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Flow equations and normal ordering

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Abstract

In this paper we consider flow equations where we allow a normal ordering which is adjusted to the one-particle energy of the Hamiltonian. We show that this flow nearly always converges to the stable phase. Starting out from the symmetric Hamiltonian and symmetry-broken normal ordering nearly always yields symmetry breaking below the critical temperature.

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1. Introduction

By applying flow equations to a Hamiltonian [1] one typically starts out from a Hamiltonian which does not show an explicit symmetry breaking even if the symmetry of the system will be broken below some temperature. As in the calculations on the Hubbard model [2–5], one can direct the flow to a form in which molecular-field approximation becomes exact. This effective Hamiltonian is still not symmetry broken. Only the molecular-field formalism breaks the symmetry below the critical temperature T_c.

In the fermionic renormalization group flow [6–10], the vertex functions will at least within weak-coupling approximations diverge at some length scale below T_c, so that the approximations become unreliable and one has to resort to other methods in this regime. Thus it is desirable to have a way to introduce symmetry breaking from the beginning. Recently Salmhofer, Honerkamp, Metzner and Lauscher [12] have added a symmetry-breaking field to the Hamiltonian and showed that this additional field leads in the symmetry broken phase.

For the Hamiltonian flow it is not necessary to add a symmetry-breaking term to the Hamiltonian. Instead it is sufficient to choose a normal ordering which is symmetry broken (compare [11]). One can show that the system will nearly always converge to the stable state, that is in the case of symmetry breaking (that is below the critical temperature) it runs to a symmetry broken state, whereas if the symmetric state is stable (above T_c) then it will run to the symmetric state.

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With this approach the normal-ordered form of the Hamiltonian shows an explicit dependence on the normal-ordering. We adjust continuously the normal ordering to the one-particle contribution of the Hamiltonian and we can show that the normal ordering has the interesting property to run in the direction of the stable state. This implies that starting out with a symmetry-broken normal ordering, then above the critical temperature it will converge to the symmetric state whereas below criticality it converges to a symmetry-broken state.

We start out from the flow equation [1]

$$\frac{\mathrm{d}H(l)}{\mathrm{d}l} = [\eta(l), H(l)], \tag{1}$$

where η is chosen so that the Hamiltonian approaches a diagonal or block-diagonal form. We write H in the normal-ordered form

$$H =: H_G :_G, \tag{2}$$

where G defines the normal ordering

$$G_{kj} = \langle a_k a_j \rangle_0. \tag{3}$$

Here we denote both creation and annihilation operators by a. Then the flow equation reads

$$\frac{\mathrm{d}H_G}{\mathrm{d}l} = [\eta, H]_G + \frac{\delta H_G}{\delta G}\frac{\partial G}{\partial l}. \tag{4}$$

The second term indicates the change of H_G due to the change of G. G itself can be described as the expectation values corresponding to a bilinear Hamiltonian H^0. Then the flow equation (4) is supplemented by a second equation for H^0. This equation describes the adaption of H^0 to the one-particle energy of H, and will be given later (46).

In the next section, we consider the effect of normal ordering on operators. Then we give the general relation between a bilinear Hamiltonian and the expectation values in thermal equilibrium. Then we return to the flow equation and show that almost always the normal ordering will approach a stable state.

2. Normal ordering

The idea behind normal ordering is to subtract expectation values

$$G_{kj} = \langle a_k a_j \rangle \tag{5}$$

from products of operator pairs a_k, a_j. More precisely, one defines normal ordering which is indicated by two colons

$$:1: = 1, \tag{6}$$

$$:\alpha A(a) + \beta B(a): = \alpha : A(a) : + \beta : B(a) :, \tag{7}$$

$$a_k : A(a): = : a_k A(a) : + \sum_j G_{kj} : \frac{\partial}{\partial a_j} A(a) :, \tag{8}$$

where α, β are c-numbers. These equations hold for bosons and fermions. In performing the derivatives for fermions one has to consider that the operators a anticommute. Iteration of (8) yields

$$a_{k_1} a_{k_2} \ldots a_{k_m} =: \left(a_{k_1} + \sum_{l_1} G_{k_1 j_1} \frac{\partial}{\partial a_{j_1}}\right)\left(a_{k_2} + \sum_{j_2} G_{k_2 j_2} \frac{\partial}{\partial a_{j_2}}\right) \ldots a_{k_m} : \tag{9}$$

which can also be written as

$$a_{k_1}a_{k_2}\ldots a_{k_m} =: \exp\left(\sum_{kj} G_{kj}\frac{\partial^2}{\partial a_j^{\text{right}}\partial a_k^{\text{left}}}\right) a_{k_1}a_{k_2}\ldots a_{k_m} : . \tag{10}$$

This is Wick's first theorem [13]. The superscripts left and right indicate that we always pick a pair of factors a and perform the derivative $\frac{\partial}{\partial a_k}$ on the left factor and the derivative $\frac{\partial}{\partial a_j}$ on the right factor, so that the factor G_{kj} depends on the sequence of the operators. The exponential appears in the equation for the following reason. If we perform the operation $G\frac{\partial^2}{\partial a\partial a}$ on m pairs of factors a, then there are due to the permutation symmetry $m!$ contributions. Therefore, in order to obtain the contribution with factor one, we have to divide the mth power of $G\frac{\partial^2}{\partial a\partial a}$ by $m!$, which yields the exponential. Note that for fermions the operators a as well as the derivatives $\frac{\partial}{\partial a}$ anticommute.

Since in the following we will change the normal ordering, it is appropriate to indicate to which expectation values G it is performed. Then we obtain quite general for operators A

$$:A_G :_G = A, \qquad A_G = \exp\left(\sum_{kj} G_{kj}\frac{\partial^2}{\partial a_j^{\text{right}}\partial a_k^{\text{left}}}\right) A(a). \tag{11}$$

If we dissect $G_{kj} = Q_{kj} + C_{kj}$, where $C_{kj} = C_{jk}$ for bosons and $C_{kj} = -C_{jk}$ for fermions, then we have

$$:A_G :_G =: A_Q :_Q, \qquad A_G = \exp\left(\frac{1}{2}\sum_{kj} C_{kj}\frac{\partial^2}{\partial a_j\partial a_k}\right) A_Q \tag{12}$$

and we need no longer to distinguish the sequence of the factors. Suppose, we have

$$H = v^{(0)} + \frac{1}{2!}\sum_{kj} v_{kj}^{(1)} a_k a_j + \frac{1}{4!}\sum_{kjmn} v_{kjmn}^{(2)} a_k a_j a_m a_n \tag{13}$$

and $v_{kj}^{(1)}$ and $v_{kjmn}^{(2)}$ are completely symmetric for bosons and antisymmetric for fermions, resp., then the normal-ordered form reads

$$H_G = v_G^{(0)} + \frac{1}{2!}v_{G,kj}^{(1)} a_k a_j + \frac{1}{4!}v_{G,kjmn}^{(2)} a_k a_j a_m a_n, \tag{14}$$

$$v_G^{(0)} = v^{(0)} + \frac{1}{2}\sum_{kj} v_{kj}^{(1)} G_{kj} + \frac{1}{8}\sum_{kjmn} v_{kjmn}^{(2)} G_{kj} G_{mn}, \tag{15}$$

$$v_{G,kj}^{(1)} = v_{kj}^{(1)} + \frac{1}{2}\sum_{mn} v_{kjmn}^{(2)} G_{mn}, \tag{16}$$

$$v_{G,kjmn}^{(2)} = v_{kjmn}^{(2)}. \tag{17}$$

Expressing A and B by A_G and B_G by means of equation (10) and then transforming back to the normal ordering, we obtain for the product of two operators:

$$: A_G(a) :_G : B_G(a) :_G =: \exp\left(\sum_{kj} G_{kj}\frac{\partial^2}{\partial b_j\partial a_k}\right) A_G(a) B_G(b) : |_{G,b=a}. \tag{18}$$

3. Expectation values for H^0

In the following we will consider only fermions. A conventional way to introduce normal ordering is to use a Hamiltonian

$$H^0 = \tfrac{1}{2}\tilde{\epsilon}_{kj} a_{k^*} a_j, \tag{19}$$

where we use the notation

$$a_k^\dagger = a_{k^*}, \qquad a_k = a_{k^*}^\dagger. \tag{20}$$

Considering a as a column vector and $a^\dagger$ as a row vector, we may write

$$\begin{aligned} &\tilde{\epsilon}_{kj} a_{k^*} a_j = (a^\dagger \quad a^T)\tilde{\epsilon} \begin{pmatrix} a \\ a^* \end{pmatrix} = (a^\dagger \quad a^T) \begin{pmatrix} A & B \\ B^\dagger & -A^T \end{pmatrix} \begin{pmatrix} a \\ a^* \end{pmatrix} \\ &A^\dagger = A, \qquad B^T = -B. \end{aligned} \tag{21}$$

Thus $\tilde{\epsilon}$ has the properties

$$\tilde{\epsilon}^\dagger = \tilde{\epsilon}, \qquad \tau\tilde{\epsilon}\tau = -\tilde{\epsilon}^T, \qquad \tau = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{22}$$

$\tilde{\epsilon}$ can be diagonalized with diagonal matrix elements ϵ_k and $-\epsilon_k$. (This diagonalization is performed by a canonical transformation which is isomorphic to a real orthogonal transformation. This can be easily seen if one introduces the Hermitean linear combinations $q_k = \frac{a_k^\dagger + a_k}{\sqrt{2}}$ and $p_k = \frac{\mathrm{i}(a_k^\dagger - a_k)}{\sqrt{2}}$.)

In thermal equilibrium one obtains for diagonal $\tilde{\epsilon}$, i.e. $\tilde{\epsilon}_{kj} = \delta_{kj}\epsilon_k$

$$\langle a_k^\dagger a_k \rangle = \frac{1}{\mathrm{e}^{\beta\epsilon_k} + 1}, \qquad \langle a_k a_k^\dagger \rangle = \frac{1}{\mathrm{e}^{-\beta\epsilon_k} + 1} \tag{23}$$

so that even when $\tilde{\epsilon}$ is not diagonal

$$\tilde{G} = \frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1} = \frac{1}{2} - \frac{1}{2}\tanh\left(\frac{\beta\tilde{\epsilon}}{2}\right) \tag{24}$$

holds with $\tilde{G}_{kj} = G_{k^* j}$. A variation of $\tilde{\epsilon}$ yields

$$\delta\tilde{G} = -\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1}\delta\,\mathrm{e}^{\beta\tilde{\epsilon}}\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1} = -\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1}\int_0^\beta \mathrm{d}\tau\,\mathrm{e}^{\tau\tilde{\epsilon}}\delta\tilde{\epsilon}\,\mathrm{e}^{(\beta-\tau)\tilde{\epsilon}}\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1}. \tag{25}$$

Thus we may write

$$\delta\tilde{G}_{kj} = -\Gamma_{kj,pq}\delta\tilde{\epsilon}_{pq} \tag{26}$$

with

$$\Gamma_{kj,pq} = \int_0^\beta \mathrm{d}\tau \left(\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1}\mathrm{e}^{\tau\tilde{\epsilon}}\right)_{kp} \left(\mathrm{e}^{(\beta-\tau)\tilde{\epsilon}}\frac{1}{\mathrm{e}^{\beta\tilde{\epsilon}} + 1}\right)_{qj}. \tag{27}$$

4. Free energy and stability

It is well known that for a given Hamiltonian H and temperature T, the free energy assumes its minimum for the corresponding statistical operator $\rho = \mathrm{e}^{-\beta H}/Z$. Thus one often determines approximately the free energy for the statistical operator $\rho^0 = \mathrm{e}^{-\beta H^0}/Z^0$ with H^0 bilinear in the operators a and determines $\tilde{\epsilon}$ so that the corresponding free energy F^0 becomes minimal. One obtains

$$F^0 = E - TS, \qquad E = v_G^{(0)}, \qquad S = -\frac{k_\mathrm{B}}{2}\,\mathrm{tr}(\tilde{G}\ln\tilde{G} + (1-\tilde{G})\ln(1-\tilde{G})). \tag{28}$$

We use that $\langle A(a)\rangle^0 = A_G|_{a=0}$. We will vary this expression. By means of

$$A_{G+\delta G} = A_G + \frac{1}{2}\sum_{kj}\delta G_{kj}\frac{\partial^2}{\partial a_j \partial a_k}A_G \tag{29}$$

$$+\frac{1}{8}\sum_{kjmn}\delta G_{kj}\delta G_{mn}\frac{\partial^4}{\partial a_j \partial a_k \partial a_n \partial a_m}A_G + O(\delta G^3), \tag{30}$$

we obtain

$$E = v_G^{(0)} + \tfrac{1}{2}v^{(1)}_{G,k^*j}\delta\tilde{G}_{kj} + \tfrac{1}{8}v^{(2)}_{G,k^*jm^*n}\delta\tilde{G}_{kj}\delta\tilde{G}_{mn} + \cdots. \tag{31}$$

A variation of S yields in first order in $\delta\tilde{G}$

$$\delta S = -\frac{k_\mathrm{B}}{2}\ln\left(\frac{\tilde{G}}{1-\tilde{G}}\right)_{jk}\delta\tilde{G}_{kj}. \tag{32}$$

Therefore, we obtain in first order in $\delta\tilde{G}$

$$\begin{aligned}\delta F^0 &= \frac{1}{2}\left(v^{(1)}_{G,k^*j} + k_\mathrm{B}T\ln\left(\frac{\tilde{G}}{1-\tilde{G}}\right)_{jk}\right)\delta\tilde{G}_{kj}\\ &= \frac{1}{2}\big(v^{(1)}_{G,k^*j} - \tilde{\epsilon}_{kj}\big)\delta\tilde{G}_{kj}.\end{aligned} \tag{33}$$

In order that F^0 is an extremum one has to choose $\tilde{\epsilon}_{kj} = v^{(1)}_{G,k^*j}$, that is the one-particle contribution of our Hamiltonian H_G has to agree with H^0. In second order in $\delta\tilde{G}$, we obtain

$$\delta F^0 = \tfrac{1}{8}v^{(2)}_{G,k^*jm^*n}\delta\tilde{G}_{kj}\delta\tilde{G}_{mn} - \tfrac{1}{4}\delta\tilde{\epsilon}_{kj}\delta\tilde{G}_{kj}, \tag{34}$$

where $\delta\tilde{\epsilon}$ is given in terms of $\delta\tilde{G}$ from (26)

$$\delta\tilde{\epsilon}_{kj} = -(\Gamma^{-1})_{kj,mn}\delta\tilde{G}_{mn}. \tag{35}$$

which yields

$$\delta F^0 = \tfrac{1}{4}\big(\tfrac{1}{2}v^{(2)}_{G,k^*jm^*n} + (\Gamma^{-1})_{kj,mn}\big)\delta\tilde{G}_{kj}\delta\tilde{G}_{mn}. \tag{36}$$

Only if this expression is positive definite then it corresponds to a stable solution. We note that Γ is positive definite and therefore Γ^{-1} exists and is positive definite, too. This can be seen if we switch to the basis in which $\tilde{\epsilon}$ is diagonal, $\tilde{\epsilon}_{kj} = \delta_{kj}\epsilon_k$. Then

$$\Gamma_{kj,pq} = \delta_{kp}\delta_{jq}\Gamma^\mathrm{d}_{kj}, \tag{37}$$

$$\Gamma^\mathrm{d}_{kj} = \frac{\mathrm{e}^{\beta\epsilon_k} - \mathrm{e}^{\beta\epsilon_j}}{(\mathrm{e}^{\beta\epsilon_k}+1)(\epsilon_k-\epsilon_j)(\mathrm{e}^{\beta\epsilon_j}+1)} > 0. \tag{38}$$

Thus Γ is diagonal with positive matrix elements along the diagonal.

These expressions are closely connected to the response function in random phase approximation. Suppose one adds a perturbation $\delta v^{(1,\mathrm{ext})}$ to the Hamiltonian H which produces a change $\delta\tilde{G}^\mathrm{ext}$ in the expectation values $\langle a_k a_j\rangle$ then we have from equations (33, 36)

$$\tfrac{1}{2}\big(\delta v^{(1,\mathrm{ext})}_{G,k^*j} + \big(\tfrac{1}{2}v^{(2)}_{G,k^*jm^*n} + (\Gamma^{-1})_{kj,mn}\big)\delta\tilde{G}_{mn}\big)\delta\tilde{G}^\mathrm{ext}_{kj} = 0. \tag{39}$$

If we now relate $\delta\tilde{G}^\mathrm{ext}$ to a perturbation $\delta v^{(1,\mathrm{eff})}$ which would have the same effect without the interaction $v^{(2)}$ according to equation (26)

$$\delta\tilde{G}^\mathrm{eff}_{mn} = -\Gamma_{mn,pq}\delta v^{(1,\mathrm{eff})}_{pq} \tag{40}$$

then we obtain

$$\delta v^{(1,\mathrm{ext})}_{G,k^*j} = \left(\tfrac{1}{2} v^{(2)}_{G,k^*jm^*n}\Gamma_{mn,pq} + \delta_{kp}\delta_{jq}\right)\delta v^{(1,\mathrm{eff})}_{p^*q}. \tag{41}$$

This factor $\frac{1}{2}v^{(2)}\Gamma + 1$ enters for example in the Lindhard expression for the static dielectric constant. One has only to introduce $v^{(2)} \propto e^2/q^2$ and

$$\Gamma^{\mathrm{d}}_{kj} = \frac{f(\epsilon_j) - f(\epsilon_k)}{\epsilon_k - \epsilon_j} \tag{42}$$

with the Fermi function $f(\epsilon)$. The dielectric constant has to be positive for a stable system.

5. Flow equations

Now we have to introduce our flow equations. We have two contributions to the change of H_G, one from the generator of the flow,

$$[\eta, H]_G = g^{(0)} + \tfrac{1}{2} g^{(1)}_{kj} a_k a_j + \cdots \tag{43}$$

and one from the change of the normal ordering which yields

$$\frac{1}{2}\frac{\partial G_{kj}}{\partial l}\frac{\partial^2}{\partial a_j \partial a_k} H = -\frac{1}{2}\Gamma_{kj,mn}\frac{\partial \tilde{\epsilon}_{mn}}{\partial l}\left(v^{(1)}_{k^*j} + \frac{1}{2} v^{(2)}_{k^*jp^*q} a_{p^*} a_q + \cdots\right). \tag{44}$$

Thus we obtain the change of $v^{(1)}$

$$\frac{\partial v^{(1)}_{k^*j}}{\partial l} = g^{(1)}_{k^*j} - \frac{1}{2}\Gamma_{pq,mn} v^{(2)}_{p^*qk^*j}\frac{\partial \tilde{\epsilon}_{mn}}{\partial l} \tag{45}$$

for the one-particle energy. On the other hand, we wish to adapt $\tilde{\epsilon}$ so that it approaches $v^{(1)}$. Therefore, we introduce a flow equation for $\tilde{\epsilon}$

$$\frac{\partial \tilde{\epsilon}_{kj}}{\partial l} = \gamma\left(v^{(1)}_{k^*j} - \tilde{\epsilon}_{kj}\right) \tag{46}$$

with some positive constant γ. Evidently for fixed $v^{(1)}$ the energy $\tilde{\epsilon}$ approaches exponentially $v^{(1)}$. From both equations, we obtain

$$\frac{\partial\left(v^{(1)}_{k^*j} - \tilde{\epsilon}_{kj}\right)}{\partial l} = g^{(1)}_{k^*j} - \gamma\left(\delta_{km}\delta_{jn} + \frac{1}{2}\Gamma_{pq,mn} v^{(2)}_{p^*qk^*j}\right)\left(v^{(1)}_{m^*n} - \tilde{\epsilon}_{mn}\right). \tag{47}$$

Thus as $g^{(1)}$ from the generator of the flow decreases also $(v^{(1)} - \tilde{\epsilon})$ will decrease provided the kernel $1 + \frac{1}{2}\Gamma v^{(2)}$ is positive definite. Otherwise the difference $(v^{(1)} - \tilde{\epsilon})$ will nearly always increase exponentially. The condition that this kernel is positive definite is equivalent to the stability obtained from F^0 in equation (36), since the kernel for F^0 differs only by the factor Γ, which itself is positive definite.

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