Effect of a lattice upon an interacting system of electrons: Breakdown of scaling and decay of persistent currents

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(received ; accepted )

PACS. 71.10-w – Theories and models for many-electron systems.
PACS. 71.10.Fd – Lattice fermion models.
PACS. 73.20.Qt – Electron solids.

Abstract. – For an interacting system of $N$ electrons, we study the conditions under which a lattice model of size $L$ with nearest neighbor hopping $t$ and $U/r$ Coulomb repulsion has the same ground state as a continuum model. For a fixed value of $N$, one gets identical results when the inter-electron spacing to the Bohr radius ratio $r_s < r_s^*$. Above $r_s^*$, the persistent current created by an enclosed flux begins to decay and $r_s$ ceases to be the scaling parameter. Three criteria giving similar $r_s^*$ are proposed and checked using square lattices.

To numerically study an interacting system of $N$ electrons, it is convenient to use a lattice model of size $L$, which can be exactly solved when $N$ and $L$ are small. To compare exact lattice results with those obtained assuming a continuum space and hence unavoidable approximations (truncations, perturbative expansions, variational approaches, fixed node Monte Carlo calculations[1],...), one needs to know the role of the lattice upon the interacting system. Using the inter-particle spacing to the Bohr radius ratio $r_s$, we define in this letter the value $r_s^*$ which characterizes the onset of the lattice effects for the ground state (GS). Assuming that $N$ is given and varying the other parameters of the lattice model, one finds that below $r_s^*$ the lattice GS is identical to the continuum GS, $r_s$ is the scaling parameter, and the persistent current $I$ created by an enclosed flux keeps its value without interaction. Above $r_s^*$, the $N$ electrons are localized by $N$ lattice sites, the GSs become different, $I$ begins to decay, and a lattice physics where $r_s$ is no longer the scaling parameter takes place.

The Hamiltonian $H_c$ describing $N$ electrons free to move on a continuum space of dimension $d$ contains one body kinetic terms, two body interaction terms plus a constant term due to the presence of the uniform positive background which can be added in order to have charge neutrality. Measuring the energies in rydbergs ($1\text{Ry} = me^4/2\hbar^2$) and the lengths in units of...
the radius $a$ of a sphere (circle in 2$d$) which encloses on the average one electron, $e$ and $m$ being the electronic charge and mass, $H_e$ reads

$$H_e = -\frac{1}{r_s} \sum_{i=1}^{N} \nabla_i^2 + \frac{2}{r_s} \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|} + \text{const},$$

which only depends on the scaling ratio $r_s = a/a_B$ when $N \to \infty$. The Bohr radius $a_B = \hbar^2/me^2$ characterizes the scale for the quantum effects. For the GS, many electrons are inside the quantum volume $a_B^d$ when $r_s$ is small and one gets a weakly coupled Fermi liquid. When $r_s$ is large, the volume per electron $a_B^d$ is large compared to $a_B^d$, and one gets an electron solid (Wigner crystal) with almost negligible quantum effects. Hereafter, though our theory could be easily extended, we restrict ourselves to polarized electrons (spinless fermions) at $d = 2$. Assuming periodic boundary conditions (BCs) for a square of size $D$, one can ignore the constant term, the electronic density $n_s = N/D^2$ and $a = 1/\sqrt{\pi n_s}$.

Let us now define a square lattice model of spacing $s$, size $L = D/s$, nearest neighbor hopping element $t = \hbar^2/(2ms^2)$ and interaction strength $U = e^2/s$. The lattice Hamiltonian $H_l$ reads:

$$H_l = t \left( 4N - \sum_{\langle j,j' \rangle} c_{j}^\dagger c_{j'} \right) + \frac{U}{2} \sum_{j \neq j'} n_{j} n_{j'}/|d_{jj'}|.$$  

The operators $c_{j}^\dagger$ ($c_{j}$) create (annihilate) a spinless fermion at the site $j$ and $\langle j, j' \rangle$ means that the sum is restricted to nearest neighbors. $d_{jj'}$ is the distance between the sites $j$ and $j'$ in unit of $s$. When one takes periodic BCs, a convention has to be chosen for the distance $d_{jj'}$. One possible definition of $d_{jj'}$ is:

$$d_{jj'} = \sqrt{\min(|j_x - j'_x|, L - |j_x - j'_x|)^2 + \min(|j_y - j'_y|, L - |j_y - j'_y|)^2}.$$  

Hereafter, we refer to the corresponding $1/|d_{jj'}|$ repulsion as the periodic singular Coulomb (PSC) repulsion, since it has a cusp when the interparticle distance $d_{jj'}$ has one of its coordinates equal to $L/2$. This cusp being unphysical, we define also the periodic regularized Coulomb (PRC) repulsion defined from

$$d_{jj'} = \frac{L}{\pi} \sqrt{\sin^2 \frac{|j_x - j'_x| \pi}{L} + \sin^2 \frac{|j_y - j'_y| \pi}{L}}.$$  

which locally coincides with the PSC repulsion, but remains analytic for all values of $d_{jj'}$ when $s \to 0$. The PRC repulsion is essentially equivalent to the Ewald repulsion obtained from the periodic repetition of the considered system. In the lattice units, $1Ry = U^2/4t$ and the ratio $r_s$ becomes:

$$r_s = \frac{UL}{2t\sqrt{\pi N}}.$$  

The question is to know whether $UL/(2t\sqrt{\pi N})$ remains a scaling parameter for $H_l$. The answer is positive if $r_s < r_s^*$. Below $r_s^*$, the lattice GS depends on the ratio $UL/t$ for a fixed value of $N$, and coincides with the continuum GS. Let us define three criteria giving $r_s^*$.

Criterion 1: In the limit $t = 0$, the $N$ electrons are localized on $N$ sites and form states $|J \rangle = c_{j_1}^\dagger \ldots c_{j_N}^\dagger |0 \rangle$ of energy $E_{Coul}(J)$. As one turns on $t$, one can expect that the lattice becomes irrelevant as each electron ceases to be localized on a single site. In analogy with the problem of a single particle in a disordered lattice, one can use the criterion first proposed by
Assuming that the values of the lattice parameters can yield a Wigner solid for a square lattice with either the PSC or PRC repulsions. A study of the case of motion of the solid when the GSs of $H$ Since the correction $E_\Delta C$ use the Kohn curvature $\expansion$. The value of $r$ gives the criterion 2 for $Nt$, $I$ for $t/U$ lattice expansion. The value of $r_s$ for which $I(U = 0) \approx I^{(N)}_t(t/U)$ gives the criterion 2 for $r_s^*$ (see Fig. 2 lower left). Instead of $I(\phi)$, one can prefer to use the Kohn curvature $C_K = \partial^2 E_0/\partial \phi^2$ evaluated at $\phi = 0$ or the GS energy change $\Delta T E_0 = E_0(\phi = 0) - E_0(\phi = \pi)$ when the BC is twisted in the $x$-direction.

**Criterion 3**: When $t/U \to 0$, the leading correction to the Coulomb energy of $H_t$ is $4Nt$. Since the correction $E_{vib}(r_s)$ to the Coulomb energy coming from the zero point vibrational motion of the solid when the GSs of $H_t$ and $H_c$ are similar cannot exceed this lattice limit $4Nt$ (see Fig. 1), $r_s^*$ is also given by the condition

$$E_{vib}(r_s) \approx 4Nt,$$

assuming that the values of the lattice parameters can yield a Wigner solid for $r_s < r_s^*$. Let us calculate the quantities used in those criteria for the case of $N = 3$ spinless fermions on a square lattice with either the PSC or PRC repulsions. A study of the case $N = 2$ can be found in Ref.[15]. For $t = 0$, as shown in the insets of Figs. 1 and 2, the configurations minimizing the PRC and PSC Coulomb energies are different. Moving one particle by a single
hop increases these energies by an amount

$$\Delta E^{(PRC)}_{\text{Coul}} \approx \frac{7\sqrt{2}\pi^3 U}{12\sqrt{3}L^3} ; \quad \Delta E^{(PSC)}_{\text{Coul}} \approx \frac{\sqrt{2}U}{L^2}$$  \hspace{1cm} (9)$$

respectively when $L$ is sufficiently large. For $U = 0$, the GS energy is given by $E_0(0) = 12t - 8t - 4t \cos(2\pi/L)$ for periodic BCs and becomes $E_0(\pi) = 12t - 8t \cos(\pi/L) - 4t \cos(3\pi/L)$ when one twists the BC in the $x$-direction. When $t/U$ is small, $\Delta_T E_0$ can be calculated at the leading order of a $t/U$-expansion [14] for $N = 3$. This gives when $L$ is large:

$$\lim_{r_s \to 0} \Delta_T E_0 \approx \frac{14\pi^2 t}{L^2} ; \quad \lim_{r_s \to \infty} \Delta_T E_0 \approx \frac{9\pi^2 t^3}{L^2 \Delta E_{\text{Coul}}}$$  \hspace{1cm} (10)$$

where $\Delta E_{\text{Coul}}$ is given by the Eqs. (9). Using these expressions, one obtains from the two first criteria:

$$r^*_s(L) = AL^\alpha$$  \hspace{1cm} (11)$$

where $\alpha = 4$ for the PRC repulsion and $\alpha = 3$ for the PSC repulsion, the constant $A$ slightly depending on the taken criterion.

For using the third criterion, one needs the zero point vibrational energy of the Wigner molecule that the three particles form for a sufficiently large $r_s < r^*_s$. Since the GSs of $H_l$ and $H_c$ are identical for $r_s < r^*_s(L)$, instead of $H_l$, one can use $H_c$ which is the sum of two decoupled terms. Denoting $\mathbf{R} = (\sum_3 \mathbf{r}_i)/3$ the coordinate of the center of mass, the first term reads $H_{C_M} = (\hbar^2/6m)\nabla^2_{\mathbf{R}}$ and corresponds to the rigid translation of the molecule while the other term contains the relative motions and the interaction. For a Wigner molecule, the second part can be simplified and expressed in terms of the normal coordinates suitable for describing the small vibrations around equilibrium.

The PRC repulsion is harmonic around equilibrium, and the three particles form a diagonal chain as indicated in the inset of Fig. 1 when $L/3$ is integer. One gets four decoupled harmonic oscillators, two corresponding to a longitudinal mode of frequency $\omega_l = \sqrt{20B}$, the two others being a transverse mode of frequency $\omega_t = \sqrt{8B}$, where $B = (\sqrt{6e^2\pi})/(24D^3 m)$. The zero point vibrational energy is then given for $N = 3$ by:

$$E_{\text{vib}}(r_s, N = 3) = \hbar(\omega_l + \omega_t) = 2\pi \frac{\sqrt{5} + \sqrt{2}}{\sqrt{18}} \left(\frac{2}{\pi}\right)^{1/4} r_s^{-\beta}$$  \hspace{1cm} (12)$$

in rydbergs where $\beta = 3/2$.

When one takes the PSC repulsion, the three relative distances at equilibrium are precisely $\mathbf{r} = (L/2, L/2)$, $\mathbf{r} = (0, L/2)$ and $\mathbf{r} = (L/2, 0)$ respectively when $L$ is even. The potentials $v(\delta \mathbf{r})$ felt by the electrons around their equilibrium positions are singular and can be expanded as $v(\delta \mathbf{r}) \approx C_1(|\delta \mathbf{r}_x| + C_2|\delta \mathbf{r}_y|$, where $C_1$ and $C_2$ depend on the equilibrium positions and are $\propto \epsilon^2/D^2 = U/L^2$. For a single particle in a 1d-potential $v(x) = C|x|$, the GS energy $\epsilon$ can be approximated by $t/B^2 + CB$ where $B$ is the GS extension and is given by $\partial \epsilon/\partial B = 0$. This yields $B \propto (C/t)^{1/3}$ and $\epsilon \propto (U^2 t/L^4)^{1/3}$. Since the 2d-potential $v(\delta \mathbf{r})$ is separable, one eventually finds:

$$E_{\text{vib}}(r_s, N = 3) \propto r_s^{-\beta}$$  \hspace{1cm} (13)$$

in rydbergs where $\beta = 4/3$. As one can see, the PSC repulsion gives a higher exponent $\beta$ when $N = 3$, which is inconsistent with the usual expansion [16] in powers of $r_s^{-1/2}$ first proposed by Wigner.
From Eq. (12) and Eq. (13), since $4Nt$ in rydbergs is given by $(4L^2)/(\pi r_s^2)$, one obtains from the third criterion similar results for $r_s^*$. As in Eq. (11), with $\alpha = 4$ for the PRC repulsion and $\alpha = 3$ for PSC repulsion.

We now present numerical results obtained using the Lanczos algorithm, after having written $H_l$ in terms of the creation (annihilation) operators of a single particle in a state of momentum $k$ and having calculated the GSs in the sub-space of total momentum $K = 0$ [14]. From the GS energy $E_0(L, U, t)$ of $K = 0$, and for a given value of $N$, we define the dimensionless ratio $F_N(L, U, t)$ by:

$$F_N(L, U, t) = \frac{E_0(L, U, t) - E_0(L, U = 0, t)}{E_0(L, U = 0, t)}.$$ (14)

The results for the PRC repulsion are shown in Figure 1. For $t = 0$, the values of $L = 6, 9, 12, 15, 18$ are commensurate with the period of the diagonal Wigner molecule shown in the inset, reducing the lattice effects. When $F_{N=3}(L, U, t)$ is plotted as a function of $r_s = (UL)/(2t\sqrt{\pi N})$, the different functions $F_{N=3}(L, U, t)$ scale without an observable lattice effect up to the $r_s^*(L)$ exactly given by criterion 3. Using Eq. (13) and $E_0(L, U = 0, t) = 12t - 8t - 4t\cos(2\pi/L)$ one can see that the numerical results coincide with the analytical result $F_{N=3} = 0.5764/\sqrt{r_s}$ valid for a continuum Wigner molecule. The function $F_{N=3}(L, U, t)$ saturates to $4Nt/E_0(L, U = 0, t)$ above $r_s^*(L)$, as indicated by the dashed lines.

The corresponding results for the PSC repulsion are shown in Fig. 2 (upper left) for even values of $L$, where the GS is a triangular molecule shown in the inset when $t/U \rightarrow 0$. Again the curves scale up to the onset $r_s^*(L)$ given by criterion 3. But, $F_{N=3} \propto r_s^{2/3}$ for intermediate
Fig. 2. – Upper left: Same as in Fig. 1 using the PSC repulsion, where the dotted-dashed line now gives the $r_s^{2/3}$ behavior due to the vibrations of the Wigner molecule. Inset: a GS configuration when $t = 0$ and $L = 24$. Upper right: Energy ratios $F_N(L, U, t)$ using the PRC repulsion for $N = 3$ ($L = 18$ solid line) and $N = 4$ ($L = 6 \circ, 8 \bigcirc, 10 \bigtriangleup$) as a function of $r_s = UL/(2t\sqrt{\pi N})$. Lower left: Dimensionless change $\Delta_T E_0(r_s)/\Delta_T E_0(r_s = 0)$ of the GS energy when the longitudinal BC is twisted for $L = 6 \bigcirc, 9 \bigtriangleup, 12 \bigtriangleup, 15 \bigtriangleup, 18 \bigtriangleup$ as a function of $r_s$ (PRC repulsion). Lower right: First energy spacing $\Delta E_{\text{Coul}}$ yielded by the hop of one particle from the $t = 0$ GS as a function of $L$. $L^{-3}$ behavior yielded by the PRC repulsion ($\bigtriangleup$) for $N = 30$. Crossover towards the $L^{-2}$ decay (dashed line) yielded by the PSC repulsion ($\bigcirc$). Inset: One GS configuration yielded by the two repulsions ($t = 0, N = 30$ and $L = 30$).

$r_s$, as implied by Eq. (12), and not $\propto r_s^{1/2}$.

In Fig. 2 (upper right), a small change of the scaling curve $F_N$ can be seen when a fourth electron is added, accompanied by the expected breakdown of the scaling behavior above $r_s^*$. When $N \to \infty$, $F_N$ should converge towards a thermodynamic limit depending only on $r_s^*$. Unfortunately, a study of this convergence is out of reach of a numerical approach using exact diagonalization.

In Fig. 2 (lower left), we illustrate the criterion 2, showing for $N = 3$ the change $\Delta_T E_0$ of the GS energy when a BC is twisted. Below $r_s^*$, $\Delta_T E_0$ does not depend on the interaction, while above $r_s^*$, one gets the lattice limit given by Eq. (10). We have checked that the same conclusions can be drawn from a study of the Kohn curvature $C_K(r_s)$.

The PSC and PRC repulsions give rise to different $r_s^*(L)$, $F_{N=3} \propto r_s^{2/3}$ for the PSC repulsion,
differing from the conventional expansion in powers of $r_s^{1/2}$. Does this difference remain for larger values of $N$? Indeed the contribution of pairs $ij$ having the coordinates of their spacings $d_{ij}$ close to $D/2$, and responsible for the $r_s^{2/3}$ behavior when $d_{ij}$ is defined by Eq. (3), becomes a surface effect $\propto N$ compared to the bulk contribution $\propto N^2$ of the remaining pairs, yielding $\Delta E_{\text{PSC}}^\text{Coul} \approx AN/L^2 + BN^2/L^3$, where $A$ and $B$ are constant. For a fixed $L$ and increasing $N$, $\Delta E_{\text{PSC}}^\text{Coul} \to BN^2/L^3$ and following criterion 1, the conventional $r_s^{1/2}$ expansion for $F_N$ should valid for the PSC repulsion too. However, for $N$ fixed and increasing $L$, the surface contribution dominates and the difference between the two repulsions remains in this limit.

To illustrate this point, we have studied a Coulomb system of $N = 30$ electrons. The electron configuration minimizing the Coulomb energy is shown in the inset of Fig. 2 (lower right) for $L = 30$, i.e. one of the values of $L$ for which the hexagonal electron lattice is commensurate with the underlying lattice. This configuration is given by the PRC and PSC repulsions. As shown in Fig. 2 (lower right) $\Delta E_{\text{Coul}}^\text{PRC}$ is in the crossover regime between the bulk regular $\propto L^{-3}$ and the singular surface $\propto L^{-2}$ behaviors, while one has the expected $L^{-3}$ for $\Delta E_{\text{Coul}}^\text{PSC}$.

We summarize the main results which we have checked using small lattice models and varying either $U/t$ or $L$ for $N = 2, 3, 4$. For $r_s < r_s^*(L)$, the GSs of $H_f$ and $H_c$ are identical, $r_s$ is the scaling parameter and $I(r_s) = I(r_s = 0)$. Above $r_s^*(L)$, $r_s$ ceases to be the scaling parameter and $I$ decays. The following relations have been obtained independently of the definition of the Coulomb repulsion: $r_s^* \propto L^\alpha$, $E_{\text{vib}} \propto r_s^{-\beta}$ and $\Delta E_{\text{Coul}} \propto UL^{-\gamma}$, with the relations $\alpha = \gamma + 1$ and $\alpha = 2/(2 - \beta)$ between the exponents.

Our motivation was to investigate whether the study of a lattice model is relevant for a continuum model, fixing $N$ and varying the lattice parameters. Another issue, of more direct physical relevance, is to study the role played by the existing lattice upon a 2D gas of correlated conduction electrons. We postpone the discussion of this question, where the lattice parameters are given, while $N$ can be varied, to a following work.

We thank X. Waintal for his help in the study of a Coulomb system of $N = 30$ electrons. One of us (ZÁN) acknowledges the support of the European Community’s Human Potential Programme under contract HPRN-CT-2000-00144 and the Hungarian Science Foundation OTKA TO34832.

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