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Grassmann Phase Space Theory for Fermions

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Abstract. A phase space theory for fermions has been developed using Grassmann phase space variables which can be used in numerical calculations for cold Fermi gases and is applicable for large fermion numbers. Numerical calculations are feasible because Grassmann stochastic variables at later times are related linearly to such variables at earlier times via c-number stochastic quantities. Large fermion number applications are possible because a Grassmann field version has been developed. Applications are shown for few mode and field theory cases.

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1. Introduction

Phase space theory is one of the basic methods for treating the physics of many-body and quantum-optical systems. It is described in several textbooks [1, 2]. Other methods for treating such systems include many-body Green functions [3], stochastic Schrodinger equations (Quantum Monte-Carlo methods) [4] and variational approaches [5]. This paper outlines a phase space theory for fermions using Grassmann phase space variables, which is usable for numerical calculations on cold Fermi gases and applicable for large fermion numbers. An example for a four-mode case will be presented. The extension of the theory for treating fermion systems in terms of fields [6] rather than separate modes is also covered, with a representative example shown. Full details are covered in the textbook by Dalton, Jeffers, Barnett: *Phase Space Methods for Degenerate Quantum Gases* [7], and a summary of the key features of Grassmann algebra and calculus is also given in Ref. [8].

1.1. C-number Phase Space Theory for Bosons

In the case of bosonic systems [1, 2] the density operator is represented by a c-number distribution function of phase space variables, with the boson annihilation, creation mode operators for each mode (which satisfy commutation rules) being associated with c-number phase space variables (α_i, α_i^+) or (α_i, α_i^*). A number of different distribution functions are used, including the Glauber-Sudarshan P ([9, 10]) Husimi Q ([11]) and Wigner W types ([12, 13]) as well as the P+ distribution [14]. Quantum correlation functions (QCF), Fock state populations and coherences are given by c-number phase space integrals over the distribution function, with the mode operators being replaced by phase space variables. The evolution eqn for the density operator is transformed into a Fokker-Planck equation (FPE) [15] for the distribution function. However, rather than solving the FPE and computing the phase space integrals to determine the QCF etc, the FPE is replaced by dynamically equivalent Ito stochastic equations (Ito SE) for c-number stochastic phase variables.that replace the original phase space variables. The QCF etc are now given by stochastic averages of products of these stochastic phase variables. The Ito SE are solved numerically and the stochastic averages computed.

1.2. Grassmann Phase Space Theory for Fermions?

The development of a phase space theory for fermions has attracted little attention by comparison. One approach involves associating c-number phase space variables with atomic spin operators [16] (the approach of Haken [17]) or pairs of fermion annihilation, creation operators [18] (Corney and Drummond - Gaussian fermion representation theory). However, in an approach similar to that for bosons, the fermion annihilation, creation operators for each mode (which satisfy anti-commutation rules) would be associated directly with phase space variables. The anti-commutation rules for the fermion annihilation, creation operators \hat{c}_i , \hat{c}_i^{\dagger} for modes $i = 1, 2, \dots n$ suggests using

Grassmann rather than c-number phase space variables, and a key paper by Cahill and Gardiner [19] presented a phase space theory for fermions, introduced via fermion coherent states and based on Grassmann phase space variables. Grassmann distribution functions of the P, Q and W types were considered, with conjugate Grassmann phase space variables (g_i, g_i^*) for each mode. Dynamical or thermal evolution was not treated. Although fermion coherent states involving Grassmann variables are widely used in particle physics ([20], [21]), phase space applications in fermion physics have been rare apart from a few papers - such as treating the Jaynes-Cummings model analytically via Grassmann phase space theory [8]. Partly this may be due to the perception (see for example, Corney and Drummond [22]) that Grassmann phase space theory would not be useful in numerical calculations - a question often asked is: How would it be possible to represent anti-commuting Grassmann variables for each single particle mode on a computer other than via huge anti-commuting matrices? There was also the issue of dealing with large numbers of fermions - each of which requires a separate mode to occupy according to the Pauli exclusion principle. However, thermal evolution based on a Matsubara equation [23] had been treated using a Grassmann phase space theory of this type by Plimak, Collett and Olsen [24] for a 1D system of spin 1/2 fermions with zero-range interactions, and numerical results were presented for number correlations between pairs of fermions with various momentum, spin cases $(+k\uparrow, -k\downarrow, -k\uparrow, +k\downarrow)$. These authors used an un-normalised B distribution function based on fermion Bargmann coherent states [19], for which a FPE was obtained where the drift vector only depended linearly on the Grassmann phase space variables - a feature the authors recognised as being vital for numerical work. Plimak et al also introduced stochastic Grassmann variables, with those at a later time (or inverse temperature, for thermal evolution) being related linearly to those at an earlier time by a stochastic c-number transformation matrix β^{-1} . However, rather than introducing Ito SE for the stochastic variables themselves, they considered an Ito SE for the transformation matrix β , their fundamental equation being an ansatz for determining the B distribution function at later times from that at an initial time via substituting stochastic Grassmann variables for the original non-stochastic phase space variable, multiplying by the determinent $(\det \beta)$ of the transformation matrix and then taking a stochastic average of the resultant product.

In this paper we follow the approach of Plimak, Collett and Olsen in also basing our work on the un-normalised B distribution, and with Grassmann number phase space variables (g_i, g_i^+) associated with each mode. Quantum correlation functions (QCF), Fock state populations and coherences are given by Grassmann phase space integrals over the B distribution function, with the mode operators being replaced by Grassmann phase space variables. We also consider FPE for the distribution function and these will involve Grassmann derivatives rather than c-number derivatives. We then replace the phase space variables by stochastic Grassmann variables. However, unlike in Ref [24] we introduce Ito stochastic equations for the stochastic Grassman variables themselves. We follow an approach for bosons described by Gardiner [25], and equate the Grassmann phase space average of an arbitrary function of the phase space variables to the stochastic average of the same function when the Grassmann phase space variables are replaced by stochastic Grassmann variables. This is so that (as in the boson case), the QCF etc are now given by stochastic averages of products of the stochastic phase variables. The time dependence of the phase space average is determined from the FPE for the distribution function and the time dependence of the stochastic average is determined from the Ito SE for the stochastic Grassmann variables, and these time dependences are required to be the same. This determines the relationship between the deterministic and noise terms in the Ito SE and the drift and diffusion terms in the FPE. It is a different approach to that based on the ansatz of Plimak et al, and our Grassmann Ito SE for the stochastic Grassmann variables are not equivalent to the c-number Ito SE for the transformation matrix obtained by Plimak, Collett and Olsen [24].

We then show how the Ito SE for the stochastic Grassmann variables can be applied in numerical calculations of stochastic averages of products of these quantities needed for determining QCF etc. Essentially, the stochastic average of a product of Grassmann stochastic phase variables at the end of a small time interval is related via a linear transformation to the set of stochastic averages of all the products of Grassmann stochastic phase variables (of the same order) at start of the time interval. The key result is showing that the linear transformation matrix relating the stochastic Grassmann phase space variables at the end of a time interval to those at its beginning is obtained just involves c-numbers, such as stochastic Wiener increments and quantities from the Ito SE for the Grassmann stochastic phase variables. By dividing a finite time interval up into small time intervals, the stochastic average of product of Grassmann stochastic phase variables at the end of the finite time interval can be obtained in steps from the stochastic averages of products of Grassmann stochastic phase variables at the initial time. Finally, the stochastic averages of products of Grassmann stochastic phase variables at the initial time are obtained from the initial density operator via expressions for QCF, Fock state populations and coherences, where the relevant phase space integrals are related to initial stochastic averages of products of Grassmann stochastic phase variables.

Finally, in order to treat problems involving large particle numbers it is often convenient to consider field annihilation and creation operators rather than those for separate modes. A phase space theory based on fields can be constructed for fermions, as is the case for bosons [26], [27]. The density operator is represented by a Grassmann distribution functional involving Grassmann fields associated with the field operators. The QCF etc are now given via Grassmann functional integrals. The distribution functional satisfies a functional Fokker-Planck equation (FFPE) involving Grassmann functional derivatives. Ito stochastic field equations (Ito SFE) can then be obtained which are equivalent to the FFPE. The detailed development of Grassmann phase space field theory is covered in Ref [7].

2. Distribution Function

2.1. Fermion Coherent States

Fermion Bargmann coherent states are defined for a set of Grassmann numbers $g \equiv \{g_1, g_2, \dots, g_i, \dots, g_n\}$ for the modes *i* by

$$|g\rangle_B = \exp\left(\sum_i (\hat{c}_i^{\dagger} g_i)\right)|0\rangle = \prod_i (1 + \hat{c}_i^{\dagger} g_i)|0\rangle = \prod_i |g_i\rangle_B$$
(1)

 $|g\rangle_B$ only depends on g_i and not on g_i^* .

The fermion Bargmann coherent states properties include the effect of \hat{c}_i and \hat{c}_i^{\dagger}

$$\hat{c}_i |g\rangle_B = g_i |g\rangle_B \qquad \hat{c}_i^{\dagger} |g\rangle_B = -\frac{\overrightarrow{\partial}}{\partial g_i} |g\rangle_B$$

$$\tag{2}$$

and they satisfy a completeness relation analogous to that for boson Bargmann coherent states.

$$\int \prod_{i} dg_i^* dg_i \exp(-g^* \cdot g) |g\rangle_B \langle g|_B = \hat{1}$$
(3)

2.2. Density Operator and Distribution Function

The canonical form of density operator in terms of fermion Bargmann states is

$$\hat{\rho} = \int \prod_{i} dg_i^+ \prod_{i} dg_i B_{can}(g, g^+) |g\rangle_B \langle g^{+*}|_B \tag{4}$$

where $\prod_i dg_i^+ = dg_1^+ dg_2^+ \cdots dg_n^+$ and $\prod_i dg_i = dg_n \cdots dg_2 dg_1$ - note the Grassmann differentials anti-commute. Each fermion mode involves pairs of Grassmann phase space variables g_i, g_i^+ . $B_{can}(g, g^+)$ is the canonical Grassmann phase space distribution function $B_{can}(g, g^+)$ and is determined from Bargmann state matrix elements of density operator

$$B_{can}(g,g^+) = \int \prod_i dg_i^{**} \prod_i dg_i^* \langle g|_B \hat{\rho} | g^{**} \rangle_B \exp\left(g \cdot g^* + g^{**} \cdot g^+\right)$$
(5)

where $\prod_i dg_i^{**} = dg_1^{**} dg_2^{**} dg_n^{**}$ and $\prod_i dg_i^{*} = dg_n^{*} \cdots dg_2^{*} dg_1^{*}$. The Grassmann distribution function $B(g, g^+)$ in (4) is actually unique, and is an even Grassmann function of $\{g_i, g_i^+\}$ of order 2^n . The use of the un-normalised $B(g, g^+)$ function is the key to numerical work (Plimak et al [24]).

2.3. QCF, Fock State Populations, Coherences

Quantum correlation functions etc are given by Grassmann phase space integrals

$$Tr\left\{ (\hat{c}_{l_1}^{\dagger})(\hat{c}_{l_2}^{\dagger})\cdots(\hat{c}_{l_p}^{\dagger})\hat{\rho}(\hat{c}_{m_q})\cdots(\hat{c}_{m_2})(\hat{c}_{m_1}) \right\}$$
$$= \int \prod_i dg_i^+ dg_i(g_{m_q})\cdots(g_{m_2})(g_{m_1})B(g,g)^+ \exp(g \cdot g^+)(g_{l_1}^+)(g_{l_2}^+)\cdots(g_{l_p}^+)(g_{l_p$$

and for Fock states defined by $|\Phi\{l\}\rangle = (\hat{c}_{l_1}^{\dagger})(\hat{c}_{l_2}^{\dagger})\cdots(\hat{c}_{l_p}^{\dagger})|0\rangle$ and $|\Phi\{m\}\rangle = (\hat{c}_{m_1}^{\dagger})(\hat{c}_{m_2}^{\dagger})\cdots(\hat{c}_{m_p}^{\dagger})|0\rangle$ the population and coherences are also phase space integrals

$$P(\Phi\{l\}) = \int \prod_{i} dg_{i}^{+} dg_{i}(g_{l_{p}}) \cdots (g_{l_{2}})(g_{l_{1}}) B(g, g^{+})(g_{l_{1}}^{+})(g_{l_{2}}^{+}) \cdots (g_{l_{p}}^{+}) (7)$$

$$c(\Phi\{m\}, \Phi\{l\}) = \int \prod_{i} dg_{i}^{+} dg_{i}(g_{l_{p}}) \cdots (g_{l_{2}})(g_{l_{1}}) B(g, g^{+})(g_{m_{1}}^{+})(g_{m_{2}}^{+}) \cdots (g_{m_{p}}^{+}) (7)$$

$$(8)$$

3. Fokker-Planck Equation

3.1. Hamiltonian

For a fermion system involving one and two particle interactions the Hamiltonian is

$$\hat{H}_f = \sum_{i,j} h_{ij} \hat{c}_i^{\dagger} \hat{c}_j + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \hat{c}_i^{\dagger} \hat{c}_j^{\dagger} \hat{c}_l \hat{c}_k \tag{9}$$

where the coefficients are given in terms of single particle states (modes) via one and two particle matrix elements

$$h_{ij} = \langle i(a)|\hat{h}(a)|j(a)\rangle \qquad V_{ijkl} = \langle i(a)|\langle j(b)|\hat{V}(a,b)|k(a)\rangle|l(b)\rangle \tag{10}$$

3.2. Master Equation

As well as Hamiltonian dynamics, Markovian relaxation due to coupling with an external reservoir is described by a master equation

$$\frac{\partial}{\partial t}\hat{\rho} = \frac{1}{i\hbar}[\hat{h},\hat{\rho}] + \frac{1}{2}\sum_{a,b}\Gamma_{ab}(2\hat{s}_B^{\dagger}\hat{\rho}\hat{s}_a - \hat{\rho}\hat{s}_a\hat{s}_B^{\dagger} - \hat{s}_a\hat{s}_B^{\dagger}\hat{\rho})$$
(11)

where for pairs fermion modes denoted $a \equiv i, j$ and $b \equiv k, l$ the transition operators \hat{s}_a and relaxation coefficients Γ_{ab} are $\hat{s}_a = \hat{c}_j^{\dagger} \hat{c}_i$, $\hat{s}_B = \hat{c}_l^{\dagger} \hat{c}_k$ and $\Gamma_{ab} \equiv \Gamma_{ij;kl}$. The symmetry features are

$$h_{ij} = h_{ji}^* \qquad V_{ijkl} = v_{jilk} = v_{klji}^* \qquad \Gamma_{ij;kl} = \Gamma_{kl;ij}^* \tag{12}$$

3.3. Dynamics in Phase Space

The dynamical equation for density operator by a Fokker-Planck equation for the distribution function, derived via the use of the following correspondence rules.

$$\hat{\rho} \Rightarrow \hat{c}_i \hat{\rho} \qquad B(g, g^+) \Rightarrow g_i B(g, g^+)
\hat{\rho} \Rightarrow \hat{\rho} \hat{c}_i \qquad B(g, g^+) \Rightarrow B(g, g^+) \left(+ \frac{\overleftarrow{\partial}}{\partial g_i^+} \right)
\hat{\rho} \Rightarrow \hat{c}_i^{\dagger} \hat{\rho} \qquad B(g, g^+) \Rightarrow \left(+ \frac{\overrightarrow{\partial}}{\partial g_i} \right) B(g, g^+)
\hat{\rho} \Rightarrow \hat{\rho} \hat{c}_i^{\dagger} \qquad B(g, g^+) \Rightarrow B(g, g^+) g_i^+$$
(13)

These rules give effect of mode operators and involve derivatives. To derive the FPE the rules are applied in succession. For the B distribution function combinations of Grassmann variables and derivatives are absent, as Plimak et al [24]) pointed out.

3.4. Fokker-Planck Equation

The Fokker-Planck equation for the B distribution function can be written in terms of right Grassmann derivatives as

$$\frac{\partial}{\partial t}B(g,g^+) = -\sum_{p=1}^{2n} (A_p B(g,g^+)) \frac{\overleftarrow{\partial}}{\partial g_p} + \frac{1}{2} \sum_{p,q=1}^{2n} (D_{pq} B(g,g^+)) \frac{\overleftarrow{\partial}}{\partial g_q} \frac{\overleftarrow{\partial}}{\partial g_p}$$
(14)

where the notation $\{g_p\} \equiv \{g_1, \dots, g_n, g_1^+, \dots, g_n^+\}$ is now used. The drift vector A is an odd Grassmann function, linearly dependent on the Grassmann variables. This key linearity feature is dependent on using B distribution function (Plimak et al [24]) and is vital for numerical work. The diffusion matrix D is an even function and is bilinearly dependent on the Grassmann variables. Unlike the boson case, it is an anti-symmetric matrix $D_{pq} = -D_{qp}$. Detailed forms for A and D when the density operator satisfies the master equation (11) are given in the Appendix 10.

4. Ito Stochastic Equations

4.1. Equivalent Dynamics in Stochastic Phase Space

As described in the Introduction, we replace the phase space variables g_p by timedependent stochastic Grassmann variables $\tilde{g}_p(t)$. We denote the *i*th member of stochastic ensemble of the $\tilde{g}_p(t)$ by $\tilde{g}_{pi}(t)$, where $i = 1, 2, \dots, m$.

The Ito stochastic equations for the stochastic Grassmann variables are given by

$$\frac{d}{dt}\tilde{g}_p(t) = C^p(\tilde{g}(t)) + \sum_a B^p_a(\tilde{g}(t))\Gamma_a(t_+)$$
(15)

where the deterministic term $C^p(\tilde{g}(t))$ and the noise factor $B^p_a(\tilde{g}(t))$ are odd Grassmann functions, and are yet to be determined. The $\Gamma_a(t_+)$ are standard c-number Gaussian-Markoff random noise terms. These have the following stochastic properties

$$\overline{\Gamma_a(t_1)} = 0 \qquad \overline{\Gamma_a(t_1)\Gamma_B(t_2)} = \delta_{ab}\delta(t_1 - t_2)$$
(16)

with the stochastic average of any odd number product being zero, and that for any even number product being determined from sums of products of the $\overline{\Gamma_a(t_1)\Gamma_B(t_2)}$. In addition, any $F(\tilde{g}(t))$ and $\Gamma_a(t_+)$ at later times t_+ are uncorrelated.

$$= \overline{F(\tilde{g}(t_1))\Gamma_a(t_2)\Gamma_B(t_3)\Gamma_c(t_4)\cdots\Gamma_k(t_l)}$$

= $\overline{F(\tilde{g}(t_1))\Gamma_a(t_2)\Gamma_B(t_3)\Gamma_c(t_4)\cdots\Gamma_k(t_l)}$ $t_1 < t_2, t_3, \cdots, t_l$ (17)

4.2. Stochastic and Phase Space Averages

For an arbitrary function $F(g, g^+)$ of the Grassmann phase space variables, the phase space average $\langle F(g, g^+) \rangle_t$ and the stochastic average of $F(\tilde{g}(t), \tilde{g}^+(t))$ after the replacement by stochastic variables $\overline{F(\tilde{g}(t), \tilde{g}^+(t))}$ are given by

$$\overline{F(\tilde{g}(t), \tilde{g}^{+}(t))} = \frac{1}{m} \sum_{i=1}^{m} f(\tilde{g}_{pi}(t))$$
(18)

$$\langle F(g,g^+)\rangle_t = \int \int dg^+ dg F(g,g^+) B(g,g^+,t)$$
(19)

where for short $F(\tilde{g}(t), \tilde{g}^+(t)) = f(\tilde{g}_{pi}(t))$.

4.3. Equivalence of FPE and Ito SE

The stochastic equations for the $\tilde{g}_p(t)$ are suitably related to the Fokker-Planck equation for the distribution function $B(g, g^+, t)$ when the phase space average of an arbitrary function $F(g, g^+)$ and stochastic average of same function always coincide. This will enable QCF, Fock state populations and coherence to either be given by a phase space integral involving the distribution function or a stochastic average involving the stochastic Grassmann phase space variables. Thus

$$\langle F(g,g^+)\rangle_t = \overline{F(\tilde{g}(t),\tilde{g}^+(t))} \tag{20}$$

By equating the time derivatives of the two averages, the following important relationships between A and D in FPE, and C and B occurring in Ito SE are found.

$$c^p(g) = -A_p(g) \tag{21}$$

$$[B(g)B^t(g)]_{qp} = d_{qp}(g) \tag{22}$$

The detailed derivation is set out in Ref [7]. The deterministic factor C in the Ito SE is easily obtained as the negative of the drift vector A in the FPE (the opposite sign to the boson case). As for bosons, the noise factor B is related to the diffusion matrix D in the FPE via $BB^t = D$, but now with $D^t = -D$. It is obtained via a construction process (see next section) involving Takagi factorisation [28, 29].

4.4. QCF, Populations and Coherences

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The QCF, Fock state populations, coherences are now given by stochastic average of product of stochastic Grassmann variables instead of phase space integrals. Thus

$$P(\Phi\{l\})_t = \overline{(\tilde{g}_{l_p}(t), \tilde{g}_{l_1}(t))(\tilde{g}_{l_1}^+(t) \cdots \tilde{g}_{l_p}^+(t))}$$
(23)

$$c(\Phi\{m\}, \Phi\{l\})_{t} = (\tilde{g}_{l_{p}}(t).\tilde{g}_{l_{1}}(t))(\tilde{g}_{m_{1}}^{+}(t)\cdots\tilde{g}_{m_{p}}^{+}(t))$$

$$\frac{Tr\left\{(\hat{c}_{l_{1}}^{\dagger})(\hat{c}_{l_{2}}^{\dagger})\cdots(\hat{c}_{l_{p}}^{\dagger})\hat{\rho}(\hat{c}_{m_{q}})\cdots(\hat{c}_{m_{2}})(\hat{c}_{m_{1}})\right\}}{(24)}$$

$$=\overline{(\tilde{g}_{m_q})\cdots(\tilde{g}_{m_2})(\tilde{g}_{m_1})\exp(\tilde{g}\cdot\tilde{g}^+)(\tilde{g}_{l_1}^+)(\tilde{g}_{l_2}^+)\cdots(\tilde{g}_{l_p}^+)}.$$
 (25)

5. Solution for Deterministic and Noise Terms - Numerics

5.1. Solution for Matrix B - Ref. [7]

From the bilinearity of the diffusion matrix elements we can write (see Appendix 10)

$$d_{pq} = \sum_{r,s} Q_{rs}^{pq} g_r g_s \tag{26}$$

where Q is a $2n^2 \times 2n^2$ complex and symmetric matrix (from $D_{pq} = -D_{qp}$) of c-numbers. The rows $\{p, r\}$ and columns $\{q, s\}$ of Q are listed as $1, 2, \dots, 2n^2$.

Using Takagi factorisation [28], [29] - with the columns of K listed as $a = 1, 2, \dots, 2n^2$ we can write

$$Q = K(K)^{t} \qquad Q_{rs}^{pq} = \sum_{a} K_{r,a}^{p} K_{s,a}^{q}$$
(27)

We define $B_a^p(g)$ in terms of c-numbers $K_{r,a}^p$ as

$$B_a^p(g) = \sum_r K_{r,a}^p g_r \tag{28}$$

It is then easily shown that $(BB^t)_{pq} = D_{pq}$, which solves the equation for the noise factor B.

5.2. Solution for Vector C - Ref. [24]

From the linearity of the drift vector elements we can write (see Appendix 10)

$$c^{p}(g) = \sum_{r} l_{r}^{p} g_{r} \tag{29}$$

where L is a $2n \times 2n$ matrix of c-numbers. Rows p and columns r are listed as $1, 2, \dots, 2n$.

5.3. Linear Relation for Grassman Stochastic Variables

Combining the results (28) and (29) for $B^p_a(g)$ and $C^p(g)$, the Ito stochastic equations can now be written as

$$\tilde{g}_p(t+\delta t) = \sum_r \left\{ \delta_{p,r} + L_r^p \delta t + \sum_a K_{r,a}^p \delta w_a(t_+) \right\} \tilde{g}_r(t) = \sum_r \Theta_{p,r}(t^+) \tilde{g}_r(t) (30)$$

where the Wiener increment is $\delta w_a(t_+) = \int_{t_+}^{t+\delta t} dt_1 \Gamma_a(t_1)$. Note there are $2n^2$ increments.

The quantity in brackets $\Theta_{p,r}(t^+)$ only involves c-numbers, and (30) shows there is a linear relationship involving a c-number stochastic transformation matrix Θ between the Grassmann stochastic phase space variables at time t and those at time $t + \delta t$. If we divide evolution between t_0 and $t_f = t_{n+1}$ into small intervals $t_i \to t_{i+1}$ with $i = 0, \dots, n$ then

$$\tilde{g}_{p}(t_{f}) = \sum_{r,s,\dots,z} \Theta_{p,r}(t_{n}^{+}) \Theta_{r,s}(t_{n-1}^{+}) \cdots \Theta_{y,z}(t_{0}^{+}) \tilde{g}_{z}(t_{0}) = \sum_{z} \Lambda_{p,z}(t_{f},t_{0}) \tilde{g}_{z}(t_{0})$$
(31)

This shows that the stochastic Grassmann variables at final time depend linearly on the SGV at earlier time via a stochastic transformation matrix that involves only c-numbers. A similar feature applies in Plimak Collett and Olsen [24]. This linearity feature is only present for the *B* distribution. For the *P* distribution the drift vector $c^p(g)$ involves cubic terms. The number of stochastic c-number Wiener increments involved is $2n^2$, which increases as square of number of modes. A similar number of increments applies in the Gaussian phase-space treatment developed by Corney and Drummond [18].

5.4. Numerics - Stochastic C-Numbers Only

By dividing the evolution between t_0 and $t_f = t_{n+1}$ into equal small intervals with $t_{i+1} = t_i + \delta t$ with $i = 0, \dots, n$, then using (30) in each factor for a product of the stochastic Grassmann variables at time $t_i + \delta t$, we can then place all the stochastic Grassmann variables for time t_i together in order and finally take the stochastic average of both sides to obtain the result

$$= \frac{\overline{\tilde{g}_p(t_i + \delta t)\tilde{g}_q(t_i + \delta t)\cdots\tilde{g}_s(t_i + \delta t)}}{\left[\Theta_{p,x}(t_i^+)\Theta_{q,y}(t_i^+)\cdots\Theta_{s,z}(t_i^+)\right]_{stochaver}} \times \overline{\tilde{g}_x(t_i)\tilde{g}_y(t_i)\cdots\tilde{g}_u(t_i)} \quad (32)$$

where the uncorrelation property (17) has been used. This shows that the stochastic average of products of $\tilde{g}_p(t_i + \delta t)$ at time $t_i + \delta t$ given by sums over stochastic averages of products of the c-number stochastic quantities in the square bracket in (32) times stochastic averages of the various products of $\tilde{g}_z(t_i)$ at time t_i . The numbers of factors in such products of stochastic Grassmann variables is the same for times t_i and t_{i+1} .

This enables a set of stochastic averages of products of Grassmann stochastic variables of a given order to be propagated over a number of small intervals in succession from an initial time to a final time. The c-number quantities in the square bracket involve Wiener increments and quantities determined from the FPE using Eqs. (21), (22), (26), (27) and (29). The stochastic averages of products of the $\tilde{g}_z(t_0)$ at the initial time t_0 are determined from initial density operator at time t_0 using (25). Thus, numerical calculations for the dynamical and thermal evolution of the QCF, Fock state populations and coherences can be carried out without having to represent the Grassmann variables themselves on a computer.

6. Application - Coherence between Cooper Pairs

6.1. Model

We consider a four mode model showing onset of coherence between Cooper pairs due to spin conserving collisions between spin 1/2 fermionic atoms. The modes involved are

$$|\phi_1\rangle = |\phi_{\mathbf{k},+}\rangle \quad |\phi_2\rangle = |\phi_{\mathbf{k},-}\rangle \quad |\phi_3\rangle = |\phi_{-\mathbf{k},+}\rangle \quad |\phi_4\rangle = |\phi_{-\mathbf{k},-}\rangle \tag{33}$$

with momenta -k, +k, spin components -, + and energies $\hbar\omega$. These are normalised in box V. Hamiltonian dynamics will be considered based on (9), with coupling constant

g describing the interaction terms.

6.2. Fock States

For the case of N = 2 fermions there are six different Fock states $|\Phi_a\rangle$

$$\begin{aligned} |\Phi_1\rangle &= \hat{c}_1^{\dagger} \hat{c}_2^{\dagger} |0\rangle \quad |\Phi_2\rangle = \hat{c}_3^{\dagger} \hat{c}_4^{\dagger} |0\rangle \quad |\Phi_3\rangle = \hat{c}_1^{\dagger} \hat{c}_4^{\dagger} |0\rangle \quad |\Phi_4\rangle = \hat{c}_2^{\dagger} \hat{c}_3^{\dagger} |0\rangle \\ |\Phi_5\rangle &= \hat{c}_1^{\dagger} \hat{c}_3^{\dagger} |0\rangle \quad |\Phi_6\rangle = \hat{c}_2^{\dagger} \hat{c}_4^{\dagger} |0\rangle \end{aligned} \tag{34}$$

The states $|\Phi_3\rangle$ and $|\Phi_4\rangle$ are degenerate Cooper pair states - involving two fermions with opposite momenta and opposite spins.

6.3. Evolution

We consider the case of the system being initially in the state $|\Phi_3\rangle$ (one fermion in mode $\phi_{\mathbf{k}(+)}$, the other in mode $\phi_{-\mathbf{k}(-)}$). The interaction term $(g/V)\hat{c}_3^{\dagger}\hat{c}_2^{\dagger}\hat{c}_4\hat{c}_1$ couples state $|\Phi_3\rangle$ to state $|\Phi_4\rangle$ (one fermion in the mode $\phi_{\mathbf{k}(-)}$, the other in mode $\phi_{-\mathbf{k}(+)}$) so a non-zero coherence between state $|\Phi_3\rangle$ and state $|\Phi_4\rangle$ should develop. This leads to anomalous number correlations of the form $\langle \hat{n}_{\pm\mathbf{k}(+)}\hat{n}_{\pm\mathbf{k}(-)}\rangle - \langle \hat{n}_{\pm\mathbf{k}(+)}\rangle\langle \hat{n}_{\pm\mathbf{k}(-)}\rangle$, studied for thermal evolution by Plimak et al ([24]).

6.4. Coherence between Cooper Pair States

Using (23), (24) the initial condition shows that the only non-zero initial stochastic averages are

$$\left(\overline{\tilde{g}_4\tilde{g}_1\tilde{g}_1^+\tilde{g}_4^+}\right)_{t=0} = 1 = -\left(\overline{\tilde{g}_4\tilde{g}_1\tilde{g}_4^+\tilde{g}_1^+}\right)_{t=0} \tag{35}$$

Applying the theory presented in previous sections for the Ito stochastic equations gives the coherence between the two Cooper pair states at time $t = \delta t$ as

$$C(\Phi_{4};\Phi_{3})_{t=\delta t} = [\{(1-i\omega\delta t) + \frac{\lambda}{\sqrt{2}}(\delta w_{6} + \delta w_{16})\}\{(1-i\omega\delta t) + \frac{\lambda}{\sqrt{2}}(\delta w_{1} + \delta w_{11})\} \times \{\frac{\lambda^{*}}{\sqrt{2}}(\delta w_{8}^{+} + \delta w_{9}^{+})\}\{\frac{\lambda^{*}}{\sqrt{2}}(\delta w_{8}^{+} + \delta w_{9}^{+})\}]_{stochaver} \left(\overline{\tilde{g}_{4}}\overline{\tilde{g}}_{1}}\overline{\tilde{g}}_{4}^{+}\overline{\tilde{g}}_{1}^{+}\right)_{t=0}.$$
(36)

where (32) has been used, and $\lambda = g/i\hbar V$. In this application the stochastic average of the quantity in square bracket is evaluated analytically, the only non-zero contributions coming from products of two Wiener increments $\overline{\delta w_8^+ \delta w_8^+} = \overline{\delta w_9^+ \delta w_9^+} = \delta t$. We find that the coherence between two Cooper pair states, $|\Phi_3\rangle$ and $|\Phi_4\rangle$ correct to order δt is

$$C(\Phi_4; \Phi_3)_{t=\delta t} = (g/i\hbar V)\delta t \tag{37}$$

a result also easily obtained from matrix mechanics.

7. Field Theory Application

7.1. Grassmann Phase Space Field Theory

In phase space treatments involving field annihilation and creation operators the density operator is represented by distribution functionals of phase space fields. Bosons involve c-number fields, for fermions we use Grassmann fields. The may be different Grassmann fields for each spin component α -thus $\psi_{\alpha}(r), \psi_{\alpha}^{+}(r)$, which are also denoted $\psi_{\alpha A}(r), A = 1, 2$. QCF, Fock state populations and coherences are given by phase space functional integrals involving the distribution functional with field annihilation, creation operators replaced by phase space fields.

The evolution eqn for the density operator leads to a functional Fokker-Planck equation for the distribution functional. As in the separate mode case, correspondence rules give the effect of field operators on the density operator, and these now involve functional derivatives

$$\hat{\rho} \Rightarrow \hat{\psi}_{\alpha}(r)\hat{\rho} \quad B[\psi] \Rightarrow \psi_{\alpha}(r)B[\psi] \qquad \hat{\rho} \Rightarrow \hat{\rho}\hat{\psi}_{\alpha}(r) \qquad B[\psi] \Rightarrow B[\psi](+\frac{\overleftarrow{\delta}}{\delta\psi_{\alpha}(r)})$$
$$\hat{\rho} \Rightarrow \hat{\psi}_{\alpha}^{\dagger}(r)\hat{\rho} \quad B[\psi] \Rightarrow (+\frac{\overrightarrow{\delta}}{\delta\psi_{\alpha}(r)})B[\psi] \qquad \hat{\rho} \Rightarrow \hat{\rho}\hat{\psi}_{\alpha}^{\dagger}(r) \quad B[\psi] \Rightarrow B[\psi]\psi_{\alpha}^{+}(r) \quad (38)$$

The FFPE are then replaced by Ito stochastic field equations for stochastic fields, and the QCF etc now given by stochastic averages of stochastic fields.

7.2. Model Hamiltonian

A model for trapped Fermi gas with spin conserving collisions of zero range between pairs of spin 1/2 fermionic atoms. Internal states $\alpha = u(\uparrow), d(\downarrow)$ can be described via Hamiltonian dynamics with

$$\hat{H} = \sum_{\alpha=u,d} \int dr \left[\frac{\hbar^2}{2m} \nabla \hat{\Psi}_{\alpha}(r)^{\dagger} \cdot \nabla \hat{\Psi}_{\alpha}(r) + \hat{\Psi}_{\alpha}(r)^{\dagger} V_{\alpha} \hat{\Psi}_{\alpha}(r) + \frac{g}{2} \hat{\Psi}_{\alpha}(r)^{\dagger} \hat{\Psi}_{-\alpha}(r)^{\dagger} \hat{\Psi}_{-\alpha}(r) \hat{\Psi}_{\alpha}(g) \right]$$

7.3. Functional FPE - B Distribution Functional

The drift term in the FFPE arise from kinetic energy and trap energy contributions

$$\begin{pmatrix} \frac{\partial}{\partial t}B[\psi(r)] \end{pmatrix}_{k} = \frac{i}{\hbar} \int ds \left[\left\{ \left(\frac{\hbar^{2}}{2m} \nabla^{2} \psi_{u1}(s)B[\ \psi(r)] \right) \frac{\overleftarrow{\delta}}{\delta \psi_{u1}}(s) \right\} + \left\{ \left(\frac{\hbar^{2}}{2m} \nabla^{2} \psi_{d1}(s)B[\ \psi(r)] \right) \frac{\overleftarrow{\delta}}{\delta \psi_{d1}}(s) \right\} - \left\{ \left(\frac{\hbar^{2}}{2m} \nabla^{2} \psi_{u2}(s)B[\psi(r)] \right) \frac{\overleftarrow{\delta}}{\delta \psi_{u2}(s)} \right\} - \left\{ \left(\frac{\hbar^{2}}{2m} \nabla^{2} \psi_{d2}(s)B[\psi(r)] \right) \frac{\overleftarrow{\delta}}{\delta \psi_{d2}(s)} \right\} \right] \tag{40}$$

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$$\left(\frac{\partial}{\partial t}B[\psi(r)]\right)_{V} = \frac{i}{\hbar}\int ds \left[-\left\{\left(V_{u}\psi_{u1}(s)B[\psi(r)]\right)\frac{\overleftarrow{\delta}}{\delta\psi_{u1}}(s)\right\} - \left\{\left(V_{d}\psi_{d1}(s)B[\psi(r)]\right)\frac{\overleftarrow{\delta}}{\delta\psi_{d1}(s)}\right\} + \left\{\left(V_{u}\psi_{u2}B[\psi(r)]\right)\frac{\overleftarrow{\delta}}{\delta\psi_{u2}}(s)\right\} + \left\{\left(V_{d}\psi_{d2}(s)B[\psi(r)]\right)\frac{\overleftarrow{\delta}}{\delta\psi_{d2}(s)}\right\}\right]$$

$$(41)$$

$$\begin{pmatrix} \frac{\partial}{\partial t} B[\psi(r)] \end{pmatrix}_{u} = \frac{i}{\hbar} \frac{g}{2} \int ds \left[\left\{ \psi_{d1}(s)\psi_{u1}(s)B[\psi(r)] \frac{\overleftarrow{\delta}}{\delta\psi_{d1}(s)} \frac{\overleftarrow{\delta}}{\delta\psi_{u1}(s)} \right\} + \left\{ \psi_{u1}(s)\psi_{d1}(s)B[\psi(r)] \frac{\overleftarrow{\delta}}{\delta\psi_{u1}(s)} \frac{\overleftarrow{\delta}}{\delta\psi_{d1}(s)} \right\} - \left\{ \psi_{d2}(s)\psi_{u2}(s)B[\psi(r)] \frac{\overleftarrow{\delta}}{\delta\psi_{d2}} (s)\frac{\overleftarrow{\delta}}{\delta\psi_{u2}(s)} \right\} - \left\{ \psi_{u2}(s)\psi_{d2}(s)B[\psi(r)] \frac{\overleftarrow{\delta}}{\delta\psi_{u2}(s)} \frac{\overleftarrow{\delta}}{\delta\psi_{d2}(s)} \right\} \right]$$
(42)

7.4. Ito Stochastic Field Equations

Application of general theory for Grassmann stochastic fields $\tilde{\psi}_{\alpha A}(r,t)$ gives

	$ \begin{array}{c} \psi_{u1}(s,t+\delta) \\ \hline \psi_{d1}(s,t+\delta) \\ \hline \psi_{u2}(s,t+\delta) \\ \hline \psi_{d2}(s,t+\delta) \\ \hline \end{array} $	$\begin{array}{c} t \\ t \\ t \\ t \\ t \\ t \end{array}$				
[$\Theta^1_{u1,u1}(t^+)$	$\Theta^1_{u1,d1}(t^+)$	0	0] [$\left[\tilde{\psi}_{u1}(s,t) \right]$
=	$\Theta^1_{d1,u1}(t^+)$	$\Theta^1_{d1,d1}(t^+)$	0	0		$\tilde{\psi}_{d1}(s,t)$
	0	0	$\Theta^2_{u2,u2}(t^+)$	$\Theta^2_{u2,d2}(t^+)$		$\tilde{\psi}_{u2}(s,t)$
	0	0	$\Theta_{d2,u2}^2(t^+)$	$\Theta_{d2,d2}^2(t^+)$		$\left[\tilde{\psi}_{d2}(s,t) \right]$
						(43)

Thus the Grassmann stochastic fields at time $t + \delta t$ are related linearly to Grassmann stochastic fields at time t via c-number stochastic quantities - ∇^2 , V_{α} and Wiener increments.

$$[\Theta^{1}(t^{+})] = \begin{bmatrix} 1 - \frac{i}{\hbar} \left\{ -\frac{\hbar^{2}}{2m} \nabla^{2} + V_{u} \right\} \delta t & \sqrt{\frac{ig}{2\hbar}} \{ \delta w_{u1,d1} + i\delta w_{d1,u1} \} \\ \hline \sqrt{\frac{ig}{2\hbar}} \{ \delta w_{u1,d1} - i\delta w_{d1,u1} \} & 1 - \frac{i}{\hbar} \left\{ -\frac{\hbar^{2}}{2m} \nabla^{2} + V_{d} \right\} \delta t \end{bmatrix}$$

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$$\left[\Theta^{2}(t^{+})\right] = \begin{bmatrix} \frac{1 + \frac{i}{\hbar} \left\{-\frac{\hbar^{2}}{2m}\nabla^{2} + V_{u}\right\} \delta t}{\sqrt{\frac{ig}{2\hbar}} \left\{\delta w_{u2,d2} + i\delta w_{d2,u2}\right\}} \\ \frac{1 + \frac{i}{\hbar} \left\{-\frac{\hbar^{2}}{2m}\nabla^{2} + V_{d}\right\} \delta t}{\sqrt{\frac{ig}{2\hbar}} \left\{-\delta w_{u2,d2} + i\delta w_{d2,u2}\right\}} \\ \end{bmatrix}$$
(44)

It is then easy to see that the Grassmann stochastic fields at any time t_f now related to Grassmann stochastic fields at initial time t_0 via c-number stochastic quantities. Also, stochastic averages of products of Grassmann stochastic fields at a later time may be computed in steps starting form such products at an initial time - and with only cnumber quantities involved in each step. Again, the stochastic averages of products of Grassmann stochastic fields at initial time t_0 determined from initial conditions.

7.5. Case of Free Field and Optical Lattice

For case of free field trap potential is zero. Here we can find a solution of the Ito stochastic field equations via spatial Fourier transforms.

$$\tilde{\psi}_{\alpha 1}(s,t) = \int \frac{dk}{(2\pi)^{3/2}} \exp(ik \cdot s) \tilde{\phi}_{\alpha 1}(k,t)$$
$$\tilde{\psi}_{\alpha 2}(s,t) = \int \frac{dk}{(2\pi)}^{3/2} \exp(-ik \cdot s) \tilde{\phi}_{\alpha 2}(k,t)$$
(45)

The Ito SFE for $\psi_{\alpha A}(s,t)$ become stochastic equations for Fourier transforms $\phi_{\alpha A}(k,t)$, with the Laplacian replaced by c-number k^2 , and the equations solved numerically. For case of optical lattice trap potential is periodic. Here we can find a solution via Bloch function transforms.

8. Summary and Future Work

A phase space theory for fermions has been developed using Grassmann phase space variables which can be used in numerical calculations for cold Fermi gases and is applicable for large fermion numbers. Numerical calculations are feasible because Grassmann stochastic variables at later times are related linearly to such variables at earlier times via c-number stochastic quantities. Large fermion number applications are possible because a Grassmann field version has been developed. Applications are shown for few mode and field theory cases.

Future work could first involve topics treated by other methods to see whether a Grassmann phase space approach provides a useful alternative description. Such topics might include: the BCS theory of superconductivity, the Landau two fluid theory of superconductivity. However future work should also involve topics that are not well understood to see whether Grassmann Phase Space Theory can be used to resolve unanswered questions. Such topics might include: the BEC/BCS crossover via Feshbach resonances in the unitary (strong interaction) regime, the Fermi-Hubbard model for ferro and antiferromagnetism in half-filled bands, 1D and 2D fermion systems.

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10. Appendix - Fokker-Planck Equation Details

10.1. Fokker-Planck Equation - Drift and Diffusion Terms

The Fokker-Planck equation is

$$\frac{\partial}{\partial t}B(g,g^{+}) = -\sum_{p=1}^{2n} (A_p B(g,g^{+})) \frac{\overleftarrow{\partial}}{\partial g_p} + \frac{1}{2} \sum_{p,q=1}^{2n} (D_{pq} B(g,g^{+})) \frac{\overleftarrow{\partial}}{\partial g_q} \frac{\overleftarrow{\partial}}{\partial g_p} \quad (46)$$

where we denote $\{g_p\} \equiv \{g_1, g_2, \dots, g_n, g_1^+, g_2^+, \dots, g_n^+\}.$

If we write the drift vector A and the diffusion matrix in terms of sub-matrices D (T is the transpose).

$$[a] = \begin{bmatrix} c^{-} \\ c^{+} \end{bmatrix} \quad [d] = \begin{bmatrix} -F^{--} & +F^{-+} \\ -(F^{-+})^{t} & +F^{++} \end{bmatrix}$$
(47)

then for the master equation in Eq.(11) the quantities giving the drift vector and diffusion matrix in terms of the Hamiltonian matrix elements and relaxation coefficients are

$$c_{i}^{-} = -\frac{1}{i\hbar} \sum_{j} h_{ij}g_{j} + \sum_{jk} (\frac{1}{2}\Gamma_{kikj})g_{j}$$

$$c_{i}^{+} = +\frac{1}{i\hbar} \sum_{j} h_{ij}^{*}g_{j}^{+} + \sum_{jk} g_{j}^{+}(\frac{1}{2}\Gamma_{kikj}^{*})$$
(48)

$$f_{ij}^{--} = \frac{1}{i\hbar} \sum_{kl} \nu_{ijkl} g_l g_k + \sum_{kl} \frac{1}{2} \{ \Gamma_{lijk} + \Gamma_{kjil} \} g_l g_k = -F_{ji}^{--}$$

$$f_{ij}^{++} = -\frac{1}{i\hbar} \sum_{kl} \nu_{ijkl}^* g_k^+ g_l^+ + \sum_{kl} \frac{1}{2} \{ \Gamma_{lijk}^* + \Gamma_{kjil}^* \} g_k^+ g_l^+ = -F_{ji}^{++}$$

$$f_{ij}^{-+} = \sum_{kl} \{ \Gamma_{jkil} \} g_l g_k^+ \qquad F_{ij}^{+-} = \sum_{kl} \{ \Gamma_{jkil}^* \} g_l^+ g_k = -F_{ji}^{-+}$$
(49)

We see that the drift vector is an odd Grassmann function, linearly dependent on Grassmann variables, and that the diffusion matrix is even and anti-symmetric $D_{pq} = -D_{qp}$, and bilinearly dependent on Grassmann variables.

10.2. New Drift, Diffusion Parameters M, L

We now write

$$-F_{ij}^{--} = \sum_{kl} m_{ikjl}^{--} g_k g_l \quad f_{ij}^{++} = \sum_{kl} m_{ikjl}^{++} g_k^+ g_l^+ \quad f_{ij}^{-+} = \sum_{kl} m_{ikjl}^{-+} g_k g_l^+ \quad F_{ij}^{+-} = \sum_{kl} m_{ikjl}^{+-} g_k^+ g_l$$
(50)

where M^{--}, M^{++}, M^{-+} and M^{+-} are four $n^2 \times n^2$ c-number matrices. Also, we introduce matrices L^-, L^+ via

$$a_i^- = -\sum_j L_{ij}^- g_j \qquad A_i^+ = -\sum_j L_{ij}^+ g_j$$
 (51)

10.3. Form of Diffusion Matrix D

By writing the diffusion matrix elements in the form

$$d_{pq} = \sum_{r,s} Q_{rs}^{pq} g_r g_s \tag{52}$$

we see that Q is a $2n^2 \times 2n^2$ complex and symmetric matrix (from $D_{pq} = -D_{qp}$), where rows are listed as p, r and columns listed as q, s. The non-zero elements of Q can be identified from the following Table

\mathbf{g}_p	\mathbf{g}_q	\mathbf{g}_r	\mathbf{g}_s	$\mathbf{Q}_{r,s}^{p,q}$	
g_i	g_j	g_k	g_l	$m_{ikjl}^{}$	
g_i	g_j^+	g_k	g_l^+	$m_{ik\ jl}^{-+}$	(53)
g_i^+	g_j	g_k^+	g_l	$m_{ik\ jl}^{+-}$	
g_i^+	g_j^+	g_k^+	g_l^+	$m_{ik\ jl}^{+\ +}$	

Note that in each $n^2 \times n^2$ sub-matrix of Q, the rows p, r are in one-one correspondence with the various i, k and the columns q, s are in one-one correspondence with the various j, l. The i, k, j, l only run from $1, 2, \dots, n$.

10.4. Form of Drift Vector A

By writing the drift vector in the form

$$a^p(g) = -\sum_r l_r^p g_r \tag{54}$$

we see that L is a $2n \times 2n$ c-number matrix with rows p and columns r listed as $1, 2, \dots, 2n$. The non-zero elements of L has non-zero elements can be identified from the following Table

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