FM85/A002

85-25

GREEN'S FUNCTIONS AND UNITARY STATES IN MANY FERMION SYSTEMS

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Talk presented at the XIV International Colloquium on Group Theoretical Methods in Physics, Seoul, August 1985

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ABSTRACT

We discuss a class of mean field hamiltonians for interacting many-fermion systems characterized by their dynamical algebras. For such systems one can easily derive the finite temperature Green's function in an algebraically explicit way. This generalized Green's function G is well-known in the case of superconductivity, for example, where it possesses the pseudo-unitary property $GG^+ = \bar{\Omega}^2 I$ (where $\bar{\Omega}^2$ is a scalar). In the case of Helium Three, however, this property of the Green's function is not automatic. By analogy with this latter case we define unitary systems (or the states of such systems) as those which satisfy this pseudo-unitary constraint. Such constrained systems are particularly easy to treat both theoretically and experimentally; and we explore some of the consequences of unitarity in the cases of coexisting superconducting and density wave systems.

The method of Green's functions is standard in field theory and many body physics, and it is unnecessary to reiterate the value of this approach in the present note. In the many body case, the Green's function G_{ij} is introduced as a thermodynamic expectation

$$G_{ij}(x\tau, x'\tau') = -\langle T_\tau(\psi_i(x\tau)\tilde{\psi}_j(x'\tau'))\rangle$$

where $\quad \langle Q\rangle = (\mathrm{tr}\; e^{-\beta\kappa}Q)/(\mathrm{tr}\; e^{-\beta\kappa}) \qquad (\beta = (k_B T)^{-1})$

for any operator Q and hamiltonian $K = H - \mu N$.

We assume that we are dealing with fermion field operators

$$\psi_i(x\tau) = e^{K\tau}\psi_i(x)e^{-K\tau} \qquad (\hbar = 1)$$

$$\tilde{\psi}_i(x\tau) = e^{K\tau}\psi_i^+(x)e^{-K\tau} \qquad (i = 1,2,\ldots,n)$$

Here x,x' are the spatial co-ordinates, and T_τ is a τ-ordering operator for the parameter τ, which is in general complex; in this latter case note that $\tilde{\psi}_i(x\tau) \neq \psi_i(x\tau)^+$. For $\tau = it$ (t = time) this gives the usual Heisenberg evolution. We shall work in the Fourier transformed case, with

$$\psi_i(x) = \mathrm{VOL}^{-\frac{1}{2}} \sum_k A_i(k)e^{ikx}$$

when the Green's function becomes

$$G_{ij}(k\tau) = -\langle T_\tau(A_i(k\tau)\tilde{A}_j(k0))\rangle$$

Using the periodicity of this latter function, period 2β, we may write

$$G_{ij}(k\omega) = \int_0^\beta G_{ij}(k\tau)e^{i\tau\omega}d\tau.$$

[For Fermi statistics ω takes values $\omega_n = (2n+1)\pi/\beta$, n = 1,2,3,...]
It is straightforward to evaluate this in the mean-field case, where we assume that our hamiltonian may be written

$$K = \sum_k K(k)$$

with $K(k) = \sum_{i,j} m_{ij}(k)A_i^+(k)A_j(k)$.

The fermion operators $A_i(k)$ satisfy the standard anticommutation relations

$$\{A_i(k),A_j^+(k')\} = \delta_{ij}\delta_{kk'} \quad .$$

Writing $X_{ij}(k) \equiv A_i^+(k)A_j(k)$, $(i,j, = 1,2,\ldots,n)$
these anticommution relations lead to the commutation relations

$$[X_{ij},X_{k\ell}] = \delta_{jk}X_{i\ell} - \delta_{i\ell}X_{kj}$$

(suppressing explicit k-dependence) which shows that our hamiltonian K is an element of a subalgebra of $\bigoplus_k g\ell(n)_{(k)}$. [If the complex coefficients $m_{ij}(k)$ are such that each $K(k)$ is hermitian - the usual case - then the dynamical algebra is a subalgebra of $u(n)$ rather than $g\ell(n)$.] Since the $\{A_i\}$ form a first rank contravariant tensor under the X_{ij}, we may readily obtain

$$A_i(k\tau) = \sum_j (e^{-m\tau})_{ij} A_j(k) = \sum_j \Lambda_{ij}(k\tau) A_j(k)$$

where m is the matrix $(m_{ij}(k))$, and $\Lambda = e^{-m\tau}$.
A standard manipulation [1] then gives for the transformed Green's function $G_{ij}(k\omega)$

$$G(k\omega) = (i\omega I - m)^{-1}.$$

As mentioned, the matrix m is hermitian. If m is also pseudo-unitary, that is

$$m^2 = \Omega_0^2 I$$

for some scalar Ω_0, then $G(k\omega)$ is explicitly invertible

$$G(k\omega) = (-i\omega I - m)/\Omega^2$$

where

$$\Omega^2 = \Omega_0^2 + \omega^2.$$

In this case G is also pseudo-unitary,

$$GG^+ = (\Omega^{-2})I.$$

These are the systems which we refer to as unitary in this note. Although this condition is highly restrictive, it is satisfied by some systems of physical interest - as we now illustrate - and makes their treatment that much simpler, both theoretically and experimentally.

An idea of just how restrictive this unitary condition is may be obtained by looking at the dynamical algebra g of the system. [In the above case, if the hamiltonian K is an element of $\bigoplus_k g_k$, with each g_k isomorphic to g, we refer to g as the dynamical or spectrum generating algebra of the system with hamiltonian K.] For a rank-ℓ

algebra g there will be invariants $I_r = \mathrm{tr}\, m^r$ $(r = 1,2,\ldots)$ associated with the matrix m of the hamiltonian K(k); at most ℓ of these will be independent. For a unitary system this number is reduced to at most two invariants, corresponding to tr m and $\mathrm{tr}\, m^2 = n\Omega_0^2$; in the traceless (semi-simple) case, there is only one invariant. Thus su(1) is automatically unitary - the case of superconductivity; but so(5)being of rank 2, unitarity imposes one condition - and this is the case for superfluid helium three (from which situation we have borrowed the nomenclature [2]). We describe the helium three case now [3]. After a Hartree-Fock linearisation, the effective hamiltonian for an interacting fermion fluid with pairing in opposite momentum (but not necessarily opposite spin) states is given by $K = \sum_k K(k)$, where

$$K(k) = \sum_{\alpha} \xi_k (a^+_{k\alpha} a_{k\alpha} + a^+_{-k\alpha} a_{-k\alpha}) + (\sum_{\alpha,\beta} V(k,\alpha,\beta) a^+_{k\alpha} a^+_{-k\beta} + \text{h.c.})$$

Choosing a basis of fermion operators $\{A_i^{(k)}\}$,

$$(A_1^{(k)}, A_2^{(k)}, A_3^{(k)}, A_4^{(k)}) = (a_{k\uparrow}, a_{k\downarrow}, a^+_{-k\downarrow}, a^+_{-k\uparrow})$$

we may write the matrix m in the spin-triplet case as

$$m = \begin{bmatrix} E & V \\ V^+ & -E \end{bmatrix}$$

where $E = \xi\tau_0$ (with $\xi_k \equiv \epsilon_k - \mu$; we suppress the momentum index) and $V = \underline{d}.\underline{\tau}$, with $d_1 = \frac{1}{2}(V_{\downarrow\downarrow} - V_{\uparrow\uparrow})$, $d_2 = -\frac{1}{2}i(V_{\uparrow\uparrow} + V_{\downarrow\downarrow})$, $d_3 = \frac{1}{2}(V_{\uparrow\downarrow} + V_{\downarrow\uparrow})$. The unitary condition $m^2 = (\Omega^2 - \omega^2)I$ leads to

$$[V, V^+] = 0$$

which is

$$\underline{d} \times \underline{d}^* = 0$$

a form given by, for example, Leggett.

For such unitary states the 4 × 4 Green's function is of course immediate, with $\Omega^2 = \omega^2 + \xi^2 + |d|^2$.

This exemplifies a characteristic feature of unitary systems; there is a single degenerate energy gap, in the helium three case given by

$|d|^2$. For a system described by a rank-ℓ spectrum generating Lie algebra we would expect ℓ "gaps". This gives a useful experimental criterion, which we now illustrate by reference to the experiment of Sooryakumar and Klein on a system of coexisting charge-density waves and superconductivity [4]. We may write the representative matrix m for the hamiltonian for this model as

$$m = \begin{bmatrix} \xi & -\Delta & \gamma & -\Delta_{-Q} \\ -\Delta^* & -\xi & -\Delta_Q^* & -\gamma \\ \gamma^* & -\Delta_Q & \xi' & -\Delta \\ -\Delta_{-Q}^* & -\gamma^* & -\Delta^* & -\xi' \end{bmatrix}$$

in a basis

$$(A_1(k), A_2(k), A_3(k), A_4(k)) = (a_{k\uparrow}, a^+_{-k\downarrow}, a_{\bar{k}\uparrow}, a^+_{-\bar{k}\downarrow}).$$

Here $\xi' \equiv \xi(k-Q) \equiv \epsilon(k-Q) - \mu$, $\bar{k} \doteq k - Q$, where Q is the characteristic wave vector for CDW propagation. The couplings for conventional superconductivity and CDW are given by Δ and γ respectively, while Δ_Q and Δ_{-Q} are so-called anomalous terms, appearing in the hamiltonian as

$$-\Delta_{-Q} a^+_{k\uparrow} a^+_{-\bar{k}\downarrow} - \Delta_Q a^+_{\bar{k}\uparrow} a^+_{-k\downarrow} + \text{h.c.}$$

The dynamical algebra here is su(4) [5], which is rank 3. The unitary condition forces $\Delta_Q = \Delta_{-Q} = 0$, and $\xi + \xi' = 0$. This last condition is known as the nesting condition. As the experiment referred to shows the presence of two energy gaps, below the appropriate lowest transition temperature, we can assert that the system is not unitary. Therefore at least one of the given conditions must fail. In a model neglecting the anomalous terms, this means that the nesting condition fails.

For the many fermion systems we have considered, the spectrum generating algebra is compact, and so has a finite-dimensional hermitian representation. Unitary states occur when all there is only one invariant associated with the matrix representing the hamiltonian. In that case the system exhibits a single energy gap, and the finite-temperature Green's function is immediately obtainable without matrix inversion in the mean field case.

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