

Hubbard-Stratonovich Transformation: Successes, Failure, and Cure

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Abstract: We recall the successes of the Hubbard-Stratonovich Transformation (HST) of many-body theory, point out its failure to cope with competing channels of collective phenomena and show how to overcome this by Variational Perturbation Theory. That yields exponentially fast converging results, thanks to the help of a variety of *collective classical fields*, rather than a fluctuating *collective quantum field* as suggested by the HST.

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1. The Hubbard-Stratonovich transformation (HST) has a well-established place in many-body theory [1] and elementary particle physics [2]. It has led to a good understanding of important collective physical phenomena such as superconductivity, superfluidity of He^3 , plasma and other charge-density waves, pion physics and chiral symmetry breaking in quark theories [3], etc. It has put heuristic calculations such as the Gorkov's derivation [4] of the Ginzburg-Landau equations [5] on a solid theoretical ground [6]. In addition, it is in spirit close [7] to the famous density functional theory [8] via the celebrated Hohenberg-Kohn and Kohn-Sham theorems [9].

The transformation is cherished by theoreticians since it allows them to re-express a four-particle interaction *exactly* in terms of a collective field variable whose fluctuations can in principle be described by higher loop diagrams. The only bitter pill is that any approximate treatment of a many-body system can describe interesting physics only if calculations may be restricted to a few low-order diagrams. This is precisely the point where the HST fails.

Trouble arises in all those many-body systems in which different collective effects compete with similar strengths. Historically, an important example is the fermionic superfluid

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He³. While BCS superconductivity was described easily via the HST by transforming the four-electron interaction to a field theory of Cooper pairs, this approach did initially not succeed in a liquid of He³ atoms. Due to the strongly repulsive core of an atom, the forces in the attractive p -wave are not sufficient to bind the Cooper pairs. Only after taking the help of another collective field that arises in the competing paramagnon channel into account, could the formation of weakly bound Cooper pairs be explained [10].

It is the purpose of this note to point out how to circumvent the fatal fucussing of the HST upon a single channel and to show how this can be avoided in a way that takes several competing channels into account to each order in perturbation theory.

2. The problem of channel selection of the HST was emphasized in the context of quark theories in [3] and in many-body systems such as He³ in [6]. Let us briefly recall how it appears. Let $x = (t, \mathbf{x})$ be the time and space coordinates, and consider the action $\mathcal{A} \equiv \mathcal{A}_0 + \mathcal{A}_{\text{int}}$ of a nonrelativistic many-fermion system

$$\mathcal{A} = \int_x \psi_x^* [i\partial_t - \xi(-i\nabla)] \psi_x - \frac{1}{2} \int_{x,x'} \psi_{x'}^* \psi_x^* V_{x,x'} \psi_x \psi_{x'}, \quad (1)$$

where we have written ψ_x instead of $\psi(x)$, and \int_x for $\int d^4x$, to save space. The symbol $\xi(\mathbf{p}) \equiv \epsilon(\mathbf{p}) - \mu$ denotes the single-particle energies minus chemical potential. Adding to \mathcal{A} also a source term $\mathcal{A}_s = \int d^4x (\psi_x^* \eta_x + \text{c.c.})$ to form $\bar{\mathcal{A}} = \mathcal{A} + \mathcal{A}_s$, the grand-canonical generating functional of all fermionic Green functions reads $Z[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{i\bar{\mathcal{A}}}$.

The HST enters the arena by rewriting the interaction part with the help of an auxiliary complex field $\Delta_{x,x'}$ as [6]

$$Z[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi \mathcal{D}\Delta^* \mathcal{D}\Delta e^{i\mathcal{A}_a[\psi^*, \psi, \Delta^*, \Delta] + i\mathcal{A}_s} \quad (2)$$

with an auxiliary action

$$\mathcal{A}_{\text{aux}} = \int_{x,x'} \left\{ \psi_x^* [i\partial_t - \xi(-i\nabla)] \delta_{x,x'} \psi_{x'} - \frac{1}{2} \Delta_{x,x'}^* \psi_x \psi_{x'} - \frac{1}{2} \psi_x^* \psi_{x'}^* \Delta_{x,x'} + \frac{1}{2} |\Delta_{x,x'}|^2 / V_{x,x'} \right\}, \quad (3)$$

Indeed, if the field $\Delta_{x,x'}$ is integrated out in (2), one recovers the original generating functional. At the classical level, the field $\Delta_{x,x'}$ is nothing but a convenient abbreviation for the composite *pair field* $V_{x,x'} \psi_x \psi_{x'}$ upon extremizing the new action with respect to $\delta \Delta_{x,x'}^*$, yielding $\delta \mathcal{A} / \delta \Delta_{x,x'}^* = (\Delta_{x,x'} - V_{x,x'} \psi_x \psi_{x'}) / 2V_{x,x'} \equiv 0$. Quantum mechanically, there are Gaussian fluctuations around this solution which are discussed in detail in [3, 6].

Expression (3) is quadratic in the fundamental fields ψ_x and reads in functional matrix form $\frac{1}{2} f_x^* A_{x,x'} f_{x'}$ with

$$A_{x,x'} = \begin{pmatrix} [i\partial_t - \xi(-i\nabla)] \delta_{x,x'} & -\Delta_{x,x'} \\ -\Delta_{x,x'}^* & [i\partial_t + \xi(i\nabla)] \delta_{x,x'} \end{pmatrix}. \quad (4)$$

where f_x denotes the fundamental field doublet (“Nambu spinor”) with $f_x^T = (\psi_x, \psi_x^*)$, and $f^\dagger \equiv f^{*T}$, as usual. Since f_x^* is not independent of f_x , we can integrate out the Fermi

fields and find

$$Z[\eta^*, \eta] = \int \mathcal{D}\Delta^* \mathcal{D}\Delta e^{i\mathcal{A}[\Delta^*, \Delta] - \frac{1}{2} \int_{x,x'} j_x^\dagger [G_\Delta]_{x,x'} j_{x'}}, \quad (5)$$

where j_x collects the external source η_x and its complex conjugate, $j_x^T \equiv (\eta_x, \eta_x^*)$, and the collective action reads

$$\mathcal{A}[\Delta^*, \Delta] = -\frac{i}{2} \text{Tr} \log [i\mathbf{G}_\Delta^{-1}] + \frac{1}{2} \int_{x,x'} |\Delta_{x,x'}|^2 / V_{x,x'}. \quad (6)$$

The 2×2 matrix \mathbf{G}_Δ denotes the propagator iA^{-1} which satisfies the functional matrix equation

$$\int_x \begin{pmatrix} [i\partial_t - \xi(-i\nabla)] \delta_{x,x'} & -\Delta_{x,x'} \\ -\Delta_{x,x'}^* & [i\partial_t + \xi(i\nabla)]_{x,x'} \end{pmatrix} \times [\mathbf{G}_\Delta]_{x',x''} = i\delta_{x,x''}. \quad (7)$$

Writing \mathbf{G}_Δ as a matrix $\begin{pmatrix} G_\rho & G_\Delta \\ G_\Delta^\dagger & \tilde{G}_\rho \end{pmatrix}$ the mean-field equations associated with this action are precisely the equations used by Gorkov [4] to study the behavior of type II superconductors.

With $Z[\eta^*, \eta]$ being the *full* partition function of the system, the fluctuations of the collective field $\Delta_{x,x'}$ can now be incorporated, at least in principle, thereby yielding corrections to these equations.

3. The basic weakness of the HST lies in the ambiguity of the decomposition of the quadratic decomposition (2) of the interaction in (1). For instance, there exists an *alternative* elimination of the two-body interaction using an auxiliary real field φ_x , and writing the partition function as

$$Z[\eta^*, \eta] = \int \mathcal{D}\psi^* \mathcal{D}\psi D\varphi \exp [i\mathcal{A}[\psi^*, \psi, \varphi] + i\mathcal{A}_s], \quad (8)$$

rather than (2), where the action is now

$$\mathcal{A}[\psi^*, \psi, \varphi] = \int_{x,x'} \left\{ \psi_x^* [i\partial_t - \xi(-i\nabla) - \varphi(x)] \delta_{x,x'} \psi_{x'} + \frac{1}{2} \varphi_x V_{x,x'}^{-1} \varphi_{x'} \right\}. \quad (9)$$

The new collective quantum field φ_x is directly related to the particle density. At the classical level, this is obtained from the field equation $\delta\mathcal{A}/\delta\varphi_x = \varphi_x - \int dx' V_{x,x'} \psi_x^* \psi_{x'} = 0$. For example, if $V_{x,x'}$ represents the Coulomb interaction $\delta_{t,t'}/|\mathbf{x} - \mathbf{x}'|$ in an electron gas, the field φ_x describes the plasmon fluctuations in the gas.

The trouble with the approach is that when introducing a collective quantum field $\Delta_{x,x'}$ or φ_x , the effects of the other is automatically included if we sum over all fluctuations. At first sight, this may appear as an advantage. Unfortunately, this is an illusion. Even the lowest-order fluctuation effect is extremely hard to calculate, already for the

simplest models of quantum field theory such as the Gross-Neveu model, since the propagator of the collective quantum field is a very complicated object. So it is practically impossible to recover the effects from the loop calculations with these propagators. Thus the use of a collective quantum field theory must be abandoned whenever collective effects of the different channels are important.

The cure of this problem comes from the development some time ago, in the treatment of path integrals of various quantum mechanical systems [11] and in the calculation of critical exponents in ϕ^4 -field theories [12], of a technique called *Variational Perturbation Theory* (VPT) [13]. This is democratic in all competing channels of collective phenomena. The important point is that it is based on the introduction of *classical collective fields* which no longer fluctuate, and thus avoid double-counting of diagrams of competing channels by quantum fluctuations.

4. To be specific let us assume the fundamental interaction to be of the *local* form

$$\mathcal{A}_{\text{int}}^{\text{loc}} = \frac{g}{2} \int_x \psi_\alpha^* \psi_\beta^* \psi_\beta \psi_\alpha = g \int_x \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow, \quad (10)$$

where the subscripts \uparrow, \downarrow indicate spin directions, and we have absorbed the spacetime arguments x in the spin subscripts, for brevity.

We now introduce auxiliary *classical* collective fields and replace the exponential of the action in the generating functional $Z[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{i\mathcal{A}}$ identically by [14]

$$\begin{aligned} e^{ig \int_x \psi_\uparrow^* \psi_\downarrow^* \psi_\downarrow \psi_\uparrow} &= e^{-\frac{i}{2} \int_x f_x^T \mathcal{M}_x f_x} \times e^{i\mathcal{A}_{\text{int}}^{\text{new}}} \\ &= e^{-\frac{i}{2} \int_x (\psi_\beta \Delta_{\beta\alpha}^* \psi_\alpha + \psi_\alpha^* \Delta_{\alpha\beta} \psi_\beta^* + \psi_\beta^* \rho_{\beta\alpha} \psi_\alpha + \psi_\alpha^* \rho_{\alpha\beta} \psi_\beta)} \times e^{i\mathcal{A}_{\text{int}}^{\text{new}}}, \end{aligned} \quad (11)$$

with the new interaction

$$\mathcal{A}_{\text{int}}^{\text{new}} = \mathcal{A}_{\text{int}}^{\text{loc}} + \frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x = \int_x \left[\frac{g}{2} \psi_\alpha^* \psi_\beta^* \psi_\beta \psi_\alpha + \frac{1}{2} (\psi_\beta \Delta_{\beta\alpha}^* \psi_\alpha + \psi_\alpha^* \Delta_{\alpha\beta} \psi_\beta^*) + \psi_\alpha^* \rho_{\alpha\beta} \psi_\beta \right]. \quad (12)$$

We now define a new free action by the quadratic form $\mathcal{A}_0^{\text{new}} \equiv \mathcal{A}_0 - \frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x = \frac{1}{2} f_x^\dagger A_{x,x'}^{\Delta,\rho} f_{x'}$, where f_x^T denotes the fundamental field doublet $f_x^T = (\psi_\alpha, \psi_\alpha^*)$. Then we rewrite $\mathcal{A}_0^{\text{new}}$ in the 2×2 matrix form analogous to (4) as $\mathcal{A}_0^{\text{new}} \equiv \mathcal{A}_0 - \frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x = \frac{1}{2} f_x^\dagger A_{x,x'}^{\Delta,\rho} f_{x'}$, with the functional matrix $A_{x,x'}^{\Delta,\rho}$ being now equal to

$$\begin{pmatrix} [i\partial_t - \xi(-i\nabla)] \delta_{\alpha\beta} + \rho_{\alpha\beta} & \Delta_{\alpha\beta} \\ \Delta_{\alpha\beta}^* & [i\partial_t + \xi(i\nabla)] \delta_{\alpha\beta} - \rho_{\alpha\beta} \end{pmatrix}. \quad (13)$$

The physical properties of the theory associated with the action $\mathcal{A}_{\text{int}}^{\text{loc}} + \mathcal{A}_s$ can now be derived as follows: first we calculate the generating functional of the new quadratic action $\mathcal{A}_0^{\text{new}}$ via the functional integral $Z_0^{\text{new}}[\eta, \eta^*] = \int \mathcal{D}\psi^* \mathcal{D}\psi e^{i\mathcal{A}_0^{\text{new}}}$. From its derivatives we find the new free propagators G_Δ and G_ρ . To higher orders, we expand the exponential

$e^{i\mathcal{A}_{\text{int}}^{\text{new}}}$ in a power series and evaluate all expectation values $(i^n/n!)\langle[\mathcal{A}_{\text{int}}^{\text{new}}]^n\rangle_0^{\text{new}}$ using Wick's theorem as a sum of products of the free particle propagators G_Δ and G_ρ . The sum of all diagrams up to a certain order g^N defines an effective collective action $\mathcal{A}_{\text{eff}}^N$ as a function of the collective classical fields $\Delta_{\alpha\beta}, \Delta_{\beta\alpha}^*, \rho_{\alpha\beta}$,

Obviously, if the expansion is carried to infinite order, the result must be independent of the auxiliary collective fields since they were introduced and removed in (11) without changing the theory. However, any calculation can only be carried up to a finite order, and that will *depend* on these fields. We therefore expect the best approximation to arise from the extremum of the effective action [11, 12, 17].

The lowest-order effective collective action is obtained from the trace of the logarithm of the matrix (13):

$$\mathcal{A}_{\Delta,\rho}^0 = -\frac{i}{2}\text{Tr} \log [i\mathbf{G}_{\Delta,\rho}^{-1}]. \quad (14)$$

The 2×2 matrix $\mathbf{G}_{\Delta,\rho}$ denotes the propagator $i[A_{x,x'}^{\Delta,\rho}]^{-1}$.

To first order in perturbation theory we must calculate the expectation value $\langle\mathcal{A}_{\text{int}}\rangle$ of the interaction (12). This is done with the help of the Wick contractions in the three channels, Hartree, Fock, and Bogoliubov:

$$\langle\psi_\uparrow^*\psi_\downarrow^*\psi_\downarrow\psi_\uparrow\rangle = \langle\psi_\uparrow^*\psi_\uparrow\rangle\langle\psi_\downarrow^*\psi_\downarrow\rangle - \langle\psi_\uparrow^*\psi_\downarrow\rangle\langle\psi_\downarrow^*\psi_\uparrow\rangle + \langle\psi_\uparrow^*\psi_\downarrow^*\rangle\langle\psi_\downarrow\psi_\uparrow\rangle. \quad (15)$$

For this purpose we now introduce the expectation values

$$\tilde{\Delta}_{\alpha\beta}^* \equiv g\langle\psi_\alpha^*\psi_\beta^*\rangle, \quad \tilde{\Delta}_{\beta\alpha} \equiv g\langle\psi_\beta\psi_\alpha\rangle = [\Delta_{\alpha\beta}^*]^*, \quad (16)$$

$$\tilde{\rho}_{\alpha\beta} \equiv g\langle\psi_\alpha^*\psi_\beta\rangle, \quad \tilde{\rho}_{\alpha\beta}^\dagger = [\tilde{\rho}_{\beta\alpha}]^*, \quad (17)$$

and rewrite $\langle\mathcal{A}_{\text{int}}\rangle$ as

$$\langle\mathcal{A}_{\text{int}}\rangle = (1/g) \int_x (\tilde{\Delta}_{\downarrow\uparrow}^*\tilde{\Delta}_{\downarrow\uparrow} - \tilde{\rho}_{\uparrow\downarrow}\tilde{\rho}_{\downarrow\uparrow} + \tilde{\rho}_{\uparrow\uparrow}\tilde{\rho}_{\downarrow\downarrow}) \quad (18)$$

Due to the locality of $\tilde{\Delta}_{\alpha\beta}$ the diagonal matrix elements vanish and $\tilde{\Delta}_{\alpha\beta} = c_{\alpha\beta}\tilde{\Delta}$, where $c_{\alpha\beta}$ is i times the Pauli matrix $\sigma_{\alpha\beta}^2$. In the absence of a magnetic field, the expectation values $\tilde{\rho}_{\alpha\beta}$ may have certain symmetries:

$$\tilde{\rho}_{\uparrow\uparrow} \equiv \tilde{\rho}_{\downarrow\downarrow} = \tilde{\rho}, \quad \tilde{\rho}_{\uparrow\downarrow} = \tilde{\rho}_{\downarrow\uparrow} \equiv 0, \quad (19)$$

so that (19) simplifies to

$$\langle\mathcal{A}_{\text{int}}\rangle = (1/g) \int_x \left[(|\tilde{\Delta}|^2 + \tilde{\rho}^2) - (\tilde{\Delta}\Delta^* + \tilde{\Delta}^*\Delta + 2\tilde{\rho}\rho) \right]. \quad (20)$$

The total first-order collective classical action $\mathcal{A}_{\Delta,\rho}^1$ is given by the sum $\mathcal{A}_{\Delta,\rho}^1 = \mathcal{A}_{\Delta,\rho}^0 + \langle\mathcal{A}_{\text{int}}\rangle$.

Now we observe that the functional derivatives of the zeroth-order action $\mathcal{A}_{\Delta,\rho}^0$ are the free-field propagators G_Δ , and G_ρ

$$\frac{\delta}{\delta\Delta_{\alpha\beta}}\mathcal{A}_{\Delta,\rho}^0 = [G_\Delta]_{\alpha\beta}, \quad \frac{\delta}{\delta\rho_{\alpha\beta}}\mathcal{A}_{\Delta,\rho}^0 = [G_\rho]_{\alpha\beta}. \quad (21)$$

Then we can extremize $\mathcal{A}_{\Delta,\rho}^1$ with respect to Δ and ρ , and find that, to this order, the field expectation values (17) are given by the free-field propagators (21) at equal arguments:

$$\tilde{\Delta}_x = g[G_\Delta]_{x,x}, \quad \tilde{\rho}_x = g[G_\rho]_{x,x}. \quad (22)$$

Thus we see that at the extremum, the action $\mathcal{A}_{\Delta,\rho}^1$ is the same as the extremal action

$$\mathcal{A}_1[\Delta, \rho] = \mathcal{A}_0[\Delta, \rho] - \frac{1}{g} \int_x (|\Delta|^2 + \rho^2). \quad (23)$$

Note how the theory differs, at this level, from the collective quantum field theory derived via the HST. If we assume that ρ vanishes identically, the extremum of the one-loop action $\mathcal{A}_1[\Delta, \rho]$ gives the same result as of the mean-field collective quantum field action (6), which reads for the present δ -function attraction $\mathcal{A}_1[\Delta] = \mathcal{A}_0[\Delta] - \frac{1}{g} \int_x |\Delta|^2$. On the other hand, if we extremize the action $\mathcal{A}_{\Delta,\rho}^1$ at $\Delta = 0$, we find the extremum from the expression $\mathcal{A}_1[\Delta, \rho] = \mathcal{A}_0[\Delta, \rho] - \frac{1}{g} \int_x \rho^2$. The extremum of the first-order collective classical action (23) agrees with the good-old Hartree-Fock-Bogoliubov theory.

The essential difference between this and the new approach arises in two ways:

- First when it is carried to higher orders. In the collective quantum field theory based on the HST the higher-order diagrams must be calculated with the help of the propagators of the collective field such as $\langle \Delta_x \Delta_{x'} \rangle$. These are extremely complicated functions. For this reason, any loop diagram formed with them is practically impossible to integrate. In contrast to that, the higher-order diagrams in the present theory need to be calculated using only ordinary particle propagators G_Δ and G_ρ of Eq. (21) and the interaction (12). Even that becomes, of course, tedious for higher orders in g . At least, there is a simple rule to find the contributions of the quadratic terms $\frac{1}{2} \int_x f_x^T \mathcal{M}_x f_x$ in (11), given the diagrams *without* these terms. One calculates the diagrams from only the four-particle interaction, and collects the contributions up to order g^N in an effective action $\tilde{\mathcal{A}}_N[\Delta, \rho]$. Then one replaces $\tilde{\mathcal{A}}_N[\Delta, \rho]$ by $\tilde{\mathcal{A}}_N[\Delta - \epsilon g \Delta, \rho - \epsilon g \rho]$ and re-expands everything in powers of g up to the order g^N , forming a new series $\sum_{i=0}^N g^i \tilde{\mathcal{A}}_i[\Delta, \rho]$. Finally one sets ϵ equal to $1/g$ [15] and obtains the desired collective classical action $\mathcal{A}_N[\Delta, \rho]$ as an expansion extending (23):

$$\mathcal{A}_N[\Delta, \rho] = \sum_{i=0}^N \tilde{\mathcal{A}}_i[\Delta, \rho] - (1/g) \int_x (|\Delta|^2 + \rho^2). \quad (24)$$

Note that this action must merely be extremized. There are no more quantum fluctuations in the *classical collective fields* Δ, ρ . Thus, at the extremum, the action (24) is directly the grand-canonical potential.

- The second essential difference with respect to the HST approach is that it is now possible to study a rich variety of possible competing collective fields without the danger of double-counting Feynman diagrams. One simply generalizes the matrix \mathcal{M}_x subtracted from \mathcal{A}_{int} and added to \mathcal{A}_{int} in (11) in different ways. For instance, we may subtract and add a vector field $\psi^\dagger \sigma^a \psi S^a$ containing the Pauli matrices σ^a and study paramagnon fluctuations, thus generalizing the assumption (??) and allowing

for a spontaneous magnetization in the ground state. Or one may do the same thing with a term $\psi^\dagger \sigma^a \nabla^i \psi A_{ia} + \text{c.c.}$ in addition to the previous term, and derive the Ginzburg-Landau theory of superfluid He³ as in [6].

An important property of the proposed procedure is that it yields good results in the limit of infinitely strong coupling. It was precisely this property which led to the successful calculation of critical exponents of all ϕ^4 theories in the textbook [12] since critical phenomena arise in the limit in which the unrenormalized coupling constant goes to infinity [18]. This is in contrast to another possibility, in principle, of carrying the variational approach to higher order via the so-called *higher effective actions* [19]. There one extremizes the Legendre transforms of the generating functionals of bilocal correlation functions, which sums up all two-particle irreducible diagrams. That does *not* give physically meaningful results [20] in the strong-coupling limit, even for simple quantum-mechanical models.

6. The mother of this approach, Variational Perturbation Theory [11], is a systematic extension of a variational method developed some years ago by Feynman and the author [16]. It converts *divergent* perturbation expansions of quantum mechanical systems into exponentially fast *converging* expansions for all coupling strength [17]. What we have shown here is that this powerful theory can easily be transferred to many-body theory, if we identify a variety of relevant *collective classical fields*, rather than a fluctuating collective *quantum field* suggested by the HST. This allows us to go systematically beyond the standard Hartree-Fock-Bogoliubov approximation.

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