Model of Antiferromagnetic Superconductivity

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Abstract

We present a simple model that supports coexistent superconductive and antiferromagnetic ordering. The model consists of a system of electrons on a simple cubic lattice that move by tunnel effect and interact via antiferromagnetic Ising spin couplings and short range repulsions: these include infinitely strong Hubbard forces that prevent double occupancy of any lattice site. Hence, under the filling condition of one electron per site and at sufficiently low temperature, the system is an antiferromagnetic Mott insulator. However, when holes are created by suitable doping, they are mobile charge carriers. We show that, at low concentration, their interactions induced by the above interelectronic ones lead to Schafroth pairing. Hence, under certain plausible but unproven assumptions, the model exhibits the off-diagonal long range order that characterises superconductivity, while retaining the antiferromagnetic ordering.

Key Words: Extended exclusion principle, antiferromagnetically induced attraction of holes, Schafroth pairing, bosonisation, ODLRO

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1. Introduction

Since the discovery of superconducting phases in certain compounds [1], it has become clear that these generally come with rich arrays of neighbouring and even coexisting ‘normal’ phases that include both magnetically ordered and insulating ones (cf. the books by Anderson [2] and Plakida [3] and references therein). There is now a huge literature devoted to quantum theories of these phase structures and this has provided a picture dominated by strong correlations due to intra-atomic Hubbard repulsive forces (see Refs. [2]-[5] for example).

However, in our view, it is still conceptually unclear how these correlations lead to superconductive ordering, and consequently we consider that there is a need for a model that reveals the mechanism behind this ordering in simple physical terms. The object of this article is to provide such a model.

The model is a version of one devised by Richmond and the author [6], long before the discovery of superconducting compounds, for the purpose of providing a treatment of magnetic ordering. It comprises a system, Σ, of $N$ electrons on a simple cubic periodicised lattice that move by tunnel effect and interact via (a) antiferromagnetic Ising couplings, (b) certain position dependent two-body repulsions of slightly longer range, and (c) infinitely strong Hubbard intra-atomic forces that prevent the occupation of each site by more than one electron and thus enforce an extended exclusion principle. Evidently, under the filling condition of one electron per site, the system is a Mott insulator. However, when the system is suitably doped, holes are created and these are mobile charge carriers. In the particular case where there are just two holes, it is a simple matter to see that they bind together when the ratio of the Ising coupling parameter to the tunnelling one is sufficiently large: the repulsive interactions (b) do not affect this result as they are dominated by the Ising coupling at sufficiently short range. Thus, the prescribed interactions lead to a Schafroth pairing [7], the bound pair constituting a boson. Since this arises from position dependent interactions, it differs from the Cooper pairing [8] of metallic superconductors, which stem from momentum dependent ones: see also the discussion by Leggett [9] of these two kinds of pairing. Further, in the physically interesting case where the number of holes is macroscopic and their density is low, the pairing prevails and the repulsive interactions (b), if sufficiently strong, prevent the formation of larger bound hole clusters. Consequently the model reduces to a dilute gas of charged bosons and, under certain natural but unproven assumptions, it executes a Bose-Einstein (BE) condensation. More precisely, it exhibits off-diagonal long range order (ODLRO), which is the generalised form of BE condensation, applicable even to systems of interacting bosons [10, 11]. As shown in Refs. [12]-[14], ODLRO implies the characteristic electromagnetic properties of superconductors with ordering represented by a macroscopic wave function.

We present our description and treatment of the system, Σ, as follows. In Section 2 we formulate the model of this system in precise mathematical terms. Here the extended exclusion principle, noted above, leads to a key modification of the canonical commutation relations [6]. Further, under the filling condition of one electron per site, it forbids any tunnelling and therefore the system reduces to an antiferromagnetic Mott insulator.
However, the introduction of holes, due to suitable doping, provides the model with charge carriers.

In Section 3, we formulate the system, $S^{(n)}$, obtained by the introduction of an arbitrary number, $n$, of holes into the ground state of $\Sigma$. Here the key Proposition 3.1, whose proof is left to the Appendix, serves to pass from the second quantisation picture, as modified by the extended exclusion principle, to a simple first quantisation picture of the $n$ hole system. In Section 4 we specialise to the situation where there are just two holes. There we show that, under conditions wherein the Ising coupling parameter is sufficiently large by comparison with the tunnelling one, the holes bind together. As noted above, this corresponds to Schafroth pairing [7]. On the other hand, we note that, in the situation where more than two holes are introduced, the repulsive interactions render the formation of larger spatial clusters of them energetically unfavourable, in that their potential energies are not minimal.

In Section 5 we invoke the observations of the previous Section in our treatment of the model $S^{(2n)}$ for $n = O(N)$ and the density $2n/N << 1$. Specifically, we assume that the pairing mechanism still prevails and that spatial clusters of more than two holes do not occur. These assumptions essentially constitute an Ansatz, according to which $S^{(2n)}$ reduces to a system of $n$ bosonic ‘atoms’, each atom being a Schafroth pair.

In Section 6, we consider the question of whether the model exhibits BE condensation, as represented by ODLRO, in a limit where $N$ becomes infinite and the hole density $\eta (= 2n/N)$ is fixed. There we note that, under conditions of strong repulsive interactions and low density $\eta$, together with a supplementary scaling assumption, this model simulates that of Lieb et al [15], which has been proved to undergo BE condensation. On this basis, we assume that the ground state of the model satisfies the ODLRO condition and hence that it is superconductive. We further assume that the magnetic ordering of $\Sigma$ prevails at sufficiently low hole density. Hence we conclude that the system is an antiferromagnetic superconductor in its ground state. This result is in line with that obtained on purely thermodynamic grounds by Kivelson et al [16].

We conclude in Section 7 with a brief discussion of open problems

2. The Model

2.1. The Lattice $X$. We assume that the model is a system, $\Sigma$, of electrons that live on the periodicised $d$-dimensional simple cubic lattice $X$ of side $L$, i.e., the discrete space $(\mathbb{Z} \text{ (mod} L))^d$, whose points $x$ are $d$-tuples $(x^1, \ldots, x^d)$, where each $x^j$ runs through the set of integers $(1, 2, \ldots, L)$ whose ends are identified with one another. Thus the number, $N$, of sites of $X$ is $L^d$. We assume that $L$ is an even integer. In anticipation of an antiferromagnetic configuration of the electrons, we resolve $X$ into interlocking subspaces $X^+$ and $X^−$, the former consisting of the points $x = (x^1, \ldots, x^d)$ for which $\sum_{j=1}^d x^j$ is even and the latter for which that sum is odd. We denote by $\mathcal{U}$ and $\mathcal{V}$ the sets of nearest neighbours of the origin, $O$, in $X$ and $X^+$, respectively.

2.2. State Space and Algebraic Structure. In general, the pure states of a
many-electron system are represented by the normalised vectors in a Fock Hilbert space $\mathcal{F}$. However, in view of the above discussed extended exclusion principle, the states of the present model are restricted to the subspace $\mathcal{H}$ of $\mathcal{F}$ for which no more than one electron can be situated at any site. We formulate the spaces $\mathcal{F}$ and $\mathcal{H}$ as follows.

The Fock space $\mathcal{F}$ may be defined in terms of a vacuum vector $\Omega$ and bounded operators $c^*(x, \lambda)$ and $c(x, \lambda)$ governing the creation and annihilation of an electron of spin $\lambda (\pm 1)$ at the site $x$. The defining properties of $\Omega$ and $c(x, \lambda)$ are that

(i) $\Omega$ is annihilated by each of the operators $c(x, \lambda)$;

(ii) $\Omega$ is cyclic with respect to the adjoints $c^*(x, \lambda)$ of these operators, i.e. the vectors obtained by action on $\Omega$ of the polynomials in these adjoints form a dense subset of $\mathcal{F}$; and

(iii) the operators $c$ and $c^*$ satisfy the canonical anticommutation relations

$$[c(x, \lambda), c^*(x', \lambda')]_+ = \delta(x, x')\delta(\lambda, \lambda')I_{\mathcal{F}} \text{ and }[c(x, \lambda), c(x', \lambda')]_+ = 0 \forall \, x, x' \in X; \, \lambda, \lambda' = \pm 1,$$

where the $\delta$ is that of Kroneker and $I_{\mathcal{F}}$ is the identity operator in $\mathcal{F}$. The number of electrons of spin $\lambda$ at the site $x$ is represented by the operator

$$\nu_{\mathcal{F}}(x, \lambda) = c^*(x, \lambda)c(x, \lambda). \quad (2.2)$$

The Hilbert space $\mathcal{H}$, which harbours the states of the system, subject to the extended exclusion condition, is the subspace $P\mathcal{F}$ of $\mathcal{F}$, where $P$ is the Gutzwiller projector [17] given by the following formula (see also Ref. [6]).

$$P = \Pi_{x \in X} \left( I_{\mathcal{F}} - \nu_{\mathcal{F}}(x, 1)\nu_{\mathcal{F}}(x, -1) \right). \quad (2.3)$$

Correspondingly, under the same condition, the creation and annihilation operators for an electron of spin $\lambda$ at the site $x$ are

$$a^*(x, \lambda) = Pc^*(x, \lambda)P \text{ and } a(x, \lambda) = Pc(x, \lambda)P, \quad (2.4)$$

respectively. Thus, under this condition, the number of electrons of spin $\lambda$ at the site $x$ is given by the operator

$$\nu(x, \lambda) = a^*(x, \lambda)a(x, \lambda), \quad (2.5)$$

which, in view of Eqs. (2.1)-(2.5), is equal to $P\nu_{\mathcal{F}}(x, \lambda)P$. The total number of particles, $\nu(x)$, and the spin, $\sigma(x)$, at $x$ are therefore given by the formulae

$$\nu(x) = \sum_{\lambda=\pm 1} \nu(x, \lambda) \quad (2.6)$$

and

$$\sigma(x) = \sum_{\lambda=\pm 1} \lambda \nu(x, \lambda). \quad (2.7)$$
Further, as the projector $P$ is the identity operator, $I$, of the space $H$, it follows from Eqs. (2.1)-(2.7) that the operators $a$, $a^*$, $\nu$ and $\sigma$ satisfy the following algebraic relations, which were established in Ref. [6].

\[
[a(x, \lambda), a(x', \lambda')]_+ = 0, \quad (2.8)
\]

\[
[a(x, \lambda), a^*(x', \lambda')]_+ = (I - \nu(x, -\lambda))\delta(x, x')\delta(\lambda, \lambda') + a^*(x, \lambda)a(x, -\lambda)\delta(x, x')\delta(\lambda, -\lambda'), \quad (2.9)
\]

\[
a^*(x, \lambda)a^*(x, \lambda') = 0 \quad \forall \ x \in X, \ \lambda, \lambda' = \pm 1. \quad (2.10)
\]

and

\[
a(x, \lambda)\Omega = 0. \quad (2.11)
\]

### 2.3. Hamiltonian of the Model.

We assume that this is the operator, $H$, in $\mathcal{H}$ that takes the form

\[
H = H^T + H^J + H^K, \quad (2.12)
\]

the three contributions representing tunnelling, Ising spin couplings and particle repulsions, respectively. These are defined so that the Ising interactions couple particles at nearest neighbouring sites, the repulsive interactions couple next nearest neighbouring ones, and the tunnelling processes are spin conserving transitions between the nearest sites that harbour particles of the same spin in the Ising antiferromagnetic ground state. Thus the Hamiltonian components are assumed to take the following forms.

\[
H^T = T\sum_{x \in X; v \in \mathcal{V}} (a^*(x, \lambda)a(x + v, \lambda) + \text{h.c.}) \equiv -T\sum_{x \in X, v \in \mathcal{V}} (a(x + v, \lambda)a^*(x, \lambda) + \text{h.c.}), \quad (2.13)
\]

\[
H^J = J\sum_{x \in X; \ u \in \mathcal{U}} \sigma(x)\sigma(x + u), \quad (2.14)
\]

; and

\[
H^K = K\sum_{x \in X; u, u'(\neq -u) \in \mathcal{U}} \nu(x)\nu(x + u + u'), \quad (2.15)
\]

where $T$, $J$ and $K$ are all positive and $\mathcal{U}$ and $\mathcal{V}$ are the subsets of $X$ defined in Section 2.1.

### 2.4. The Filling Condition, Mott Insulation and Antiferromagnetic Order

Under the filling condition, where the total number of electrons is equal to $N$, the number of lattice sites, the extended exclusion principle signifies that each site of $X$ is occupied by precisely one electron. Hence this condition signifies that the state space of $\Sigma$ is reduced to the subspace of $\mathcal{H}$ for which the following vectors $\Psi(\lambda)$, which correspond to spin configurations $\{\lambda(x)|x \in X\}$ form an orthogonal basis.

\[
\Psi(\lambda) = [\Pi_{x \in X}a^*(x, \lambda(x))]\Omega. \quad (2.16)
\]

It follows from this formula and Eqs. (2.6)-(2.10) that

\[
a^*(x, \lambda'(x))\Psi(\lambda) = 0, \quad (2.17)
\]
\[ \nu(x)\Psi(\lambda) = \Psi(\lambda) \quad \forall \, x \in X. \quad (2.18) \]

and

\[ \sigma(x)\Psi(\lambda) = \lambda(x)\Psi(\lambda). \quad (2.19) \]

It now follows from Eqs. (2.10), (2.13) and (2.16) that

\[ H^T\Psi(\lambda) = 0, \quad (2.20) \]

which signifies that the extended exclusion prevents any tunnelling and thus produces Mott insulation. Further, by Eqs. (2.15) and (2.18), \( H^K \) reduces to a constant, namely \( NKd \), on \( \Psi(\lambda) \). Therefore, in view of Eqs. (2.12) and (2.20), the effective Hamiltonian reduces to \( H^J \), and consequently the equilibrium state of the system is antiferromagnetically ordered below the critical Ising temperature. Hence the ground states of the model are just those of the Ising system, as governed by the Hamiltonian \( H^J \). There are just two of these, which we denote by \( \Phi \) and \( \Phi' \) and which, by Eqs. (2.14) and (2.19), are simultaneous eigenvectors of the \( \sigma(x) \)'s with corresponding eigenvalues \( \{s(x) = \pm 1 \, \forall \, x \in X^\pm\} \) and \( \{s(x) = \mp 1 \, \forall \, x \in X^\pm\} \), respectively. Our treatment of the model will be centred on operations applied to the state vector \( \Phi \); the corresponding treatment based on \( \Phi' \) and its modifications could be carried out analogously.

It follows from the above specifications that

\[ \sigma(x)\Phi = s(x)\Phi \quad \forall \, x \in X \quad (2.21) \]

where

\[ s(x) = 1 \quad \forall \, x \in X^+ \quad \text{and} \quad -1 \quad \forall \, x \in X^-, \quad (2.22) \]

and

\[ \Phi = [\Pi_{x \in X} a^*(x, s(x))] \Omega. \quad (2.23) \]

We remark here that it may be assumed, without loss of generality, that

\[ H\Phi = 0, \quad (2.24) \]

since this equation is validated by adding the constant \(-NKd\) to the r.h.s. of Eq. (2.12).

Suppose now that the spin configuration \( \{s(x)|x \in X\} \), corresponding to the ground state \( \Phi \), is modified by reversal of the spins in a subset \( \Delta \) of \( X \). The resultant state of \( \Sigma \) then becomes

\[ \Phi_{\Delta} = [\Pi_{x \in X \setminus \Delta} a^*(x, s(x))] [\Pi_{x \in \Delta} a^*(x, -s(x))] \Omega. \quad (2.25) \]

It then follows that, corresponding to Eq. (2.24) for the ground state \( \Phi \),

\[ H\Phi_{\Delta} = E(\Delta)\Phi_{\Delta}, \quad (2.26) \]

where \( E(\Delta) \) is the energy required to reverse the spins in \( \Delta \) when the system is in the ground state \( \Phi \).
3. Holes in the Antiferromagnetically Ordered Ground State

We now consider the modification of the state $\Phi$ by the introduction of $n$ holes, denoting the resultant system by $S^{(n)}$. We represent the creation of a hole at the site $x$ by the operator $\alpha(x)$, defined by the equation

$$\alpha(x) = a(x, s(x)) \forall x \in X. \quad (3.1)$$

The algebraic properties of the operators $\alpha(x)$ then follow from this formula and Eqs. (2.8)-(2.11).

3.1. The System $S^{(n)}$. We define $S^{(n)}$ to be the system of $n$ holes in the state $\Phi$ and represent its pure states by the linear combinations of the actions on $\Phi$ of the monomials of order $n$ in the $\alpha(x)$'s. Thus, in view of the anticommutation relations of the latter, these state vectors take the form

$$C_n(f) := (n!)^{-1/2} \sum_{x_1, \ldots, x_n \in X} f(x_1, \ldots, x_n) \alpha(x_1) \ldots \alpha(x_n) \Phi, \quad (3.2)$$

where $f$ is an element of the Hilbert space, $\mathcal{H}^{(n)}$, of antisymmetric function on $X^n$ with $l^2(X^n)$ inner product. It follows from these specifications that

$$\langle C_n(f), C_n(g) \rangle_{\mathcal{H}} = \langle f, g \rangle_{\mathcal{H}^{(n)}} \forall f, g \in \mathcal{H}^{(n)}. \quad (3.3)$$

Thus, $C_n$ is an isomorphism of $\mathcal{H}^{(n)}$ into $\mathcal{H}$ and therefore the pure states of $S^{(n)}$ are faithfully represented by the vectors in $\mathcal{H}^{(n)}$. Correspondingly, the observables of $S^{(n)}$ are represented by the self-adjoint operators in this space. The following Proposition, which will be proved in the Appendix, provides the correspondence between first and second quantisation pictures of $S^{(n)}$ under the condition of the extended exclusion principle.

**Proposition 3.1.** It follows from the above definitions that $H$ induces a self-adjoint operator $H^{(n)}$ in $\mathcal{H}^{(n)}$, which we take to be the Hamiltonian of $S^{(n)}$, according to the following formula.

$$HC_n(f) = C_n(H^{(n)}f) \forall f \in \mathcal{H}^{(n)}. \quad (3.4)$$

where

$$H^{(n)} = -T \sum_{j=1}^{n} \Delta_{V_j} + \sum_{j,k=1}^{n} V(x_j - x_k), \quad (3.5)$$

$$V(x_j - x_k) = -J \sum_{u \in U} \left( \delta(x_j, x_k + u) + \delta(x_j, x_k - u) \right) +$$

$$K \sum_{u, u' \neq -u} \left( \delta(x_j, x_k + u + u') + \delta(x_j, x_k - u - u') \right). \quad (3.6)$$

and $\Delta_{V_j}$ is the versions for the site $x_j$ of the discretised Laplacian $\Delta_V$ defined by the formulae

$$\Delta_V f(x) = \sum_{v \in V} [f(x + v) + f(x - v) - 2f(x)]. \quad (3.7)$$

Evidently, the first and second sums in Eq. (3.5) correspond to the kinetic and potential energy, respectively, of $S^{(n)}$.  

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Discussion. This Proposition signifies that \( \mathcal{H}^{(n)} \) is the state space and \( H^{(n)} \) is the Hamiltonian for the system, \( S^{(n)} \), of \( n \) holes in the state \( \Phi \). We take this to be the model of the \( n \) hole system at sufficiently low values of the ambient temperature and hole density \( n/N \), even though this model differs from that of \( n \) holes in the full system \( \Sigma \), since that can also carry holes in the modifications, \( \Phi_\Delta \), of \( \Phi \) by reversals of finite numbers of spins, as defined by Eq. (2.25). In fact our neglect of these modifications is based on the assumption that they do not significantly affect the qualitative features of the equilibrium states of the model at sufficiently low temperature and hole density \( n/N \). The heuristic basis of this assumption is the following. First, in the absence of holes, the energy cost, given by Eq. (2.26), of the spin reversals would freeze them out at sufficiently low temperatures. The creation of holes, however, would change this situation since their interaction with the spin reversals would render this freezing incomplete. Nevertheless, we anticipate that this interaction is effectively very weak at sufficiently low hole density and consequently that the equilibrium properties of \( S^{(n)} \) should simulate those of \( n \) holes in the full system \( \Sigma \) at sufficiently low temperatures and hole density.

4. Binding of Hole pairs.

Suppose now that just a pair of holes is introduced into the system when that is in its ground state. In order to obtain a condition for their binding, we first note that, by Eqs. (3.5)-(3.7), the Hamiltonian \( H^{(1)} \) for a single hole is \(-T\Delta V\) and, by Eq. (3.6), its spectrum is \([0, T]\). Hence, the condition for the existence of bound states of the pair of holes is that the spectrum of \( H^{(2)} \) is at least partly in \( \mathbb{R}_- \) or, equivalently, that there exists an element \( h^{(2)} \) of \( H^{(2)} \) such that \( (h^{(2)}, H^{(2)}h^{(2)}) < 0 \). The following proposition provides just such a condition.

**Proposition 4.1.** A sufficient condition for the binding of the hole pair is that

\[
J > \gamma T, \tag{4.1}
\]

where \( \gamma \) is the number of elements of \( V \), i.e. \( 2d(d-1) \).

**Proof.** Choose

\[
h^{(2)}(x_1, x_2) = 2^{-1/2} [\delta(x_1, a)\delta(x_2, b) - \delta(x_1, b)\delta(x_2, a)], \tag{4.2}
\]

where \( a \) and \( b \) are nearest neighbouring points of \( X \). Then by Eqs. (3.5)-(3.7) and (4.2),

\[
(h^{(2)}, H^{(2)}h^{(2)}) \leq 2(\gamma T - J), \tag{4.3}
\]

Hence, Eq. (4.1) is a sufficient condition for a bound state.

4.1. Internal and External Descriptions. We now define \( y \) and \( z \) to be the relative displacement and the centre of the coordinate pair \((x_1, x_2)\) respectively, i.e.

\[
y = x_1 - x_2 \quad \text{and} \quad z = \frac{1}{2}(x_1 + x_2). \tag{4.4}
\]
Thus y and z run over the spaces $X$ and $X/2 := \{ (\xi/2) | \xi \in X \}$, respectively. We refer to y and z as the internal and external coordinates, respectively, of the pair. Defining $\tilde{X}$ to be the subspace of $X \times (X/2)$ comprising the pairs $(y, z)$ for which $(z \pm y/2) \in X$, we re-express the wave functions $f(x_1, x_2)$ as vectors in the Hilbert space $\mathcal{H}^{(2)} := \{ \tilde{f} \in l^2(\tilde{X}) | \tilde{f}(-y, z) = -\tilde{f}(y, z) \}$, according to the formula

$$\tilde{f}(y, z) := f(x_1, x_2) = f(z + y/2, z - y/2).$$

We define the representation spaces for the internal and external observables to be the Hilbert spaces $\mathcal{H}_{\text{int}} := \{ g \in l^2(X) | g(x) = -g(-x) \}$ and $\mathcal{H}_{\text{ext}} := l^2(X/2)$, respectively. It follows from these specifications that $\mathcal{H}^{(2)} = \mathcal{H}_{\text{int}} \otimes \mathcal{H}_{\text{ext}}$. We denote by $U$ the unitary transformation $f \rightarrow \tilde{f}$ of $\mathcal{H}^{(2)}$ onto $\mathcal{H}^{(2)}$ given by Eq. (4.5).

We denote by $W$ the density matrix in $\mathcal{H}^{(2)}$ representing the zero temperature state of $S^{(2)}$. Then this state may also be represented in $\mathcal{H}^{(2)}$ by its unitary transform

$$\hat{W} = UWU^*.$$

We denote by $\hat{W}_{\text{int}}$ the density matrix in $\mathcal{H}_{\text{int}}$ representing the interior state of the pair, as defined by the formula

$$\hat{W}_{\text{int}} = \text{Tr}_{\text{ext}}(\hat{W}),$$

where $\text{Tr}_{\text{ext}}$ signifies partial trace over $\mathcal{H}_{\text{ext}}$.

4.2. Hamiltonian Operators. In view of Eq. (4.5), the Hamiltonian operator for the pair is given by the operator $\hat{H}^{(2)}$ in $\mathcal{H}^{(2)}$ defined by the formula

$$[\hat{H}^{(2)} \tilde{f}] (y, z) = [H^{(2)} f] (z + y/2, z - y/2).$$

It follows from Eqs. (3.5)-(3.7), (4.5) and (4.8) that

$$[\hat{H}^{(2)} \tilde{f}] (y, z) = -T \sum_{v \in V} \left( \tilde{f}(y + v, z + v/2) + \tilde{f}(y - v, z - y/2) + \tilde{f}(y - v, z + v/2) + \tilde{f}(y + v, z - v/2) - 4 \tilde{f}(y, z) \right) + V(y) \tilde{f}(y, z).$$

Consequently, defining displacement operators $D_{\text{int}}(a)$ and $D_{\text{ext}}(b)$ in $\mathcal{H}^{(2)}$ by the equations

$$[D_{\text{int}}(a) \tilde{f}] (y, z) = \tilde{f}(y - a, z) \text{ and } [D_{\text{ext}}(b) \tilde{f}] (y, z) = \tilde{f}(y, z - b),$$

$$\hat{H}^{(2)} = -T \sum_{v \in V} \left[ G_{\text{int}}(v) G_{\text{ext}}(v) - 4 \right] + V(y),$$

where

$$G_{\text{int}}(v) = D_{\text{int}}(v) + D_{\text{int}}(-v)$$

and

$$G_{\text{ext}}(v) = D_{\text{ext}}(v/2) + D_{\text{ext}}(-v/2).$$
We define the exterior Hamiltonian for the pair to be the partial mean of $\hat{H}^{(2)}$ w.r.t. its internal variables, as governed by the density matrix $\hat{W}_{\text{int}}$, i.e.

$$\hat{H}_{\text{ext}} = \text{Tr}_{\text{int}}(\hat{W}_{\text{int}}\hat{H}^{(2)}),$$

(4.14)

where $\text{Tr}_{\text{int}}$ is the partial trace over $\hat{H}^{(2)}_{\text{int}}$. Hence, by Eq. (4.11) with the constant term $-4$ in the square brackets excluded,

$$\hat{H}_{\text{ext}} = -T\sum_{v \in \mathcal{V}} \text{Tr}_{\text{int}}(\hat{W}_{\text{int}}G_{\text{int}}(v))G_{\text{ext}}(v) + \text{Tr}_{\text{int}}(\hat{W}_{\text{int}}V(y))$$

(4.15)

We now note that the Hamiltonian of the model $\Sigma$ is invariant under interchanges of the principal axes of the lattice $X$, and we assume that the density matrix $W$ retains this symmetry. By Eqs. (4.7) and (4.12), this implies that the values of the partial trace $\text{Tr}_{\text{int}}(\hat{W}_{\text{int}}G_{\text{int}}(v))$ is independent of $v$. We denote this quantity by $g$, a constant. Further, since Eq. (4.7) implies that $\text{Tr}_{\text{int}}(\hat{W}_{\text{int}}V(y))$ is also a constant, it follows from these observations that Eq. (4.15), as modified by the addition of certain harmless constants, takes the following explicit form.

$$\hat{H}_{\text{ext}} = -\hat{T}\Delta_{\mathcal{V}},$$

(4.16)

where $\Delta_{\mathcal{V}}$ are the discretised Laplacians defined by Eq. (3.7) and

$$\hat{T} = gT.$$  

(4.17)

Thus the Hamiltonian $H_{\text{ext}}$ is that of a particle that moves freely on the space $X/2$.

**4.2. Discount of Larger Clusters of Holes.** The proof of Prop. 4.1 exploited the fact that the potential energy of the pair, as given by the second sum in Eq. (3.5), is minimised when the two holes are nearest neighbours. One may reasonably ask whether larger stable clusters of holes may be formed in the case when there are more than two of them. Although we do not have a definite answer to this question, we shall now show that clusters of more than two holes cannot minimise the potential energy if the repulsion parameter $K$ is sufficiently large; and consequently that, in this case, the mechanism of bound pairing does not extend to larger clusters of holes. Our argument runs as follows.

We define a cluster to be a set of holes that occupies a subset, $C$, of $X$ such that

(i) each point of $C$ has a nearest neighbour in that set, and

(ii) at least one element of each pair of nearest neighbours in $C$ has another nearest neighbour in $C$.

Suppose that now $a$ and $b$ are a nearest neighbouring pair within a cluster $C$. Then at least one of these points, say $b$, has another nearest neighbour, $c$, in $C$. Hence, by Eqs. (3.6), the particle at $a$ is coupled to that at $b$ with energy $-2J$ and to that at $c$ with energy $2K$. Further, the number of nearest neighbours of $a$ in $C$ cannot exceed $2d$, while the number of its next nearest neighbours is at least 1. Hence the increment in the potential energy of the system due to the transfer of the hole to another region is no greater than
2dJ – K. Thus the potential energy is not minimised by clusters of more than two holes if \( K > 2dJ \). Of course, this does not rule out the possibility that some quantum mechanism might lead to cluster-like correlations, but we shall ignore that possibility in the treatment that follows. This procedure amounts to an Ansatz.

5. Bosonisation

We now pass to a treatment of the 2\(n\) hole system \( S^{(2n)} \), with \( n = O(N) \), and the density \( \eta = 2n/N \ll 1 \). In accordance with the observation of the previous Section, we assume that the pair binding mechanism, established for the case where there are just two holes, still prevails for \( S^{(2n)} \), and that the repulsive interactions prevent the formation of bound clusters of more than two holes.

Thus we base our treatment on the Ansatz that the holes of \( S^{(2n)} \) combine into \( n \) pairs. Evidently these are bosons, as its wave functions \( f(x_1, x_2, \ldots, x_{2n}) \) change sign under interchanges \( x_j \leftrightarrow x_k \) of single positions and therefore remain invariant under interchanges \( (x_j, x_{j+1}) \leftrightarrow (x_k, x_{k+1}) \) of pairs. Hence the pairs behave as bosonic atoms, and we shall refer to them as such. We formulate the model of these \( n \) atoms by a natural generalisation of the derivation, in Section 4.1, of the exterior Hamiltonian of just one of these.

To this end, we resolve the set \((x_1, x_2, \ldots, x_{2n})\) of hole coordinates into pairs whose relative displacements are \( y_1, \ldots, y_n \) and whose centres are \( z_1, \ldots, z_n \), respectively. Thus the coordinates of the \( n \) pairs of holes comprising \( S^{(2n)} \) are

\[ (z_1 + y_1/2, z_1 - y_1/2), (z_2 + y_2/2, z_2 - y_2/2), \ldots, (z_n + y_n/2, z_n - y_n/2). \]

To formulate the internal and external features of \( S^{(2n)} \), we define the Hilbert spaces \( \hat{H}^{(n)}_{\text{int}}, \hat{H}^{(n)}_{\text{ext}} \) and \( \hat{H}^{(2n)} \) to be the natural \( 2n \) hole generalisations of the spaces \( \hat{H}_{\text{int}}, \hat{H}_{\text{ext}} \) and \( \hat{H}^{(2)} \), respectively, on which the description of pairs was based in Section 4. Thus we define \( \hat{H}^{(2n)} \) to be \( \hat{H}^{(n)}_{\text{int}} \otimes \hat{H}^{(n)}_{\text{ext}} \), where \( \hat{H}^{(n)}_{\text{ext}} \) and \( \hat{H}^{(n)}_{\text{int}} \) are the bosonic and fermionic spaces given by the symmetric (resp. antisymmetric) elements, of \( l^2((X/2)^n) \) (resp. \( l^2(X^n) \)), with the added restriction that the latter elements change sign under reversal of each component \( y_j \) of the points \((y_1, \ldots, y_n)\) of the underlying space \( X^n \).

We take the internal state of each of these atoms to be given by the canonical copy of that of a single pair, as represented by the density matrix, \( \hat{W}_{\text{int}} \), formulated in Section 4.1; and we assume that, in view of the diluteness of the atomic system, these states may be treated as statistically independent. Thus the density matrix in \( \hat{H}^{(n)}_{\text{int}} \) representing the internal state of \( S^{(2n)} \) is

\[ \hat{W}^{(n)}_{\text{int}} = \bigotimes_{j=1}^{n} \hat{W}_{\text{int}, j}, \tag{5.1} \]

where each \( \hat{W}_{\text{int}, j} \) is a copy of the internal density matrix, \( \hat{W}_{\text{int}} \) for one pair.

By Eqs. (3.5)-(3.7) and the representation by Eq. (4.5) of the positions of a pair in terms of its internal and external coordinates, the Hamiltonian for \( S^{(2n)} \) is the operator \( \hat{H}^{(2n)} \) in \( \hat{H}^{(2n)} \) given by the formula

\[ \hat{H}^{(2n)} = \sum_{j=1}^{n} \hat{H}^{(2)}_j + \sum_{j,k,(j>k)=1}^{n} \tilde{V}(z_j - z_k | y_j, y_k), \tag{5.2} \]
where $\hat{H}^{(2)}_j$ is the copy of $\hat{H}^{(2)}$ representing the Hamiltonian of the $j$th atom and $\tilde{V}(z_j - z_k|y_j, y_k)$ is the energy of interaction between the $j$th and $k$th atom, given by the formula

$$
\tilde{V}(z_j - z_k|y_j, y_k) = V(z_j - z_k + (y_j + y_k)/2) + V(z_j - z_k - (y_j + y_k)/2) + V(z_j - z_k + (y_j - y_k)/2) + V(z_j - z_k - (y_j - y_k)/2).
$$

(5.3)

We define the exterior Hamiltonian for $S^{(2n)}$ to be the partial mean w.r.t. the internal state $\hat{W}^{(n)}_{\text{int}}$ of the Hamiltonian $\hat{H}^{(2n)}$, i.e.

$$
\hat{H}^{(n)}_{\text{ext}} = \text{Tr}_{\text{int}}(\hat{W}^{(n)}_{\text{int}} H^{(2n)}).
$$

(5.4)

where $\text{Tr}_{\text{int}}$ signifies the partial trace over the Hilbert space $\hat{H}^{(n)}_{\text{int}}$. Thus $\hat{H}^{(n)}_{\text{ext}}$ is effectively the Hamiltonian for a system of $n$ bosonic atoms, considered as point particles. It follows now from Eqs. (5.1), (5.2) and (5.4), together with the normalisation condition for $\hat{W}^{(n)}_{\text{int}}$, that

$$
\hat{H}^{(n)}_{\text{ext}} = \sum_{j=1}^{n} \hat{H}_{j,\text{ext}} + \sum_{j,k,(>j)=1}^{n} \nabla(z_j - z_k),
$$

(5.5)

where $\hat{H}_{j,\text{ext}}$ is a copy of $\hat{H}_{\text{ext}}$, as defined by Eq. (4.16), and represents the exterior Hamiltonian for the $j$th atom, and

$$
\nabla(z - z') = \sum_{y,y' \in X} \text{Tr}(\hat{W}^{(n)}_{\text{int}} \tilde{V}(z - z'|y, y')) \forall z, z' \in X/2,
$$

(5.6)

It follows from Eqs. (4.16) and (5.6) that the exterior Hamiltonian for $S^{(2n)}$ is

$$
\hat{H}^{(n)}_{\text{ext}} = -\hat{T} \sum_{j=1}^{n} \Delta \nu_j + \sum_{j,k,(>j)=1}^{n} \nabla(z_j - z_k).
$$

(5.7)

Thus the model reduces that of a system, $\Sigma_b$, of charged interacting bosons. We note that, by Eqs. (3.6) and (5.6), the interactions are of short range.

6. Conditions for ODLRO, Superconductivity and Antiferromagnetism.

We recall that O. Penrose and Onsager [10] presented a generalised version of Bose-Einstein condensation, pertinent to systems of interacting bosons and subsequently termed off-diagonal long range order (ODLRO) by Yang [11]. For systems of charged particles, the combination of this property and the basic requirements of gauge covariance, translational invariance and thermodynamical stability implies superconductive electrodynamics [12-14]. The condition that a state of the charged bosonic system $\Sigma_b$ possess the property of ODLRO may be expressed in the following way. Denoting the density matrix for the state, in coordinate representation, by $\rho(z_1, \ldots, z_n|z'_1, \ldots, z'_n)$, the single particle density matrix is defined to be

$$
\rho_1(z|z') = \sum_{z_2, \ldots, z_n} \rho(z, z_2, \ldots, z_n|z', z_2, \ldots, z_n).
$$

(6.1)
The ODLRO condition for the state $\rho$ is essentially that $\rho_1(z|z')$ factorises into a product of the form $\overline{\phi(z)}\phi(z')$ when the points $z$ and $z'$ are widely separated. To be precise, bearing in mind that the state $\rho$ depends on the size parameter $N$, the ODLRO condition at fixed particle density $\eta := 2n/N$ is that there exists a (non-zero) function $\phi$ on $X/2$ such that

$$\lim_{|c| \to \infty} \lim_{N \to \infty} 2n/N = \eta [\rho_1(z|z' + c) - \overline{\phi(z)}\phi(z' + c)] = 0.$$ (6.2)

This condition defines $\phi$, which is termed the macroscopic wave function, up to an arbitrary constant phase factor. It has been proved to be satisfied not only by ideal bose gases below condensation temperatures but also by a certain class of dilute interacting bose gases [15, Ths. 5.1 and 7.4] in their ground states. Moreover, it has been cogently argued by O. Penrose and Onsager [10] that the superfluid phase of $He_4$ is characterised by ODLRO. However, no general conditions have as yet been established for the occurrence of ODLRO in systems of interacting particles. In particular, the conditions of Lieb et al [15] are not strictly applicable to the present model $\Sigma_b$ in that (a) they are based on a continuum, rather than a lattice, model, (b) their interactions are wholly repulsive, and (c) the length, $L$, of the side of their containing volume is proportional to $n$ rather than $n^{1/d}$. This signifies that the particle density is proportional to $N^{d-1-1}$, which vanishes in the limit $N \to \infty$. Nevertheless, we consider that (a) and (b) do not represent essential qualitative differences of the present model from that of Ref. [15] since, on the one hand, we expect the difference between the lattice and continuum models to be irrelevant to their large scale properties, while, on the other hand, the two-body interactions of $\Sigma_b$ are predominantly repulsive if $K/J$ is sufficiently large. However, the observation (c), as it stands, marks a serious difference between the two models and, in order to overcome it, we need an assumption to the effect that the density of $\Sigma_b$ becomes $N$- independent in the thermodynamic limit. This appears to be quite plausible since low particle densities $\eta$ do not appear to be radically different, from the physical standpoint, from those of the form $N^{d-1-1}$. In view of these observations, we make the following assumption.

(I) Given that $J$ is large enough to produce Schafroth pairing in the system $\Sigma$, the ground state of $\Sigma_b$ possesses the property of ODLRO if the ratio $K/J$ is sufficiently large and the density $\eta$ sufficiently low.

Further, we assume that the spin correlations of the original fermionic system $\Sigma$ remain close to those of its hole-free states when the hole density $\eta$ is suitably low. Thus we supplement assumption (I) with the following one.

(II) At sufficiently low hole density, the ground state of the original system $\Sigma$ retains its antiferromagnetic ordering.

Thus, assuming the validity of (I) and (II), we conclude that at sufficiently low hole density, and for a suitable range of values of the parameters $T$, $J$ and $K$, the system $\Sigma$ supports both ODLRO and magnetic ordering at zero temperature. Hence as the ODLRO property, together with the basic conditions of gauge covariance, translational invariance and thermodynamical stability ensures that the model exhibits superconductive electrodynamics [12-14], we conclude that the system is an antiferromagnetic superconductor at zero temperature.
7. Concluding Remarks.

We have shown that the many electron system, $\Sigma$, formulated in Sections 2 and 3, exhibits Schafroth pairing of holes; and that, consequently, the resultant pairs form a bosonic system, $\Sigma_b$. Under the assumptions (I) and (II) discussed in Section 6, together with the conditions of sufficiently low hole density $\eta$ and strong interelectronic repulsions, the ground state of $\Sigma_b$ possesses the property of ODLRO, which characterises superconductivity. Hence assuming that, at sufficiently low hole density, the ground state of $\Sigma$ retains the magnetic ordering it possesses under the filling condition of one electron per lattice site, the system exhibits superconductive-cum-antiferromagnetic order.

Among the challenging problems that remain are those of
1. providing a firm basis for the assumption, made in the discussion at the end of Section 3, that the model $S^{(n)}$ represents the system of $n$ holes in the original system $\Sigma$;
2. establishing the validity of assumptions (I) and (II) of Section 6 under appropriate conditions on the parameters of the model;
3. extending the theory to non-zero temperatures; and
4. providing a corresponding theory of ferromagnetic superconductivity, for which there is experimental evidence in Refs. [18] and [19].

Appendix: Proof of Prop. 3.1.

As a preliminary to the proof of Prop. 3.1, we define

\[
\alpha_-(x) := a(x, -s(x)) \forall x \in X
\]  

and establish the following lemma.

**Lemma A.1.** The above definitions and assumptions imply that

\[
\alpha_-(x)\Phi = 0 \forall x \in X
\]  

**Proof.** By Eqs.(2.9), (3.1) and (A.1),

\[
\alpha_-(x)\alpha^*(x) + \alpha^*(x)\alpha_-(x) = \alpha^*(x)\alpha_-(x)
\]  

and hence

\[
\alpha_-(x)\alpha^*(x) = 0. \forall x \in X.
\]  

Furthermore, by Eq. (2.23) and (3.1),

\[
\Phi = [\Pi_{x' \in X} \alpha^*(x')]\Omega
\]

and, in view of the anticommutation relation (2.8) and Eq. (3.1), we may move the factor $\alpha^*(x)$ of the r.h.s. of this formula to the left of all the other factors, where, in view of Eq.
(A.3), it is annihilated by the action of $\alpha_-(x)$. Eq. (A.2) follows immediately from this observation.

**Proof of Prop. 3.1.** By Eqs. (2.24) and (3.2),
\[
HC_n(f) = [H, D_n(f)]\Phi. \tag{A.4}
\]
where
\[
D_n(f) := (n!)^{-1/2}\sum_{x_1, \ldots, x_n \in X} f(x_1, \ldots, x_n) \alpha(x_1) \cdot \alpha(x_n). \tag{A.5}
\]
Hence, defining
\[
H^{(n)T} := -T\sum_{j=1}^n \Delta_{\nu,j}, \tag{A.6}
\]
\[
H^{(n)J} := -J\sum_{j,k, (j > k)}\sum_{u \in \mathcal{U}} \left(\delta(x_j, x_k + u) + \delta(x_j, x_k - u)\right), \tag{A.7}
\]
and
\[
H^{(n)K} := K\sum_{j,k, (j > k)}\sum_{u, u' \in \mathcal{U}} \left(\delta(x_j, x_k + u + u') + \delta(x_j, x_k - u - u')\right), \tag{A.8}
\]
we see from Eqs. (2.12), (3.5), (3.6) and (A.4)-(A.8) that in order to establish the formula (3.4), it suffices to prove that
\[
[H^{T}, D_n(f)]\Phi = D_n(H^{(n)T} f)\Phi, \tag{A.9}
\]
\[
[H^{J}, D_n(f)]\Phi = D_n(H^{(n)J} f)\Phi, \tag{A.10}
\]
and
\[
[H^{K}, D_n(f)]\Phi = D_n(H^{(n)K} f)\Phi, \tag{A.11}
\]

**Proof of Eq. (A.9).** By Eq. (A.5),
\[
[H^{T}, D_n(f)]\Phi =
\]
\[
(n!)^{-1/2}\sum_{x_1, \ldots, x_n \in X} \sum_{j=1}^n f(x_1, \ldots, x_n) \alpha(x_1) \cdot \alpha(x_j-1)[H^{T}, \alpha(x_j)]_- \alpha(x_{j+1}) \cdot \alpha(x_n)\Phi \tag{A.12}
\]
and, by Eqs. (2.13) and (3.1),
\[
[H^{T}, \alpha(x_j)]_- = -T\sum_{x \in X, \lambda = \pm 1, v \in \mathcal{V}} \left[ a^*(x, \lambda)a(x + v, \lambda) + a^*(x + v, \lambda)a(x, \lambda), a(x, s(x_j)) \right]_- \tag{A.13}
\]
In view of the anticommutation relations (2.8) and (2.9), together with Eqs. (3.1) and (A.1), this formula reduces, after some manipulation, to the following equation.
\[
[H^{T}, \alpha(x_j)]_- = -T\sum_{v \in \mathcal{V}} \left[ (\alpha(x_j + v) + \alpha(x_j - v))(I - \alpha^*_-(x_j)\alpha_-(x_j)) + \alpha^*_-(x_j)\alpha(x_j)(\alpha_-(x_j + v) + \alpha_-(x_j - v)) \right]. \tag{A.13}
\]
Furthermore, by Eqs. (2.8), (3.1) and (A.1), the terms $\alpha_- (x_j)$ and $(\alpha_- (x_j + v) + \alpha_- (x_j - v))$ commute or anticommute with $\alpha(x_{j+1}) \ldots \alpha(x_n)$, according to whether $(n - j)$ is odd or even; and, by Lemma (A.1), they annihilate $\Phi$. Consequently, by Eq. (A.13), the commutator $[H^T, \alpha(x_j)]_-$ may be replaced by $-T \sum_{\sigma \in V} \bigl( \alpha(x_j + v) + \alpha(x_j - v) \bigr)$ in the formula (A.12). On transferring the action of this operator to the function $f$, we arrive at Eq. (A.9), with $H^{(n)}_T$ given by Eq. (A.6), up to a harmless additive constant.

**Proof of Eq. (A.10).** By Eqs. (2.14) and (A.5),
\[
[H^J, D_n(f)]_-(x) = (n!)^{-1/2} \sum_{j=1}^n f(x_1, \ldots, x_n) \alpha(x_1) \cdot \alpha(x_{j-1}) [H^J, \alpha(x_j)]_- \alpha(x_{j+1}) \cdot \alpha(x_n)
\]
and, by Eqs. (2.7)-(2.9), (2.14) and (3.1),
\[
[H^J, \alpha(x_j)]_- = J \sum_{x \in X, u \in U} (\sigma(x)[\sigma(x + u), \alpha(x_j)]_- + [\sigma(x), \alpha(x_j)]_- \sigma(x + u)) =
\]
\[
Js(x_j) \sum_{x \in X, u \in U} (\delta(x + u, x_j) \sigma(x) \alpha(x_j) + \delta(x, x_j) \alpha(x_j) \sigma(x + u)) =
\]
\[
Js(x_j) \sum_{u \in U} (\sigma(x_j - u) \alpha(x_j) + \alpha(x_j) \sigma(x_j + u)).
\]
Hence since, by Eqs. (2.5), (2.7)-(2.9) and (3.1), $\alpha(x_j)$ commutes with $\sigma(x_j - u)$,
\[
[H^J, \alpha(x_j)]_- = Js(x_j) \sum_{u \in U} \alpha(x_j)(\sigma(x - u) + \sigma(x + u)).
\]
Further, since
\[
[\sigma(x_j \pm u), \alpha(x_{j+1}) \ldots \alpha(x_n)]_- \Phi =
\]
\[
\sum_{k=j+1}^n \alpha(x_{j+1}) \ldots \alpha(x_k)[\sigma(x_j \pm u), \alpha(x_k)]_- \alpha(x_{k+1}) \ldots \alpha(x_n) \Phi
\]
and since, by Eqs. (2.5), (2.7)-(2.9) and (3.1),
\[
[\sigma(x_j \pm u), \alpha(x_k)]_- = \delta(x_j \pm u, x_k) s(x_j \pm u) \alpha(x_k),
\]
it follows from Eqs. (2.21), (A.16) and (A.17) that
\[
\sigma(x_j \pm u) \alpha(x_{j+1}) \ldots \alpha(x_n) \Phi =
\]
\[
s(x_j \pm u) \alpha(x_{j+1}) \ldots \alpha(x_n) \Phi - \sum_{k=j+1}^n \delta(x_j \pm u, x_k) s(x_j \pm u) \alpha(x_{j+1}) \ldots \alpha(x_n) \Phi.
\]
Since, for $u \in U$, the sites $x_j$ and $(x_j + u)$ are nearest neighbours and therefore carry opposite spins in the antiferromagnetic configuration,
\[
s(x_j) s(x_j - u) = -1.
\]
Hence, by Eqs. (A.15), (A.18) and (A.19),
\[
[H^J, \alpha(x_j)]_- \alpha(x_{j+1}) \ldots \alpha(x_n) \Phi =
\]

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\[ 4dJ \alpha(x_j) \Phi - J \sum_{u \in \mathcal{U}} \sum_{k=j+1}^{n} \left( \delta(x_j, x_k + u) + \delta(x_j, x_k - u) \right) \alpha(x_j) \Phi \]

It follows from this equation and Eq. (A.14) that Eq. (A.10) is satisfied, with \( H^{(n)}_{\alpha} \) given by Eq. (A.4), up to an irrelevant additive constant \( 4dJ \).

**Proof of Eq. (A.11).** Noting that, by Eqs. (2.5), (2.6) and (3.1),

\[
[\nu(x), \alpha(x')] = -\alpha(x) \delta(x, x'),
\]

we see that it is a simple matter to prove (A.11) by replacing \( s(x), \sigma(x), u \) and \( J \) by \( \nu, 1, u + u' \) and \( K \), respectively, in the proof of (A.10). This completes the proof of the Proposition.

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