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Exchange effects in a two-dimensional Fermi liquid

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Abstract. We investigate the possibility of simulating exchange effects in a two-dimensional fermion liquid within a model of distinguishable particles. For this purpose, we intend to reproduce both bulk and microscopic properties of the system of N indistinguishable particles, as predicted by the Landau theory of Fermi liquids adapted to describe a single atomic monolayer, by means of a Hartree calculation of the ground state, the single particle spectrum and the effective interaction of a system of N distinguishable particles interacting via a coordinate-dependent plus momentum-dependent interaction. It is shown that for given original two-body interactions of the same microscopic properties as the original quantum liquid within a substantial range of single particle momenta.

1. Introduction

Since the advent of Landau's theory of Fermi liquids [1], liquid ³He became the best established paradigm of such systems [2, 3]. The fundamental concepts of the theory have also been applied to nuclear and neutron star matter [4]. More recently, the possibility of building up two-dimensional Fermi liquids in the laboratory, arose from the recognition of the existence of Andreev states [5] in mixtures of liquid ³He and ⁴He, together with the observed formation of atomic monolayers that may exhibit properties like a T^2 dependence of the surface tension [6], surface second sound [7], superfluidity [8] and Heisenberg ferromagnetism [9]. The need to review the standard theories of Fermi liquids in order to adapt them to lower dimensionalities is a natural outcome of these experimental facts.

On the other hand, numerical experiments driven by computer simulations are now a common tool in condensed matter physics as alternatives to both laboratory experiments and theoretical approaches. However, while the procedure to set up numerical dynamics of classical particles is well understood, simulations of quantum systems such as the quantum molecular dynamics (QMD) approach [10] are appreciably more complicated due to the restrictions imposed by the indistinguishability of the particles. In addition to the difficulties associated with the numerical implementation of QMD and related methods, their theoretical foundation has not been fully established. A way to circumvent the momentum space restrictions posed by the Pauli principle on fermion systems, and perform either classical molecular dynamics or classical Monte Carlo calculations, has been succesfully applied to aspects of nuclear dynamics [11–16]. The idea already advanced by Wilets and collaborators [17, 18] is to mimic the antisymmetric character of the many-particle wavefunction by means of a repulsive two-particle potential that depends upon the relative momentum of the interacting pair. In a recent work [19], the Hamiltonian dynamics of one and two

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particles subjected to such momentum-dependent interactions, in addition to a soft barrier repulsion that approaches a hard disk interaction, has been presented with the aim of getting some insight on the possible modifications of hard disk molecular dynamics [20–22] when momentum space restrictions are enforced into the picture.

The construction of image systems of quantum liquids, made up of distinguishable particles that interact through two-body potentials acting on the relative phase space of the collision partners is an interesting field, in view of the possibility of performing numerical experiments based on classical molecular dynamics. However, it should be kept in mind that for an interacting many-body system, the fundamental entity that enters the ground state energy, the excitation spectrum and particle collisions is the effective interaction in the medium. It then appears that consistent attempts to model a system of indistinguishable particles by means of distinguishable ones should give a reliable description of elementary excitations and scattering properties of the original liquid, in addition to thermodynamic properties such as the equation of state, bulk incompressibility or sound velocity, and the lowest multipole Landau parameters. The aim of the present work is to analyse within a simple, however non-trivial approach, the conditions under which a two-dimensional Fermi liquid can be mimicked by a system of distinguishable particles.

To this end, in section 2 we briefly review the notation and major ingredients entering the Landau theory of Fermi liquids adapted to the two-dimensional case. In the remainder of the paper, we compare two situations, namely (a) an N-body system interacting through a pairwise interaction $V_c(r)$ whose total energy is provided by the Hartree–Fock (HF) description and (b) an N-body system interacting with a phase space potential $V_c(r) + V_m(q)$, where q is the relative momentum of the given pair, with total energy computed in the Hartree (H) frame where exchange effects in the total wavefunction are not considered. Attention is paid to the quasiparticle excitation spectrum and to the quasiparticle effective interaction as given by the Landau theory of Fermi liquids; the potential of (b) is then chosen to provide the best match with the quantities computed in (a). In sections 3 and 4 we discuss respectively the application to a Woods–Saxon and to a Lennard-Jones potential, the latter endowed with a finite repulsive core to make mean field calculations feasible. The conclusions and perspectives are summarized in section 5.

2. The two-dimensional Fermi liquid

The system we wish to investigate consists of N interacting fermions confined to a twodimensional box of area A. Since the details of Landau's theory of Fermi liquids usually refer to three-dimensional systems (see, for example, [2, 3]), here we briefly discuss the necessary modifications for monolayers. Let us first recall a few essential issues of the theory. We shall always refer to a liquid in thermodynamical equilibrium at temperature T, characterized by a single fermion distribution $n_k^0 = \{1 + \exp[(\varepsilon_k - \mu)/T]\}$. From the total energy $E_0(\{n_k^0\})$ one may obtain the single particle (sp) spectrum

$$\varepsilon_k = \frac{\delta E}{\delta n_k} \tag{2.1}$$

and the effective quasiparticle interaction

$$f_{kk'} = \frac{\delta^2 E}{\delta n_k \delta n_{k'}} \tag{2.2}$$

where the symbol δ denotes functional differentiation and $E = E^0 + \delta E$ is the energy when occupation number fluctuations $\{\delta n_k\}$ take place in the liquid.

The effective quasiparticle interaction is usually represented by its dimensionless multipolar strengths on the Fermi surface or Landau parameters $F_l^{\alpha} = v_F f_l^{\alpha}$, where v_F is the density of sp states on the Fermi surface and f_l^{α} is the amplitude of the expansion of $f_{kk'}^{\alpha}$ in terms of a set of orthogonal functions of the angle between k and k', for each spin channel $\alpha = s$ (symmetric) or $\alpha = a$ (antisymmetric). For the two-dimensional situation, this expansion takes the form

$$f_{\boldsymbol{k}\boldsymbol{k}'}^{\alpha} = \sum_{l} f_{l}(\boldsymbol{k}, \boldsymbol{k}') \mathrm{e}^{\mathrm{i}l\varphi}$$
(2.3)

where $\cos \varphi = \hat{k} \cdot \hat{k}'$. Accordingly, the Landau parameters are taken as

$$F_l^{\alpha} = \nu_F f_l^{\alpha}(k_F, k_F) \tag{2.4}$$

where $k_F = \sqrt{2\pi\rho}$ is the radius of the Fermi circle and with the level density per unit area

$$\nu_F = \frac{m_F^*}{\pi\hbar^2}.\tag{2.5}$$

In the above expression, m_F^* is the effective mass for quasiparticles lying on the twodimensional Fermi level and is related to the symmetric dipolar Landau parameter by

$$\frac{m^*}{m} = 1 + F_1^s. (2.6)$$

By contrast, the dipole correction is reduced by a factor of $\frac{1}{3}$ in the three-dimensional system [2, 3].

Hereafter we will restrict ourselves to the zero temperature case. The HF formulation is well known and for a two-dimensional system of area A, the total energy can be written as

$$E_0^{HF} = 2\sum_k \frac{\hbar^2 k^2}{2m} + \frac{2}{A} \sum_{kk'} \tilde{V}(0) - \frac{1}{A} \sum_{kk'} \tilde{V}(k - k')$$
(2.7)

where $\rho = N/A$ is the total density and $\tilde{V}(q)$ is the Fourier transform of the interaction potential V(r); $q \equiv k - k'$ is the transferred momentum and k, k' the relative momenta of the particles respectively after and before the interaction event. The sp spectrum and effective interaction easily follow as

$$\varepsilon_{k} = \frac{\hbar^{2}k^{2}}{2m} + \tilde{V}(0)\rho - \frac{1}{A}\sum_{k'}\tilde{V}(k-k')$$
(2.8)

$$f_{\boldsymbol{k},\boldsymbol{k}'} = \frac{1}{A} [\tilde{V}(0) - \delta_{\sigma\sigma'} \tilde{V}(\boldsymbol{k} - \boldsymbol{k}')]$$
(2.9)

where all summations upon momenta are restricted to the interior of the Fermi circle.

A straightforward calculation leads us to the following expression for the total HF energy per particle:

$$\frac{E_0}{N}(\rho) = \left[\frac{\pi\hbar^2}{2m} + \frac{\tilde{V}(0)}{2}\right]\rho - \int_0^\infty \mathrm{d}r \, V(r) \frac{J_1^2(k_F r)}{r}$$
(2.10)

from which we may obtain the pressure $P(\rho) = \rho^2 \partial [E_0/N] / \partial \rho$ as

$$P(\rho) = \left[\frac{\pi\hbar^2}{2m} + \frac{\tilde{V}(0)}{2}\right]\rho^2 - \rho\frac{E_0}{N} - \sqrt{2\pi}\rho^{3/2}\int_0^\infty \mathrm{d}r \, V(r)J_0(k_F r)J_1(k_F r) \tag{2.11}$$

and the incompressibility modulus $K^{-1} = \rho \partial P / \partial \rho$

$$K^{-1}(\rho) = \left[\frac{\pi\hbar^2}{2m} + \frac{\tilde{V}(0)}{2}\right]\rho^2 - \pi\rho^2 \int_0^\infty \mathrm{d}r \, r \, V(r) [J_0^2(k_F r) - J_1^2(k_F r)]. \tag{2.12}$$

Furthermore, the single quasiparticle energy is

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} + \tilde{V}(0)\rho - k_F \int_0^\infty \mathrm{d}r \ J_0(kr) J_1(k_F r) V(r)$$
(2.13)

the effective mass as a function of sp momentum takes the form

$$\frac{m^*(k)}{m} = 1 + \frac{mk_F}{\hbar^2 k} \int_0^\infty \mathrm{d}r \, r \, V(r) \, J_1(kr) \, J_1(k_F r) \tag{2.14}$$

and the multipolar amplitudes of the effective interaction in each spin channel read

$$f_l^s(k,k') = \frac{V(0)}{A} \delta_{l0} - \frac{\pi}{A} \int_0^\infty \mathrm{d}r \, r \, V(r) J_l(kr) J_l(k'r) \tag{2.15}$$

$$f_l^a(k,k') = f_l^s(k,k') - \frac{V(0)}{A}\delta_{l0}.$$
(2.16)

With the above expressions for the momentum-dependent Landau fields $f_l^{\alpha}(k, k')$, a simple calculation permits us to verify both equation (2.6) and the relationship

$$K^{-1} = \rho^2 \frac{1 + F_0^s}{\nu_F} \tag{2.17}$$

that also holds in the three-dimensional case.

Let us now consider an image system consisting of N distinguishable particles in a ground state described by a Hartree product of plane waves. The total energy reads, in general,

$$E_0^{\rm H} = 2\sum_{k} \frac{\hbar^2 k^2}{2m} + \frac{1}{2} \sum_{kk'} \sum_{\sigma\sigma'} \langle k\sigma k'\sigma' | V_{\rm H} | k\sigma k'\sigma' \rangle$$
(2.18)

with summations restricted to momenta below k_F and with the phase space potential

$$V_{\rm H}(r,q) = V_c(r) + V_m(\hat{q}) \frac{\delta(r-r_0)}{2\pi r} \delta_{\sigma\sigma'}.$$
 (2.19)

While the term $V_c(r)$ is the usual coordinate-dependent interaction, the new contribution $V_m(\hat{q})$ depends upon the relative momentum of the particles that come together at the interaction distance r_0 . More generally, the momentum-dependent force should be allowed to act whenever the two particles are sufficiently close in coordinate space to experience a momentum change due to the non-vanishing interaction force; in this sense, the Dirac's delta in equation (2.19) is a limiting representation of a bell-like kernel spreading through the active interaction region. This is the simplest form of taking into account the local character of the momentum change, making room for analytical expressions that permit one to reproduce the desired effects. For the full phase space interaction, one gets, instead of formulae (7) to (9),

$$E_0^{\rm H} = 2\sum_{k} \frac{\hbar^2 k^2}{2m} + \frac{2}{A} \sum_{kk'} \tilde{V}_{\rm H}(0) + \frac{1}{A} \sum_{kk'} \tilde{V}_m(k - k')$$
(2.20)

$$\varepsilon_{k} = \frac{\hbar^{2}k^{2}}{2m} + \tilde{V}_{\rm H}(0)\rho + \frac{1}{A}\sum_{k'}\tilde{V}_{m}(k-k')$$
(2.21)

$$f_{k,k'} = \frac{1}{A} [\tilde{V}_{\rm H}(0) + \delta_{\sigma\sigma'} \tilde{V}_m(k - k')].$$
(2.22)

3. The smoothed square potential

Let us first consider a simple barrier or well of the form

$$V(r) = \frac{V_r}{1 + e^{b_r (r^2 - r_0^2)}}$$
(3.1)

where V_r and r_0 respectively measure the strength and range of the interaction, r being the relative distance between particles and b_r the size of the region where the interaction forces are non-vanishing. The direct and exchange matrix elements entering the effective qp interaction can be shown to be

$$\langle \boldsymbol{k}\boldsymbol{k}'|V|\boldsymbol{k}\boldsymbol{k}'\rangle = \frac{\pi V_r}{A} \left[r_0^2 + \frac{1}{b_r} \ln(1 + \mathrm{e}^{-b_r r_0^2}) \right]$$
(3.2)

$$\langle \boldsymbol{k}\boldsymbol{k}'|\boldsymbol{V}|\boldsymbol{k}'\boldsymbol{k}\rangle = \frac{2\pi}{A} \int_0^\infty \mathrm{d}\boldsymbol{r}\,\boldsymbol{r}\,\boldsymbol{V}(\boldsymbol{r})J_0(|\boldsymbol{k}-\boldsymbol{k}'|\boldsymbol{r}) \tag{3.3}$$

where we have used the integral representation of the zeroth Bessel function

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{ix \cos \varphi}.$$
 (3.4)

Let us now specialize the interaction terms in equation (2.19) as follows. Let V_c take the smoothed square form with renormalized strength and width $V_r^{\rm H}$, $b_r^{\rm H}$ and let the momentum dependent potential be a repulsion given by

$$V_m(q) = \frac{V_q}{1 + e^{b_q(q^2 - q_0^2)}}.$$
(3.5)

After some algebra, we obtain the multipolar amplitudes of the new effective interaction

$$f_l^s(k,k') = \frac{\tilde{V}_{\rm H}(0)}{A} \delta_{l0} + \frac{1}{4\pi} \int_0^{2\pi} \frac{\cos\varphi \,\mathrm{d}\varphi}{1 + \mathrm{e}^{b_q(k^2 + k'^2 - 2kk'\cos\varphi - q_0^2)}}$$
(3.6)



Figure 1. Total energy of the liquid in the mean field approximation as a function of the density for the parameter values of table 1. The full curve corresponds to the energy computed in the Hartree–Fock frame, while asterisks indicate results from Hartree calculations.



Figure 2. Quasiparticle energy as a function of single particle momentum in units of the Fermi momentum. Details are the same as in figure 1.



Figure 3. Dimensionless effective interaction as a function of transferred momentum in units of the Fermi momentum. Details are the same as in figure 1.

$$f_l^a(k,k') = f_l^s(k,k') - \frac{\tilde{V}_{\rm H}(0)}{A} \delta_{l0}.$$
(3.7)

For the selected phase space potential, the summations in equations (2.20) and (2.21) can neither be carried out analytically nor cast into an integral form as in equations (2.10) to (2.15). Consequently, we have computed them explicitly as follows. For a fixed density,



Figure 4. Dimensionless multipolar amplitudes of the quasiparticle effective interaction as functions of momenta in units of the Fermi momentum obtained in the Hartree–Fock frame with the parameters of table 1; (*a*) l = 0; (*b*) l = 1; (*c*) l = 2.

we fit the effective interaction $f^{s}(q)$ computed in the HF frame to the formula

$$f_{\rm H}^s = \frac{1}{A} \left[\tilde{V}_r(0) + \frac{1}{2} V_m(q) \right].$$
(3.8)



Figure 4. (Continued)

This fit leaves us with a set of parameters for the Hartree potential. The quasiparticle and the total energy are then obtained as

$$\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m} + 2\sum_{\boldsymbol{k}\boldsymbol{k}'} f^s_{\boldsymbol{k}\boldsymbol{k}'} \tag{3.9}$$

$$E_0^{\rm H} = 2\sum_{k} \varepsilon_k - 2\sum_{kk'} f_{kk'}^s.$$
 (3.10)

The summations are carried over all sp states lying at the nodes of a lattice with side $2\pi/\sqrt{A}$ in momentum space; the number of particles is chosen higher than the numerical bound N_{max} for which the ratio E_0^H/N becomes independent of N. This is an important computational detail, in view of the fact that the *HF* results are exact in the thermodynamic limit, i.e. integrations over momentum space have been fully performed.

The major results of this section are presented in figures 1 to 7. They correspond to the set of parameters displayed in table 1. The value of b_r has been chosen to yield a sharp well or barrier, intending to mimic hard disks in the latter case. The value of V_r has been selected to give a stable system at low densities, since a detailed study of the HF energy for the two-body interaction (2.10) shows that no saturation point is reached, regardless of the sign and strength of V_r . Indeed, while for repulsive interactions the system is never bound, for attractive ones it collapses at high densities. This behaviour is due to the fact that the exchange contribution to the interaction matrix elements becomes essentially constant for densities above unity and its size is not sufficient to counterbalance the large kinetic-plus-direct interaction term proportional to the density.

Figure 1 displays the total energy per particle E/N as a function of the density, while in figure 2 we plot the quasiparticle energy ε_k in terms of the sp momentum, and in figure 3 the dimensionless effective interaction $F(q) = v_F f^s(q)$ in the spin symmetric channel as a function of transferred momentum. The full curves denote HF results and asterisks correspond to the H case. In figures 4(a)–(c) we show the HF multipolar amplitudes $F_l(k, k')$ of the dimensionless effective interaction F(k, k') for l = 0, 1, 2, while those in figure 5 have been computed from the H energy. It is seen that the overall agreement is excellent.



Figure 5. Same as figure 4 for the Hartree results.

In particular, it is surprising that although the fit was performed for a fixed density, the total energy coincides over a large density range. Furthermore, we find that in spite of the fact that the agreement between the respective multipoles of the effective interaction, as well as that of the Landau parameters, is remarkable, the H calculations give slightly smoother surfaces than the HF ones. This fact can be easily attributed to the loss, in the H frame, of the quantal oscillations contained in the exchange matrix elements.



Figure 5. (Continued)



Figure 6. Same as figure 2 for the bounded Lennard-Jones potential.

4. The bounded Lennard-Jones potential

We now choose for the particle interaction a Lennard-Jones shape with a finite barrier at short distances, of the form

$$V(r) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] & r \ge \sigma \\ b \left[1 - \left(\frac{r}{\sigma}\right)^{8} \right] & r < \sigma \end{cases}$$
(4.1)



Figure 7. Same as figure 3 for the bounded Lennard-Jones potential.

Table 1. Total energy, pressure, incompressibility and the first three symmetric Landau parameters obtained in the fit of the HF results with the smoothed squared interaction to the H potential. The parameters of the corresponding potentials are shown in the two columns at the right. The fit was performed for a density $\rho = 0.5$ and the H calculations correspond to a particle number N = 882.

	Hartree-Fock	Hartree		Hartree-Fock	Hartree
E	0.344	0.339	b_r	10	10
Ρ	0.129	0.128	V_r	-0.85	-0.92
K^{-1}	0.192	0.194	b_q		0.18
F_0^s	-0.728	-0.725	V_q		5
F_1^s	0.112	0.103	q_0		1.4
F_2^s	0.018	0.010			

Table 2. Same as in table 1 for the bounded Lennard-Jones interaction. The fit was performed at the saturation density $\rho_s = 1.2$.

Hartree-Fock	Hartree		Hartree-Fock	Hartree
-0.310	-0.315	ε	2	2.518
1.47	1.45	b	2	1.9
-0.730	-0.736	b_q		0.95
-0.119	-0.116	$\dot{V_q}$		12.8
0.094	0.094	q_0		0.39
		α		-4.5
		β		2.78
		γ		1.9
		δ		4.15
	Hartree–Fock -0.310 1.47 -0.730 -0.119 0.094	Hartree–Fock Hartree -0.310 -0.315 1.47 1.45 -0.730 -0.736 -0.119 -0.116 0.094 0.094	Hartree–Fock Hartree -0.310 -0.315 ε 1.47 1.45 b -0.730 -0.736 b_q -0.119 -0.116 V_q 0.094 0.094 q_0 α β γ	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$

where both ε and b are regarded as parameters. In this case, only the direct matrix element can be computed exactly, giving

$$\langle \boldsymbol{k}\boldsymbol{k}'|\boldsymbol{V}|\boldsymbol{k}\boldsymbol{k}'\rangle = \frac{1}{A}\frac{2}{5}\pi\sigma^2(2b-3\varepsilon)$$
(4.2)

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Figure 8. Same as figure 4 for the bounded Lennard-Jones potential.

It can be verified that there exists a range of values (ε, b) where the system saturates at a density near unity. Hereafter, we will discuss the results obtained at saturation density for the choice $\varepsilon = b = 2$. The first observation is the oscillatory character of the HFeffective interaction. Since at zero temperature transferred momenta larger than $2k_F$ are not relevant to investigating scattering properties of the system, we concentrate on values of qbelow $2k_F$. We are able to reproduce the shape of the effective interaction adopting, for the Hartree formalism, the momentum-dependent potential

$$V_m(q) = P(q) \frac{V_q}{1 + e^{b_q(q^2 - q_0^2)}} + [1 - P(q)] \left[\alpha J_0 \left(\beta \frac{q}{k_F} - \gamma \right) + \delta \right].$$
(4.3)



Figure 8. (Continued)

Here P(q) is a smooth step function

$$P(q) = \frac{1}{1 + e^{(q^2 - q_c^2)}}$$
(4.4)

with $q_c = 0.9k_F$. The parameters α , β , γ and δ are given in table 2.

The calculation procedure is identical to that described in the previous section and the results for the quasiparticle energy and for the effective interaction are shown in figures 8 and 9, respectively, while the multipolar fields are plotted in figures 10 and 11. In this case, the fit was performed at the saturation density $\rho_s = 1.2$. As in the Woods–Saxon case, we find excellent agreement for all microscopic quantities. However, in contrast to the preceding situation, the total energies do not coincide for densities other than the one selected for the fit. Furthermore, the pressure is not reproduced at ρ_s , due to the fact that the latter is not the saturation density (i.e. P = 0) for the H system. It should be kept in mind that the smoothed square potential, with the chosen values of V_q and b_q , gives rise to a relatively weak repulsion in a broad momentum region. By contrast, the purely repulsive contribution here discussed is one order of magnitude stronger than the smoothed squared one and considerably more localized.

5. Summary and conclusions

In this work, we have presented the formalism corresponding to the Landau theory of Fermi liquids applied to a two-dimensional system. We have employed the prescription of the theory to extract both bulk and microscopic magnitudes of an interacting N fermion system on a surface, starting from the total energy computed in the HF approximation. We have shown that in model situations corresponding to the choice of a Woods–Saxon or a Lennard-Jones pairwise interaction, it is possible to find a phase space potential that, when acting among particles whose exchange correlations have been suppressed in the total wavefunction, yields the same quasiparticle effective interaction as obtained from the



Figure 9. Same as figure 5 for the bounded Lennard-Jones potential.

solution of the HF problem. We have observed as well that such potentials provide an excellent agreement with the sp spectra, with the lowest multipolar fields that expand the effective interaction and with the total energy. For the smoothed square potential, the agreement comprises the total energy as a function of the density, as well as pressure and incompressibility modulus.

A further approach would be to attempt, by means of phase space interactions, a fit of the two-body scattering amplitudes obtained as solutions of the Bethe Salpeter equation in the Landau limit [3]. Such a possibility would provide an image system of the quantum liquid that is free from exchange correlations, however yielding similar kinetic behaviour



Figure 9. (Continued)

as the original fluid. The corresponding phase space potential could then be a basis for a molecular dynamics investigation of the rich hydrodynamics and kinetics of classical twodimensional systems, for which very efficent algorithms are presently available [20–22]. We believe that this perspective opens an interesting field of research, in view of the fact that present simulations of fermion dynamics that resort to phase space potentials mostly design the latter to account only for the equation of state of the quantum system.

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