The Hubbard–Stratonovich Transformation and Exchange Boson Contributions

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Abstract. The Hubbard - Stratonovich transformation of many - body theory is reconsidered in various versions. Learning from its failures in coping with competing channels of collective phenomena, a combined Hubbard - Stratonovich transformation is proposed to overcome these difficulties. That yields a variety of fluctuating bosonic quantum fields describing the competition of different phases in the system under consideration. As a consequence of results, the validity of the Hubbard - Stratonovich transformation and its relation to a given order parameter are discussed.

1. Introduction
One of the most powerful techniques in the functional integral formalism is the use of the so-called Hubbard - Stratonovich transformation which is an exact mathematical transformation invented by Russian physicist R. L. Stratonovich [1] and popularized by British physicist J. Hubbard [2]. Since its birth, the Hubbard - Stratonovich transformation has a well - established place not only in many - body theory but also in elementary particle physics [3, 4]. It has led to a good understanding of important collective physical phenomena such as superconductivity, superfluidity of He⁳, plasma and other charge - density waves, pion physics and chiral symmetry breaking in quark theories, etc. It has put heuristic calculations such as the Gorkov’s derivation [5] of the Ginzburg - Landau equations [6] on a solid theoretical ground. In addition it is in spirit close to the famous density functional theory via the celebrated Hohenberg - Kohn and Kohn - Sham theorems. The transformation is cherished by theoreticians since it allows them to re-express a two - body interaction exactly in terms of a bosonic collective field variable whose fluctuations, i.e. exchange bosons 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 Hubbard - Stratonovich transformation fails. Trouble arises in all those many - body systems in which different exchange boson effects compete with similar strengths. Historically, an important example is the fermionic superfluid He⁳. While BCS superconductivity was described easily via the Hubbard - Stratonovich transformation by transforming the two - body 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
motivated by many physical considerations. Normally, for bosonic Hubbard-Stratonovich to make the Hubbard-Stratonovich transformation a meaningful operation, it has to be the help of another exchange boson field that arises in the competing paramagnon channel into account, could the formation of weakly bound Cooper pairs be explained.

2. The Hubbard–Stratonovich Transformation
While the term of Hubbard-Stratonovich transformation may sound very impressive, the essence of this transformation is nothing but a straightforward manipulation of a Gaussian integral with respect to complex or Grassmann variables. In order to make this fact more transparent for a generic two-body interaction, let’s briefly recall how it appears. Consider a non-relativistic many-body fermionic system described by a Hamiltonian:

$$ H = H_0 + H_1, $$

where

$$ H_0 = \sum_{\sigma} \sum_{k} \varepsilon_{\sigma}(k) \psi_{\sigma}^\dagger(k) \psi_{\sigma}(k), $$

where

$$ H_0 $$

is unperturbed Hamiltonian describing the system of free electrons, the symbols $$ \psi_{\sigma}(k) $$ and $$ \psi_{\sigma}^\dagger(k) $$ denote the annihilation and creation operators of the electrons with the spin projection $$ \sigma = \uparrow, \downarrow $$ respectively, and $$ \varepsilon_{\sigma}(k) $$ is the dispersion of the free electrons; and

$$ H_1 = \sum_{\sigma_1,\sigma_2,\sigma_1',\sigma_2'} \sum_{k,k',q} V_{\sigma_1\sigma_2\sigma_1'\sigma_2'}(k,k',q) \psi_{\sigma_1}^\dagger(k - \frac{q}{2}) \psi_{\sigma_2}^\dagger(k + \frac{q}{2}) \psi_{\sigma_1'}(k + \frac{q}{2}), $$

$$ H_1 $$

is a generic effective two-body interaction term of interacting electrons written in the normal order, which may cover the contributions of other interactions in the system such as electron-phonon interaction, spin-spin interaction, ... even impurity - electron and impurity - impurity interactions. In both mathematical and physical aspects, the generic effective interaction term is very complicated and has no exact and explicit analytical expression.

The Hubbard–Stratonovich transformation enters the arena by rewriting the two-body interaction term (3) with the help of an auxiliary complex field $$(\varphi)_{\sigma,\sigma'}(k, -q, \tau)$$ as

$$\begin{align*}
\exp \left\{ (-1)^{\beta} \int_0^\beta d\tau \sum_{\sigma_1,\sigma_2,\sigma_1',\sigma_2'} \sum_{k,k',q} V_{\sigma_1\sigma_2\sigma_1'\sigma_2'}(k,k',q) (\psi_{-\sigma}^\dagger(\psi_{\sigma})_{\sigma_1\sigma_2'}(k, -q, \tau) \\
&\quad - \frac{i}{\hbar} \int [D\varphi^*][D\varphi] \exp \left\{ - S_0 [\varphi^*, \varphi] \right\} \\
&\quad - (i)^{\beta} \int_0^\beta d\tau \sum_{\sigma,\sigma'} \sum_{k,q} \left\{ (\varphi)_{\sigma}^\dagger(\varphi)_{\sigma'}(k, -q, \tau) (\psi_{-\sigma}^\dagger(\psi_{\sigma})_{\sigma'}(k, -q, \tau) \\
&\quad + (\psi_{-\sigma}^\dagger(\psi_{\sigma})_{\sigma'}(k, -q, \tau)) (\varphi)_{\sigma'}(k, -q, \tau) \right\} \right\},
\end{align*}$$

where

$$ S_0 [\varphi^*, \varphi] = \int_0^\beta d\tau \sum_{\sigma_1,\sigma_2,\sigma_1',\sigma_2'} \sum_{k,k',q} (\varphi)_{\sigma_1\sigma_2'}^*(k', -q, \tau) (V)_{\sigma_2\sigma_1'}^{-1}(k', k, q) (\varphi)_{\sigma_1\sigma_2}(k, -q, \tau). $$

The Hubbard–Stratonovich transformation is actually explicit and exact. However, in practice, to make the Hubbard–Stratonovich transformation a meaningful operation, it has to be motivated by many physical considerations. Normally, for bosonic Hubbard–Stratonovich
transformation, the interaction is split by choosing a composite operator consisted of two fermionic field operators which are called bifermionic. The version of the transformation in (4) corresponds to the type of pairing which is referred to decoupling in the direct channel or in other words, in the "density" channel. However, there are, at least, two other inequivalent choices of pairing up the fermionic operators to construct the fermionic bilinear term of the generic two - body interaction which are decoupling in the “exchange” channel generated by choice of the fermionic pairings \((\psi^\dagger \psi)^{\sigma_a}_{\sigma} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right)\), and \((\psi^\dagger \psi)^{\overline{\sigma}}_{\sigma'} \left( \mathbf{k}', \mathbf{k}, \mathbf{q} \right)\), and decoupling the in Cooper channel corresponding to following bifermionic operators \((\psi \psi)_{\sigma_1 \sigma_2} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right)\) and \((\psi^\dagger \psi^\dagger)_{\sigma_2 \sigma_1} \left( \mathbf{k}', \mathbf{k}, -\mathbf{q} \right)\). This is always not clear why one kind of pairing is chosen but not others. The existence of there pairing possibilities may lead to the impression of a certain arbitrariness to the Hubbard - Stratonovich transformation philosophy. Indeed, the “right” choice of the decoupling field should be only motivated by physical reasoning. This is to emphasis that the transformation as such is always exact, no matter what channel is chosen. Besides the physical reasoning of the system under consideration, the mathematical structure of the two - body interaction term has also an important role in choosing the “right” channel for the Hubbard - Stratonovich transformation. In the mathematical context, the “right” choice of the decoupling corresponds to the existence of the auxiliary bosonic Gaussian integral \(W\) (5), i. e. the positiveness and the existence of the inverse of two - body matrix element \((V)^{-1}_{\overline{\sigma}_a \sigma_1 \overline{\sigma}_2 \sigma_2} \left( \mathbf{k}', \mathbf{k}, \mathbf{q} \right)\).

For every type of bifermionic operators as “density”, “exchange” and “Cooper” pairings, the Hubbard - Stratonovich transformation requires a corresponding inverse of two - body matrix element such as

\[
\sum_{\sigma, \sigma'} \sum_{\mathbf{k}', \mathbf{q}'} V_{\sigma_1 \sigma_2} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right) (V_d)^{-1}_{\overline{\sigma}_a \sigma_1 \sigma_2} \left( \mathbf{k}', \mathbf{k}_1, \mathbf{q} \right) = \delta_{\mathbf{k} \mathbf{k}_1}, \delta_{\overline{\sigma}_1 \sigma_2} \delta_{\overline{\sigma}_1 \sigma_2'},
\]

\[
\sum_{\sigma, \sigma'} V_{\sigma_1 \sigma_2} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right) (V_{\text{ex}})^{-1}_{\sigma_2 \overline{\sigma}_2 \sigma_2} \left( \mathbf{k}', \mathbf{k}, \mathbf{q} \right) = \delta_{\sigma_1 \sigma_2} \delta_{\overline{\sigma}_1 \overline{\sigma}_2},
\]

\[
\sum_{\sigma_1, \sigma_2} V_{\sigma_1 \sigma_2} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right) (V_{\text{C}})^{-1}_{\sigma_2 \overline{\sigma}_1 \overline{\sigma}_1} \left( \mathbf{k}', \mathbf{k}, \mathbf{q} \right) = \delta_{\sigma_1 \sigma_2}, \delta_{\sigma_2 \sigma_4},
\]

respectively.

The existence of different inverses for the two - body matrix elements \(V_{\sigma_1 \sigma_2} \left( \mathbf{k}, \mathbf{k}', \mathbf{q} \right)\) gives some additional arguments to physical insights of the system under consideration, deciding the existence of the corresponding order parameter.

In fact, in the most well - known microscopic models of interacting fermion systems, the two - body matrix element is dramatically simplified and its spin - dependence is actually neglected. Such way of simplification leads to the fact that all three possible decoupling schemes are always posible and can be applied to the interacting electron systems, or in other words, without spin - dependence of two - body matrix elements all possible kinds of order parameters can coexist in a theoretical calculations leading to “false” physical interpretation of the given system. And the only thing to justify physical properties of a real physical system described by these microscopic models is physical reasoning.

In order to verify this arguments, another version of the Hubbard - Stratonovich transformation
based on a simple and always valid bosonic Gaussian integral

\[
\mathcal{W} = \int \left[ D\phi^* \right] \left[ D\phi \right] \exp \left\{ -\frac{1}{\beta} \int_0^\beta d\tau \sum_{\sigma_1,\sigma'_1, k, q} (\phi)^*_\sigma (k, -q, \tau) (\phi)_{\sigma'_1} (k, -q, \tau) \right\}, \tag{9}
\]

is performed.

This version, however, requires the existence of term \((V)_{\sigma_1,\sigma_2,\sigma'_1,\sigma'_2}^{1/2} (k, k', q)\) and its inverse for each corresponding pairing.

Once the mathematical structure of the two-body interaction term confirms the possible order parameters which would appear in the systems, the standard techniques can be used to obtain physical quantities without difference among decoupling schemes. The simplest physical reasoning to include spin-dependence to the two-body matrix element is the contributions of exchange bosons reflecting the interactions between conducting electrons and bosonic background fluctuations which cause the rise of selected competing channels. Mathematically, the exchange boson contributions of background fluctuations would lead to additional spin-dependent terms to two-body interaction, which allows the existence of specified version of the inverse two-body matrix element.

3. Discussions and Conclusions

The validity of the Hubbard - Stratonovich transformations in different decoupling schemes as “density”, “exchange” and “Cooper” channels is discussed and shows that spin-dependent dependence of two-body matrix elements plays an important role in the existence of a certain phase in the systems. The roles of exchange bosons in the spin-dependence of two-body matrix element are also discussed. This can motivate to attain a proper comprehension of formalism and that the functional integral formalism is a very systematic technique, free of ambiguity.

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References

[1] R. L. Stratonovich. On a method of calculating quantum distribution functions. Soviet Physics Doklady, 2:461, 1958.
[2] J. Hubbard. Calculation of partition functions. Phys. Rev. Lett., 3(2):77–78, 1959.
[3] H. Kleinert. Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics. World Scientific, Singapore, 3rd edition, 2004.
[4] John W. Negele and Henri Orland. Quantum Many-Particle Systems, volume 68 of Frontiers in Physics. Addison Wesley, 1988.
[5] L. P. Gor’kov. Microscopic Derivation of the Ginzburg-Landau Equations in the Theory of Superconductivity. Sov. Phys. JETP, 36:1304–1307, 1959.
[6] V. L. Ginzburg and L. D. Landau. To The Theory of Superconductivity. Sov. Phys. JETP, 20:1064, 1950.