+n_\delta-(i_\alpha+i_\beta+i_\gamma+i_\delta)} e^{-2\zeta^2}. \quad (B1)$$
In previous equation the summation must be intended over four independent of $s_\theta = 0 \ldots n$ with $\theta = \alpha, \beta, \gamma, \delta$. With the substitution
\[
\int d\zeta (2\zeta)^\alpha e^{-2\zeta^2} = \delta_{\alpha,2N} \sqrt{2}^{\alpha-3} \Gamma[(\alpha + 1)/2]
\] (B2)
($\delta_{\alpha,2N}$ indicates that $\alpha$ must be an even number) Eq. (B1) becomes
\[
U_x = \frac{1}{\pi l_x} \sum_{\bar{s}} \frac{\Xi(\bar{s})}{\sqrt{2}^{||\bar{n}||+3}} \Gamma \left[ \frac{||\bar{n}|| - ||\bar{s}|| + 1}{2} \right] \delta_{||\bar{n}||,2N}
\] (B3)
with
\[
\bar{a} = \{a_\alpha, a_\beta, a_\gamma, a_\delta\} \quad 1\text{-norm:} \quad ||\bar{a}|| = \sum_\theta a_\theta
\] (B4)
and
\[
\Xi(\bar{s}) = \prod_\theta \frac{1}{\sqrt{n_\theta}} \left( \frac{n_\theta}{s_\theta} \right) H_{s_\theta}(0)
\] (B5)
where $\Xi(\bar{s}) = 0$ for odd $i_\theta$. The $\delta$ function in Eq. (B3) should be written as $\delta_{||\bar{n}||-||\bar{s}||,2N}$. However the condition $||i_\theta|| = \text{even}$ already implies $||\bar{s}|| = \text{even}$. We are then allowed to write in Eq. (B3):
\[
\delta_{||\bar{n}||-||\bar{s}||,2N} = \delta_{||\bar{n}||,2N}.
\]

We solve now the radial part of the interaction term integral written in Eq. (B3)
\[
U_\rho = \int \int \frac{d^2\eta}{\pi} \mathcal{L}_{J_\alpha,m_\alpha}(\eta) \mathcal{L}_{J_\beta,m_\beta}(\eta) \mathcal{L}_{J_\gamma,m_\gamma}(\eta) \mathcal{L}_{J_\delta,m_\delta}(\eta),
\]
where $\eta = (\rho, \phi)$ and $d^2\eta = \rho d\rho d\phi$. Following [36], we express $\mathcal{L}_{J_\alpha,m_\alpha}(\rho, \phi)$ in terms of a finite sum:
\[
\mathcal{L}_{J_\alpha,m_\alpha}(\rho, \phi) = e^{2im_\alpha \phi} e^{-\rho^2/\ell_\perp^2} \frac{1}{\sqrt{(J_\alpha + m_\alpha)!(J_\alpha - m_\alpha)!}} \prod_{q_\alpha} \left( \frac{(-1)^{J_\alpha - q_\alpha} \left( \frac{\rho}{\ell_\perp} \right)^{2q_\alpha}}{(J_\alpha - q_\alpha)!(q_\alpha + m_\alpha)!(q_\alpha - m_\alpha)!} \right)
\] (B6)
Hence the radial part of $\mathcal{L}_{J_\alpha,m_\alpha}(\bar{\rho}, \phi)$ can be written as
\[
R_{J_\alpha,m_\alpha}(\bar{\rho}) = \frac{e^{-\bar{\rho}/\ell_\perp^2/2}}{\ell_\perp} \sum_{q_\alpha = |m_\alpha|}^{J_\alpha} \Lambda_\alpha \left( \frac{\bar{\rho}}{\ell_\perp} \right)^{2q_\alpha}
\] (B7)
where
\[
\Lambda_\alpha = \frac{(-1)^{J_\alpha - q_\alpha} \sqrt{(J_\alpha + m_\alpha)!(J_\alpha - m_\alpha)!}}{(J_\alpha - q_\alpha)!(q_\alpha + m_\alpha)!(q_\alpha - m_\alpha)!}.
\] (B8)
Substituting Eq. (B7) into Eq. (29) we have
\[
U_\rho = \frac{2\delta_{m_\alpha+m_\gamma,m_\beta+m_\delta}}{\pi l_\perp^4} \sum_{q_\alpha=|m_\alpha|}^{J_\alpha} \sum_{q_\beta=|m_\beta|}^{J_\beta} \sum_{q_\gamma=|m_\gamma|}^{J_\gamma} \sum_{q_\delta=|m_\delta|}^{J_\delta}
\times \Lambda_\alpha \Lambda_\beta \Lambda_\gamma \Lambda_\delta \int_0^\infty d\rho \frac{\rho}{\pi l_\perp^2} \left( \frac{\rho}{l_\perp} \right)^{2||\bar{q}||} e^{-2\bar{\rho}^2} \tag{B9}
\]
that, with the same notation of Eq. (B3), becomes
\[
U_\rho = \frac{\delta_{m_\alpha+m_\gamma,m_\beta+m_\delta}}{\pi l_\perp^4} \sum_{\bar{q}=|\bar{m}|}^{\bar{J}} \Lambda \left( \bar{J}, \bar{m}, \bar{q} \right) \frac{\Gamma \left( ||\bar{q}|| + \frac{3}{2} \right)}{2||\bar{q}|| + 3/2} \tag{B10}
\]
with
\[
\Lambda \left( \bar{J}, \bar{m}, \bar{q} \right) = \prod_{\theta=\alpha,\beta,\gamma,\delta} \Lambda_\theta . \tag{B11}
\]

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