A Wilsonian Approach to Displacive Metal-Insulator Transitions and application to Vanadium Dioxide

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The physics of tight-binding type electron momentum states is reformulated in terms of an SU(2) lattice gauge theory and a Wilson action. Allowing the lattice to fluctuate introduces curvature, with the construction of the curvature form following the usual approach however the three phonons in three dimensions require three gauge fields, and therefore an SU(2) structure. Symmetry-breaking is incorporated by applying the SU(2) interaction vertices simultaneously on neighbouring unit cells, which allows both spin-ordering and Peierls pairing, and this generates linear combinations of neighbouring electron position state wavefunctions, lowering the crystal symmetry and opening a band gap. The occurrence of strong electron-phonon coupling accompanied by phonon softening is incorporated easily as it simply adds a constant to the tight-binding phase at each lattice site, thus modifying the ground state lattice structure.

Over the course of the last century tremendous progress has been made in describing the physics of materials using first quantum mechanics, and subsequently ideas and machinery from Quantum Field Theory. However, despite this progress, and the huge effort which has been poured into this search for understanding, precise descriptions of certain phenomena have remained stubbornly intractable. One such problem is a mathematical description of the metal-insulator-structural phase transition of vanadium dioxide. VO\textsubscript{2} is a 3d\textsuperscript{1} system which exists in a metallic, tetragonal structure above \( \sim 340 \) K, and when pure or unstrained adopts a monoclinic P2\textsubscript{1}/c structure (usually called “M\textsubscript{1}”) below \( T_c \).

There has been an intense debate about the nature of the insulating phase ranging for some decades, as the atomic rearrangements in going from Tetragonal to the Monoclinic structure are highly reminiscent of the Peierls mechanism: the vanadium chains which run parallel to the tetragonal c-axis dimerize (and also experience an antiferroelectric distortion, see Figure 1a-b), which suggest a band description of the metal-insulator transition from perturbation theory\cite{Booth}. However the tetragonal electron liquid exhibits the characteristics of a strongly correlated system near \( T_c \) and thus the insulating state resulting from this would be expected to be a Mott-Hubbard insulator\cite{Hubbard}. Strong support for the Mott scenario was voiced by Mott himself\cite{Mott} due to the appearance of the “M\textsubscript{2}” structure upon doping with holes, extra electrons or by inputting stress/strain\cite{Stress}. This structure is also Monoclinic (although C2/m rather than P2\textsubscript{1}/c)\cite{Struct} however in this form the dimerization and antiferroelectric distortion occur individually, and not together, each occurring on a neighbouring vanadium chain (see Figure 1c).

There is no doubt however that the M\textsubscript{2} form is a Mott insulator, as DMFT\cite{DMFT} and modified GW calculations\cite{GW} confirm, however the most significant aspect of this resolution is that the antiferroelectric chains are also antiferromagetically ordered, while the dimerized chains show no such order\cite{Chain}.

This coincidence of antiferroelectricity and antiferromagnetism led the author to propose a Yang-Mills description of electron-phonon interactions in metal oxides\cite{Yang}, which can manifest spin-ordering via the transverse phonons, and pairing via the longitudinal phonons separately. In that study the basic interaction structure was determined, including the spinor grouping, however the adaptation to mass generation, i.e. metal-insulator transitions focussed the electronic structure, and ignored the underlying lattice.

In this work the formalism of lattice QCD\cite{Lattice} is adapted to the description of crystal lattices and their fluctuations to describe crystal structure transformations which are accompanied by spin ordering and metal-insulator transitions.

For the purposes of this discussion the high symmetry electronic structure is metallic, and thus the fermions obey a Weyl equation as per the discussion of Booth and Russo\cite{Booth_Russo}. A momentum state in the tight-binding representation is given by:

\[ \psi_k(\mathbf{r}) = \sum_{\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) e^{i\mathbf{kR}} \]  

(1)

where \( \phi(\mathbf{r}) \) is a single or a sum of position state wavefunctions such as orbitals, and \( \mathbf{R} = n\mathbf{a} \) is a lattice vector, i.e. some integer multiple of the unit cell constant. We see that in this representation, the lattice enters in the phase which is applied to the position state wavefunctions. To parallel transport we need a Unitary: \( U(x, \mu) \), which translates our wavefunction, from which we can construct a derivative:

\[ \partial_\mu \psi(x) = \frac{1}{a} \left( U(x, \mu) \psi(x + a\hat{\mu}) - \psi(x) \right) \]  

(2)

where \( a\hat{\mu} \) is a unit cell vector, and the definition of the momentum state (equation 1) requires only the forward derivative, and thus no Fermion doubling problem arises\cite{Doubling}.
of where these fluctuations reflect a change in the position of the atoms rather easily:

This formulation allows us to introduce fluctuations in the positions of the atoms rather easily:

where these fluctuations reflect a change in the position of \( \psi(x) \), not its neighbour. The fluctuations will be small (or the lattice will be destroyed) and thus we can write:

\[
U(x, \mu)\psi(x + (a + \delta a)\hat{\mu}) \rightarrow e^{ik\alpha_n\hat{\mu}}(1 + ik\delta\alpha_n\hat{\mu})\psi(x)
\]  

(6)

Therefore:

\[
\partial_\mu\psi(x) \rightarrow \partial_\mu\psi(x) + ie^{ik\alpha_n\hat{\mu}}\frac{\delta\alpha_n}{\alpha_n}\hat{\mu}\psi(x)
\]

(7)

Thus the fluctuation is normalized to the original interposition dependence. Since the coupling of phonons to electron momentum states is highly wavevector dependent, we absorb this into a coupling parameter \( g(k) \) which also contains the constant phase term:

\[
ie^{ik\alpha_n\hat{\mu}}\frac{\delta\alpha}{\alpha} \rightarrow ig(k)\delta\alpha_n\hat{\mu}
\]

(8)

Assuming that the fluctuations are local, i.e. differ from site to site on the lattice, we can proceed by quantizing the displacement in the usual way, we shift \( \delta\alpha_n\hat{\mu} \) to \( \hat{A}_\mu(x) \) where:

\[
\hat{A}_\mu(x) = \int \frac{d^3p}{2\pi^22E_p} \sum_\lambda \left[ \hat{a}_\mu \epsilon_\mu^\lambda(p)e^{ip_\mu x} + \hat{a}_\mu^\dagger \epsilon_\mu^\lambda(p)e^{-ip_\mu x} \right]
\]

(9)

where now \( \hat{a}^\dagger/\hat{a} \) create and annihilate polarization vectors \( \epsilon_\mu^\lambda(p) \) which describe the motion of the atomic position, and the \( \lambda \) are the basis vectors of the spacetime. The variation in space and time is given by the \( e^{-ip_\mu x} \) term, and for phonons there may be non-linear dispersion.

Now:

\[
ie^{ik\alpha_n\hat{\mu}}\frac{\delta\alpha}{\alpha} \psi(x) = ig(k)\hat{A}_\mu(x)\psi(x)
\]

(10)

However, \( \psi(x) \) is a spinor, and thus the derivative \( \partial_\mu\psi(x) \) needs to give us information on the change of the spinor variables as a function of space and time. This requires resolving the spinor variables into 4-components, a time component, and three spatial components, such that their changes can be evaluated. The spatial components are just the spin vector \( \mathbf{S} \) which are resolved using the Pauli matrices, and the time component is just given by the identity matrix. Thus the derivative term becomes \( \sigma^\mu\partial_\mu \), and accounting for helicity means that we double stack the Pauli matrices into gamma matrices (and change the signs on the spatial matrices of the left-handed spinor to make sure the Weyl equation is still obeyed):

\[

L_{\text{spinor}} = i\bar{\psi}(x)\gamma^\mu\partial_\mu\psi(x) - g(k)\bar{\psi}(x)\gamma^\mu\hat{A}_\mu(x)\psi(x)
\]

(11)

Thus this lattice formulation is now equivalent to the usual covariant derivative of an interacting set of fermion and vector boson fields.

An action for the bosonic sector can be constructed using a modification of the usual Wilsonian Lattice approach by defining plaquettes, and summing over the

![Diagram](image-url)
parallel transporters evaluated around them, which generates a curvature form $F_{\mu \nu}$. This starts from the usual definition of the parallel-transporting Unitaries defining transport around a plaquette, $x \to x + a\mu \to x + a\mu + av \to x + av \to x$, in the same manner as lattice QCD, which is given by:\[13\]

$$O_{\mu \nu}(x) = U(x, \mu)U(x + a\mu, \nu)U^{-1}(x + a\nu, \mu)U^{-1}(x, \nu)$$

(12)

If:

$$U(x, \mu) \rightarrow e^{ik(\alpha + \delta a)\bar{\mu}}$$

(13)

we can write:

$$O_{\mu \nu}(x) = e^{iA_\mu(x)}e^{iA_\nu(x+a\mu)}e^{-iA_\mu(x+av)}e^{-iA_\nu(x)}$$

(14)

Using the Baker-Campbell-Hausdorff expression on the first two, and last two terms separately:

$$e^{iA_\mu(x)}e^{iA_\nu(x+a\mu)} = \exp\left[(A_\mu(x) + A_\nu(x) + a\mu)
+ \frac{1}{2} (A_\mu(x), A_\nu(x) + a\mu)] + ...\right]$$

(15)

and

$$e^{-iA_\mu(x+av)}e^{-iA_\nu(x)} = \exp\left[-(A_\mu(x) + av) + A_\nu(x)
+ \frac{1}{2} (A_\mu(x) + av), A_\nu(x)] + ...\right]$$

(16)

and combing these terms in the same manner, i.e. using the BCH expression:

$$O_{\mu \nu}(x) = \exp\left(\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + [A_\mu(x), A_\nu(x)] + ...\right)
= e^{F_{\mu \nu}}$$

(17)

which is the exponentiated curvature form of the vector field $A_\mu(x)$. For an Abelian vector field the commutator drops out, however as we have three phonons, we must use a $2 \times 2$ linear transformation, parametrised by the Pauli matrices:\[10\]

$$\sigma_a \cdot W_\mu^a \rightarrow \tilde{W}_\mu^a$$

(18)

where $a = 1, 2, 3$ labels the generator, $\mu$ is a spacetime index and the $\sigma_a$ are the usual Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(19)

therefore we have:

$$\tilde{W}_\mu^a = \begin{bmatrix} W_\mu^3 & W_\mu^1 - iW_\mu^2 \\ W_\mu^1 + iW_\mu^2 & -W_\mu^3 \end{bmatrix}$$

(20)

By grouping the electron momentum states appropriately, the actions of the SU(2) phonons/bosons can be made to incorporate wide range of phenomena such as magnetic ordering and the BCS theory (for a more detailed explanation see Booth and Russo:\[10\]):

$$\left(\begin{array}{c} \tilde{c}_k^\dagger \\ \tilde{c}_-^\dagger \\ \tilde{c}_+^\dagger \end{array}\right) = \begin{array}{c} \text{up} \\ \text{top} \\ \text{bottom} \end{array}$$

(21)

This structure can be neatly arranged into colours and generations:

| Colour | Generation |
|-------|------------|
| a     | up         |
| b     | top        |

| Colour | Generation |
|-------|------------|
| a     | down       |
| b     | bottom     |

The electron phonon interactions then take the form:

$$g_{\alpha} \bar{\psi} \gamma^\alpha W_\mu^a \psi =
\left[\begin{array}{c} \psi^\alpha_a(x) \\ \bar{\psi}^\alpha_b(x) \end{array}\right] \times
\gamma^\mu \left(\begin{array}{c} W_\mu^3(x) \\ W_\mu^1 - iW_\mu^2(x) \\ -W_\mu^3(x) \end{array}\right)$$

(22)

where the gamma matrices are expressed (in the chiral basis) in two-component form as:

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

(23)

and thus

$$\bar{\psi} = \psi^\dagger \gamma^0 \psi = (\bar{\psi}_a, \bar{\psi}_b) = (\psi^\dagger_a^0, \psi^\dagger_b^0)$$

(24)

As we now have an SU(2) theory, equation \[17\] requires summing over the traces of the generators:

$$O_{\mu \nu}(x) = \text{tr} F_{\mu \nu} + ...$$

(25)

As the fluctuations are small, we can expand the exponential:

$$O_{\mu \nu}(x) = N + \frac{1}{2}\text{tr}(F_{\mu \nu})^2 + ... = N + \mathcal{L}_{\text{gauge}}$$

(26)

The linear term drops out due to the tracelessness of the SU(2) generators. This leads to the pure Gauge plaquette action:\[13\]

$$S_G[U] = \sum_p [1 - O_{\mu \nu}]$$

(27)

where the sum is over all plaquettes, $p$. This now gives us a vector field component to the action, as well as a spinor field component which is coupled to it.

The key concept with respect to phase transitions in this formalism is that the bosons live on the links between the fermions. For a mononuclear unit cell this means they live on the boundaries of the unit cells, the region between the spinor variables. In a previous paper\[10\]}
was noted that the linear combinations $W^1_\mu (x) - iW^2_\mu (x)$ and $W^1_\mu (x) + iW^2_\mu (x)$ cannot manifest at the same site in a crystal. They arise from an out of phase motion of the atoms and thus a phase must be added to one of the combinations to enforce this. Alternatively, this phase difference can be wired into the interaction vertex by applying them on neighbouring sites, which is a more intuitive expression of the fact that the bosons live on the links between fermions in this formalism. Thus:

$$
\begin{pmatrix}
\psi_a(x) \\
\psi_b(x)
\end{pmatrix} \rightarrow
\begin{pmatrix}
\psi_a(x_1) \\
\psi_b(x_2)
\end{pmatrix}
$$

(28)

Thus the interaction vertex becomes (illustrated schematically in Figure 2):

$$
g_a \bar{\psi} \gamma^\mu \tilde{W}^\alpha_\mu \psi =
g_{(1,2,3)} \left( \bar{\psi}_a'(x'), \bar{\psi}_b'(x') \right) \times
\gamma^\mu
\begin{pmatrix}
W^3_\mu (x_1) & W^1_\mu - iW^2_\mu (x_2) \\
W^1_\mu + iW^2_\mu (x_1) & -W^3_\mu (x_2)
\end{pmatrix}
\begin{pmatrix}
\psi_a(x_1) \\
\psi_b(x_2)
\end{pmatrix}
$$

(29)

Remembering that:

$$
\tilde{W}^3_\mu (x) \sim \sum_p \bar{\alpha}^i \epsilon^i_\mu(p) e^{-ipx}
$$

(30)

the negative sign of the $\sigma_3$ matrix reverses the direction of the polarization vector of the $W^3_\mu$ mode at $x_2$, and thus this vertex now contains a pairing of neighbouring atoms, as per the displace transition of VO$_2$. The $W^1_\mu + iW^2_\mu (x_1)$ and $W^1_\mu - iW^2_\mu (x_1)$ (i.e. the transverse phonons) when contracted with the $\gamma$-matrices (and appropriate polarization vectors) result in spin raising and lowering operators respectively[14] and thus this vertex can also ordering neighbouring spins antiferromagnetically, again, reminiscent of the ordering seen in the M$_2$ VO$_2$ structure.[9]

Setting $g_1W^1_1 = g_aW^2_2$ and all other polarization vector components to zero to illustrate this most clearly we get a term:

$$
\left( \bar{\psi}_a', \bar{\psi}_b' \right) \times
\begin{pmatrix}
0 & g_1W^1_1(x_1)(\gamma^1 + i\gamma^2) \\
g_1W^1_1(x_2)(\gamma^1 - i\gamma^2) & 0
\end{pmatrix}
\begin{pmatrix}
\psi_a \\
\psi_b
\end{pmatrix}
$$

(31)

If both $\psi_a$ and $\psi_b$ are in eigenstates of $S_Z$, and remembering:

$$
\gamma^i = \begin{pmatrix}
0 & \sigma^i \\
-\sigma^i & 0
\end{pmatrix}
$$

(32)

this gives the familiar spin raising and lowering operators, $S^+ = \sigma^1 + i\sigma^2$, and $S^- = \sigma^1 - i\sigma^2$:

$$
\bar{\psi}_a'g_1W^1_1(x_2) \begin{pmatrix}
0 & \hat{S}^- \\
-\hat{S}^- & 0
\end{pmatrix} \psi_b
+ \bar{\psi}_b'g_1W^1_1(x_1) \begin{pmatrix}
0 & \hat{S}^+ \\
-\hat{S}^+ & 0
\end{pmatrix} \psi_a
$$

(33)

with the negative sign in the $\gamma^i$ accounting for the opposite helicities of the two-component spinors in each four-component spinor such that the Weyl equation for each is satisfied. We can now conveniently relabel the linear combinations of the $W^1_\mu, W^2_\mu$ bosons as $\tilde{W}^3_\mu (x_1)$ and $\tilde{W}^3_\mu (x_2)$.

Applying the full vertex (i.e. non-zero polarization vector components for $W^3_\mu$ as well as the other two) along a chain of atoms with say a single itinerant electron inhabiting a sum of tight-binding momentum states at each site as a simple example (although the system cannot obviously be one-dimensional, it must be embedded in a three-dimensional space to have three phonon modes), the temporal and spatial variation of the SU(2) mode is given by:

$$
e^{-ipx} e^{i(kx - \omega t)}
$$

(34)

where it is assumed that the SU(2) mode is collective, i.e. the 4-momentum for the individual bosons is the same, and where $\omega$ is the energy of the modes. For a classical mass-spring oscillator this would be $\sqrt{\frac{k}{m}}$ where $k$ is the spring constant and $m$ the mass. Obviously in the case of phonons in metal oxides, the dispersion will have non-linearities particularly at high wavevector, and the energy ($\omega$) required to produce a phonon in an interacting system will have a self-energy component which comes from the electron-phonon and phonon-phonon interactions. Phonon softening, i.e. a decrease in $\omega$ can occur if these self-energy terms are large and negative. In the case of vanadium dioxide it is experimental fact that there is a unit cell doubling coinciding with pairing of the vanadium atoms, and an antiferroelectric distortion orthogonal to it. This turns the correlated metallic electron state above $T_c$ into an insulator below $T_c$, however it is still not entirely clear which insulating paradigm this structure belongs to. However, for the purposes of this discussion we simply state that a large negative self-energy exists, and do not dwell on its origin.

Thus if we have an increasingly large negative self-energy for the formation of a mode with a particular wavevector (for example as $T_c$ is approached from above), as the energy of the mode decreases, we expect that the
coupling will increase: it is more likely for the crystal to populate a low energy mode by Boltzmann statistics. If this increasing population feeds back into the self energy, however, the spin ordering may be enhanced by electron self-energy terms (on the different signs of the $\hat{W}_\mu^3$ polarization vectors), and spin ordering just above $T_c$, both characteristics of the metal-insulator transitions of vanadium dioxide systems.

Returning to the issue of strong coupling, as the system approaches $T_c$ from above the expansion of equation 6 becomes invalid, however the result is simply that the interaction vertices contribute a static (remembering that this becomes a VEV) exponential term to the momentum state description of equation [38] which modifies the atomic positions, producing a ground state with different symmetry. From equations [39] and [40], it is obvious that $\delta a$ fluctuates in space and time, and ignoring the constant terms, for a single boson we have:

$$\delta a_n \mu \simeq \epsilon_\mu(x) e^{-i\omega t}$$

and the VEV can be written:

$$\langle \delta a_n \mu \rangle = \langle \epsilon_\mu(x) \rangle$$

Thus the RHS of equation [5] becomes:

$$e^{ik(a_n + \delta a_n)\hat{\mu}} \psi(x) \rightarrow e^{ik(a_n + \langle \epsilon_\mu(n) \rangle)\hat{\mu}} \psi(x)$$

where now position is denoted by the index $n$, and we can write:

$$a_n + \langle \epsilon_\mu(n) \rangle = a'_n$$

giving:

$$U(x, \mu) \psi(x + a'_n \hat{\mu}) = e^{ika'_n \hat{\mu}} \psi(x)$$

For the SU(2) vertex the polarization vector components of the three bosons simply add to give a single vector, with a result identical to equation [43]. Therefore we see that the consequence of strong coupling when combined with a VEV is to simply modify the ground state lattice structure. Thus we see that the above formalism describes crystal phase transitions accompanied by spin ordering and the opening of a gap in the electronic structure.

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1 J. B. Goodenough, Journal of Solid State Chemistry 3, 490 (1971).
2 J. P. Pouget, H. Launois, M. Rice, Tim, P. D. Dernier, A. Gossard, G. Villeneuve, and P. Hagenmüller, Phys. Rev. B 10, 1801 (1974).
3 M. M. Qazilbash, M. Brehm, B.-G. Chae, P.-C. Ho, G. O. Andreev, B.-J. Kim, S. J. Yun, a. V. Balatsky, M. B. Maple, F. Keilmann, H.-T. Kim, and D. N. Basov, Science 318, 1750 (2007).
4 J. Hubbard, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 276, 383 (1963).
5 N. F. Mott and L. Friedman, Philosophical Magazine 30, 389 (1974).
6 J. H. Park, J. M. Coy, T. S. Kusirga, C. Huang, Z. Fei,
7. S. Hunter, and D. H. Cobden, *Nature* **500**, 431 (2013).
8. W. H. Brito, M. C. Aguiar, K. Haule, and G. Kotliar, *Phys. Rev. Lett.* **117**, 056402 (2016).
9. J. M. Booth, D. W. Drumm, P. S. Casey, J. S. Smith, and S. P. Russo, *J. Chem. Phys.* **244110**, 1 (2016).
10. J. P. Pouget and H. Launois, *Journal de Physique* **C4**, 49 (1976).
11. C. Gattringer and C. Lang, *Quantum Chromodynamics on the Lattice* (Springer-Verlag, Berlin Heidelberg, 2010).
12. C. Gattringer and C. Lang, in *Quantum Chromodynamics on the Lattice* (Springer-Verlag, Berlin-Heidelberg, 2010) Chap. 5, pp. 110–111.
13. R. Sommer, “Introduction to Lattice Gauge Theories,” (2005).