

Dynamical mean-field equations for strongly interacting fermionic atoms in arbitrary potential traps

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received 2 June 2006; accepted in final form 27 July 2006

published online 16 August 2006

PACS. 03.75.Ss – Degenerate Fermi gases.

PACS. 05.30.Fk – Fermion systems and electron gas.

PACS. 34.50.-s – Scattering of atoms and molecules.

Abstract. – We derive a set of general dynamical mean-field equations for strongly interacting fermionic atoms in arbitrary slowly varying potential traps. Our derivation generalizes the ansatz of the crossover wave function to the inhomogeneous case. The equations reduce to a time-dependent Gross-Pitaevskii equation on the BEC side of the resonance. We discuss an iteration method to solve these mean-field equations, and present the solution for a harmonic trap as an illustrating example, which self-consistently verifies the approximations made in our derivation.

The recent experimental advance in ultracold atoms has allowed controlled studies of strongly interacting Fermi gases in various types of potential traps, with the interaction strength tunable by an external magnetic field through the Feshbach resonance [1]. For homogeneous strongly interacting Fermi gases at zero temperature, the physics is captured by the variational crossover wave function [2–4], which interpolates the BCS and the BEC theories. For strongly interacting atoms in a potential trap, there are currently two main methods to deal with the resultant inhomogeneity: one is the local density approximation (LDA) [4, 5], which neglects the kinetic terms associated with the spatial variation of the order parameters; the other is based on the numerical simulation of the Bogoliubov-de-Gennes (BDG) equations [6, 7]. Both of these methods have found wide applications recently [4–7], but each of them also has its own limitation: the LDA becomes inadequate in cases where variations of the order parameters have significant impacts; the BDG equations take into account exactly the spatial variation of the order parameter, but its numerical solution is typically time-consuming, which limits its applications only to very special types of potentials.

In this work, we develop a different method to describe both the static properties and the dynamics of strongly interacting fermionic atoms in arbitrary but slowly varying potential traps. Our starting point is a variational state which is a natural generalization of the crossover wave function to the inhomogeneous and dynamical cases. The key simplification in our derivation comes from the assumption that the spatial variation of the order parameter is small within the size of the Cooper pairs. This assumption is similar to the one in the derivation of the Ginzberg-Landau equation for the weakly interacting fermions [8], but we avoid the

use of perturbation expansions so that the order parameter here in general does not need to be small [8, 9]. With such an assumption, we derive a set of dynamical mean-field equations for the bare molecular condensate and the Cooper-pair wave functions. This set of equations can be solved iteratively, and its zeroth-order approximation, which neglects the order-parameter variation, gives the LDA result. On the BEC side of the Feshbach resonance (with the chemical potential $\mu \leq 0$), these mean-field equations can be reduced to a generalized dynamical Gross-Pitaevskii (GP) equation [8–10], with the effective nonlinear interaction for the bare molecules derived from a fermionic gap equation. When one goes deeper into the BEC region, the nonlinear interaction resumes the conventional GP form, and one can derive an effective scattering length for the bare molecules. We solve the dynamical mean-field equations for a harmonic trap as a simple illustrating example to self-consistently verify the approximations made in our derivation. Another recent work also addresses the dynamics of a trapped Fermi gas across a Feshbach resonance [11]. The set of equations derived therein are semiclassical hydrodynamic equations, which, after linearization, can be applied to calculate the dynamical properties of the system. In contrast, our work follows the time-dependent variational approach. By reducing the dynamical mean-field equations to a time-dependent nonlinear GP equation on the BEC side of the resonance, we provide a complementary perspective to the problem.

Our starting point is the two-channel field Hamiltonian [3, 4, 12]

$$\begin{aligned}
 H = & \sum_{\sigma} \int \Psi_{\sigma}^{\dagger} [-\nabla^2 / (2m) + V(\mathbf{r}, t)] \Psi_{\sigma} d^3\mathbf{r} + \int \Psi_b^{\dagger} [-\nabla^2 / (4m) + \gamma + 2V(\mathbf{r}, t)] \Psi_b d^3\mathbf{r} + \\
 & + \alpha \int [\Psi_b^{\dagger} \Psi_{\downarrow} \Psi_{\uparrow} d^3\mathbf{r} + \text{H.c.}] + U \int \Psi_{\uparrow}^{\dagger} \Psi_{\downarrow}^{\dagger} \Psi_{\downarrow} \Psi_{\uparrow} d^3\mathbf{r}, \quad (1)
 \end{aligned}$$

which describes the interaction between the fermionic atom fields Ψ_{σ}^{\dagger} ($\sigma = \uparrow, \downarrow$ labels atomic internal states) in the open channel and the bosonic bare molecule field Ψ_b^{\dagger} in the closed channel. In this Hamiltonian, m is the atom mass, and $V(\mathbf{r}, t)$ is the trap potential which could vary both in space and in time. Note that we have assumed that the trap frequencies for a composite boson and for a single atom are the same, so that the potential that a boson feels is twice as a single atom does. The bare atom-molecule coupling rate α , the bare background scattering rate U , and the bare energy detuning of the closed channel molecular level relative to the threshold of the two-atom continuum γ are connected with the physical ones α_p , U_p , γ_p through the standard renormalization relations [4]. The values of the physical parameters α_p , U_p , γ_p are determined, respectively, from the resonance width, the background scattering length, and the magnetic-field detuning relative to the Feshbach resonance point (see, *e.g.*, the explicit expressions in ref. [13]). Note that following the standard two-channel model, direct collisions between the bosonic bare molecules are neglected, as their contribution is negligible near a broad Feshbach resonance [3, 4, 12].

At almost zero temperature and with a slowly varying potential $V(\mathbf{r}, t)$, the state of the Hamiltonian (1) can be assumed to evolve according to the following variational form:

$$|\Phi(t)\rangle = \mathcal{N} \exp \left[\int f(\mathbf{r}, \mathbf{r}', t) \Psi_{\uparrow}^{\dagger}(\mathbf{r}) \Psi_{\downarrow}^{\dagger}(\mathbf{r}') d^3\mathbf{r} d^3\mathbf{r}' \right] \exp \left[\int \phi_b(\mathbf{r}, t) \Psi_b^{\dagger}(\mathbf{r}) d^3\mathbf{r} \right] |\text{vac}\rangle, \quad (2)$$

where \mathcal{N} is the normalization factor, $\phi_b(\mathbf{r}, t)$ is the condensate wave function for the bare molecules, and $f(\mathbf{r}, \mathbf{r}', t)$ is the Cooper-pair wave function. This variational state is a natural generalization of the crossover wave function to the inhomogeneous and dynamical cases [14]. Without the fermionic field, this variational state would have the same form as the one in the derivation of the dynamical GP equation for the weakly interacting bosons [10].

To derive the evolution equations for the wave functions $\phi_b(\mathbf{r}, t)$ and $f(\mathbf{r}, \mathbf{r}', t)$, we follow the standard variational procedure to minimize the action $S = \int dt [\langle \dot{\Phi} | \Phi \rangle - \langle \Phi | \dot{\Phi} \rangle] / (2i) - \langle \Phi | H | \Phi \rangle$, where $|\Phi\rangle$ and H are specified in eqs. (1) and (2). Under the ansatz state (2), Wick's theorem implies the decomposition $U \langle \Psi_{\uparrow}^{\dagger} \Psi_{\downarrow}^{\dagger} \Psi_{\downarrow} \Psi_{\uparrow} \rangle \approx U \langle \Psi_{\uparrow}^{\dagger} \Psi_{\downarrow}^{\dagger} \rangle \langle \Psi_{\downarrow} \Psi_{\uparrow} \rangle$ (the additional Hartree-Fock terms, which only slightly modify the effective $V(\mathbf{r}, t)$, are not important when there is pairing instability [8] and are thus neglected here). It turns out that to get the expression of the action S , the critical part is the calculation of the pair function $F^*(\mathbf{r}_1, \mathbf{r}_2, t) \equiv \langle \Psi_{\uparrow}^{\dagger}(\mathbf{r}_1) \Psi_{\downarrow}^{\dagger}(\mathbf{r}_2) \rangle$. Under the ansatz state (2), the pair function satisfies the following integral equation (we drop the time variables in $F^*(\mathbf{r}_1, \mathbf{r}_2, t)$ and $f^*(\mathbf{r}, \mathbf{r}', t)$ when there is no confusion):

$$F^*(\mathbf{r}_1, \mathbf{r}_2) = f^*(\mathbf{r}_1, \mathbf{r}_2) - \int f^*(\mathbf{r}_1, \mathbf{r}_3) f^*(\mathbf{r}_4, \mathbf{r}_2) F(\mathbf{r}_4, \mathbf{r}_3) d^3 \mathbf{r}_3 d^3 \mathbf{r}_4. \quad (3)$$

To solve this integral equation, we write both $F^*(\mathbf{r}_1, \mathbf{r}_2)$ and $f^*(\mathbf{r}_1, \mathbf{r}_2)$ in terms of the new coordinates $\mathbf{r} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r}_- = \mathbf{r}_1 - \mathbf{r}_2$. Then, we take the Fourier transformation of eq. (3) and its conjugate with respect to the relative coordinate \mathbf{r}_- . The Fourier transforms of $F(\mathbf{r}, \mathbf{r}_-)$ and $f(\mathbf{r}, \mathbf{r}_-)$ are denoted by $F_{\mathbf{k}}(\mathbf{r})$ and $f_{\mathbf{k}}(\mathbf{r})$, respectively. In this Fourier transformation, we assume $|\partial_{\mathbf{r}} f| \ll |\partial_{\mathbf{r}_-} f|$ and $|\partial_{\mathbf{r}} F| \ll |\partial_{\mathbf{r}_-} F|$. Physically, it corresponds to the assumption that the order parameter is slowly varying within the size of the Cooper pairs. Under this assumption, we derive from eq. (3) and its conjugate the following simple relation between the Fourier components:

$$F_{\mathbf{k}}(\mathbf{r}) = f_{\mathbf{k}}(\mathbf{r}) / [1 + |f_{\mathbf{k}}(\mathbf{r})|^2]. \quad (4)$$

This relation is critical for the explicit calculation of the action S .

We can now express the action S in terms of the variational wave functions $f_{\mathbf{k}}(\mathbf{r}, t)$ and for $\phi_b(\mathbf{r}, t)$. From the functional derivatives $\delta S / \delta f_{\mathbf{k}}^*(\mathbf{r}, t) = 0$ and $\delta S / \delta \phi_b^*(\mathbf{r}, t) = 0$, we get the following evolution equations for $f_{\mathbf{k}}(\mathbf{r}, t)$ and for $\phi_b(\mathbf{r}, t)$:

$$i\partial_t f_{\mathbf{k}} = [2\epsilon_{\mathbf{k}} + H_0(\mathbf{r}, t)] f_{\mathbf{k}} + \Delta(\mathbf{r}, t) - \Delta^*(\mathbf{r}, t) f_{\mathbf{k}}^2, \quad (5)$$

$$i\partial_t \phi_b = [\gamma + H_0(\mathbf{r}, t)] \phi_b + (\alpha/U) \Delta_f(\mathbf{r}, t), \quad (6)$$

where $H_0(\mathbf{r}, t) \equiv -\nabla^2 / (4m) + 2V(\mathbf{r}, t)$, $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$ (m is the atomic mass), $\Delta_f(\mathbf{r}, t) \equiv (U/8\pi^3) \int d^3 \mathbf{k} f_{\mathbf{k}}(\mathbf{r}, t) / [1 + |f_{\mathbf{k}}(\mathbf{r}, t)|^2]$, and $\Delta(\mathbf{r}, t) \equiv \alpha \phi_b(\mathbf{r}, t) + \Delta_f(\mathbf{r}, t)$. The two equations (5) and (6) represent a central result of this work: they completely determine the evolution of the wave functions $f_{\mathbf{k}}$ and for ϕ_b , just as the GP equation determines the condensate evolution for the weakly interacting bosons. In the stationary case with a time-independent trap, one just needs to replace $i\partial_t f_{\mathbf{k}}$ and $i\partial_t \phi_b$, respectively, with $2\mu f_{\mathbf{k}}$ and $2\mu \phi_b$, where μ is the atom chemical potential.

The evolution equations (5) and (6) are a set of coupled nonlinear differential equations. They can be solved through direct numerical simulations (for instance, through the split-step method), but as the potential $V(\mathbf{r}, t)$ is typically slowly varying both in \mathbf{r} and in t , the following iterative method may prove to be more efficient. In this case, we expect both $\phi_b(\mathbf{r}, t) e^{i2\mu t}$ and $f_{\mathbf{k}}(\mathbf{r}, t) e^{i2\mu t}$ to be slowly varying in \mathbf{r} and t . We can then introduce the following effective potentials: $V_{eff}(\mathbf{r}, t) \equiv \phi_b^{-1}(\mathbf{r}, t) [-i\partial_t - \nabla^2 / (4m) + 2\mu] \phi_b(\mathbf{r}, t) / 2$ and $V_{eff}^{\mathbf{k}}(\mathbf{r}, t) \equiv f_{\mathbf{k}}^{-1}(\mathbf{r}, t) [-i\partial_t - \nabla^2 / (4m) + 2\mu] f_{\mathbf{k}}(\mathbf{r}, t) / 2$, both of which should be small. With these introduced potentials, we can solve $f_{\mathbf{k}}(\mathbf{r}, t)$ from eq. (5) as

$$f_{\mathbf{k}} = -(E_{\mathbf{k}} - (\epsilon_{\mathbf{k}} - \mu_{eff}^{\mathbf{k}})) / \Delta^*, \quad (7)$$

where $\mu_{eff}^{\mathbf{k}} \equiv \mu - V(\mathbf{r}, t) - V_{eff}^{\mathbf{k}}(\mathbf{r}, t)$, $\mu_{eff} \equiv \mu - V(\mathbf{r}, t) - V_{eff}(\mathbf{r}, t)$, $\Delta = \alpha\phi_b[1 - U(\gamma - 2\mu_{eff})/\alpha^2]$, and $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu_{eff}^{\mathbf{k}})^2 + \Delta^2}$. Substituting eq. (7) into eq. (6), we get the following effective gap equation:

$$1/U_T = - (1/8\pi^3) \int d^3\mathbf{k} \left(\frac{1}{2E_{\mathbf{k}}} - \frac{1}{2\epsilon_{\mathbf{k}}} \right), \quad (8)$$

where $1/U_T = 1/[U_p - \alpha_p^2/(\gamma_p - 2\mu_{eff})] = 1/[U - \alpha^2/(\gamma - 2\mu_{eff})] + \int d^3\mathbf{k} [1/(16\pi^3\epsilon_{\mathbf{k}})]$ (the latter equality comes from the renormalization relation between γ, α, U and γ_p, α_p, U_p [4]).

Under the zeroth-order approximation, we assume $V_{eff}(\mathbf{r}, t) \simeq V_{eff}^{\mathbf{k}}(\mathbf{r}, t) \simeq 0$, which leads to $\mu_{eff}^{\mathbf{k}} = \mu_{eff} = \mu - V(\mathbf{r}, t)$ in $E_{\mathbf{k}}$. In this case, the gap equation (8), together with the number equation $N = \int n(\mathbf{r}, t)d^3\mathbf{r}$, where N denotes the total atom number and $n(\mathbf{r}, t) = 2|\phi_b|^2 + (2/8\pi^3) \int d^3\mathbf{k} |f_{\mathbf{k}}|^2 / (1 + |f_{\mathbf{k}}|^2)$ is the local atom density, completely solves the problem, the result of which corresponds to a solution under the local density approximation in the adiabatic limit. Thus we recover the LDA result under the zeroth-order approximation which completely neglects $V_{eff}(\mathbf{r}, t)$ and $V_{eff}^{\mathbf{k}}(\mathbf{r}, t)$. It is then evident how to go beyond the LDA.

We can use the LDA result $\phi_b^{(0)}(\mathbf{r}, t), f_{\mathbf{k}}^{(0)}(\mathbf{r}, t)$ as the zeroth-order wave functions to calculate the first-order effective potentials $V_{eff}^{(1)}(\mathbf{r}, t)$ and $V_{eff}^{\mathbf{k}(1)}(\mathbf{r}, t)$ through their definition equations. Substituting these effective potentials into the gap equation (8) and eq. (7), we can find out the next order wave functions $\phi_b^{(1)}(\mathbf{r}, t), f_{\mathbf{k}}^{(1)}(\mathbf{r}, t)$. This iterative process should converge if the effective potentials are small (*i.e.*, the order parameters are slowly varying in \mathbf{r} and t).

In the following, we consider a different simplification of the basic equations (5) and (6) on the BEC side of the resonance with the chemical potential $\mu \leq 0$ (note that it is not required to be in the deep BEC region). On this side, we expect the wave functions $\phi_b(\mathbf{r}, t)$ and $f_{\mathbf{k}}(\mathbf{r}, t)$ to have similar dependence on \mathbf{r} and t , so we assume $V_{eff}(\mathbf{r}, t) \simeq V_{eff}^{\mathbf{k}}(\mathbf{r}, t)$. This approximation will be self-consistently tested and we will see that it is well satisfied when $\mu \leq 0$. Under this approximation, $\mu_{eff}^{\mathbf{k}} = \mu_{eff}$, while μ_{eff} can be solved from the gap equation (8) as a function of $|\phi_b|^2$. Substituting this solution μ_{eff} into the definition equation of V_{eff} , we get

$$i\partial_t\phi_b = [-\nabla^2/(4m) + 2V(\mathbf{r}, t) + 2\mu_{eff}] \phi_b. \quad (9)$$

This equation has the same form as the dynamical GP equation for the weakly interacting bosons except that the collision term is now replaced by a general nonlinear potential μ_{eff} [10], a function of $|\phi_b|^2$ with its shape determined by the gap equation (8). We have numerically solved eq. (8) for the function $\mu_{eff}(|\phi_b|^2)$ at several different detunings for ${}^6\text{Li}$, and the shapes of these functions are shown in fig. 1. We can see that μ_{eff} becomes almost linear in $|\phi_b|^2$ when one goes further into the BEC region. In that limit, eq. (9) reduces to an exact GP equation, and we can define an effective scattering length a_{eff} for the bare molecular condensate with $d\mu_{eff}/d(|\phi_b|^2) = 2\pi a_{eff}/(2m)$. This effective scattering length a_{eff} is shown in fig. 1(d) as a function of the field detuning for ${}^6\text{Li}$. We should note, however, that the effective scattering length for the bare molecules is in general very different from the one for the dressed molecules [4, 9, 15]. The dressed molecules are dominantly composed of Cooper pairs of atoms in the open channel (for instance, when the chemical potential $\mu \approx 0$, the population fraction of the bare molecules is only about 0.1% for ${}^6\text{Li}$). As the bare molecules have a very low density near the resonance, they in general have a large effective scattering length to compensate for that, as is shown in fig. 1(d). The effective scattering lengths for the bare and the dressed molecules coincide with each other only in the deep BEC region with the population dominantly in the closed channel. In this limit, we have checked that the dependence of the

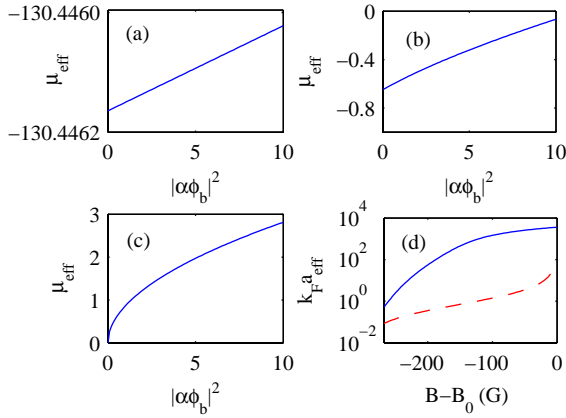


Fig. 1 – (a), (b), (c) The effective potential μ_{eff} as a function of $|\alpha\phi_b|^2$, with the field detuning $B - B_0$ given by -268 G (a), -107 G (b), and 0 G (c), respectively. Both μ_{eff} and $|\alpha\phi_b|$ are in the unit of $E_F = k_F^2/2m$, where $k_F = (3\pi^2 n_0)^{1/3}$ is a convenient inverse length scale corresponding to a density $n_0 = 3 \times 10^{13} \text{ cm}^{-3}$ as is typical for the MIT ${}^6\text{Li}$ experiment [1]. (d) The effective scattering lengths as a function of the field detuning. The solid line is for the bare molecules (see the definition in the text) while the dashed one is for the atoms.

effective scattering length on the field detuning is in agreement with a different calculation in ref. [16] under the two-channel model (we can only apply the two-channel model in this limit because of a large closed channel population [4, 17]). Experimentally, the scattering length between the dressed molecules can be measured from the collective excitations of the trapped Fermi gas [18] or from the in-trap radius of the condensate cloud [19]; while it is difficult to measure the scattering length between the bare molecules.

The simplified equation (9) determines the distribution of the bosonic molecules. This solution, combined with eq. (7), then fixes the distribution of the fermionic atoms. As a simple illustrating example, we use them to solve the Fermi condensate shape function in a harmonic trap on the BEC side of the resonance. We take the values of the parameters corresponding to ${}^6\text{Li}$, and assume a total of $N \sim 10^5$ atoms trapped in a time-independent potential $V(\mathbf{r}) = \frac{1}{2}m\omega\mathbf{r}^2$ with $\omega/2\pi \sim 100$ Hz, as is typical in the experiments [1]. Figures 2(a) and (b) show the condensate shape functions in two different regions with the magnetic field detunings $B - B_0$ given, respectively, by -268 G and -107 G. The first detuning corresponds to a point deep in the BEC region with $(k_F a_s)^{-1} \sim 11$, where a_s is the atom scattering length at that detuning and k_F^{-1} is a convenient length unit defined in the caption of fig. 1. The second one corresponds to the onset of the bosonic region with the atom chemical potential $\mu \sim 0$ and $(k_F a_s)^{-1} \sim 0.8$. We have shown in fig. 2 the number distributions for the bare molecules and the fermi condensate. One can see that these distribution functions are smooth in space, without the artificial cutoff at the edge of the trap as in the LDA result. The closed channel population (the total bare molecule fraction) is calculated to be about 33% and 0.1%, respectively, for these two detunings.

An important goal of the calculation of this simple example is to self-consistently check the approximations made in our derivation. First, to derive the basic equations (5), (6), we have assumed that the order parameter should be slowly varying over the size of the Cooper pairs. From fig. 2, we see that the characteristic length for the variation of the

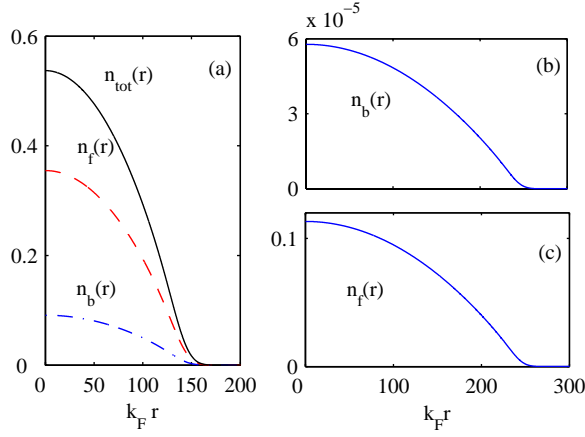


Fig. 2 – The radial distributions of the bare-molecule density (n_b), the Fermi-atom density (n_f), and the total density (n_{tot}) in a harmonic trap with the field detuning $B - B_0$ given by -268 G (a), and -107 G (b) and (c), respectively. All the densities are in the unit of n_0 (see the value in the caption of fig. 1).

order parameter is typically of $100k_F^{-1}$, while the size of the Cooper pair is well below k_F^{-1} at these detunings [17]. Therefore, this approximation should be well satisfied for typical experiments. Second, from the basic equations (5), (6) to the simplified equation (9), we have used the approximation $V_{eff}(\mathbf{r}, t) \simeq V_{eff}^k(\mathbf{r}, t)$. To check the validity of this approximation, we calculate the effective potentials $V_{eff}(\mathbf{r})$ and $V_{eff}^k(\mathbf{r})$ (time independent in this case) with our solutions of $\phi_b(\mathbf{r})$ and $f_{\mathbf{k}}(\mathbf{r})$ from the stationary harmonic trap, and the results are shown in fig. 3. It is clear that the difference $|V_{eff}(\mathbf{r}) - V_{eff}^k(\mathbf{r})|$ is small compared with the magnitude

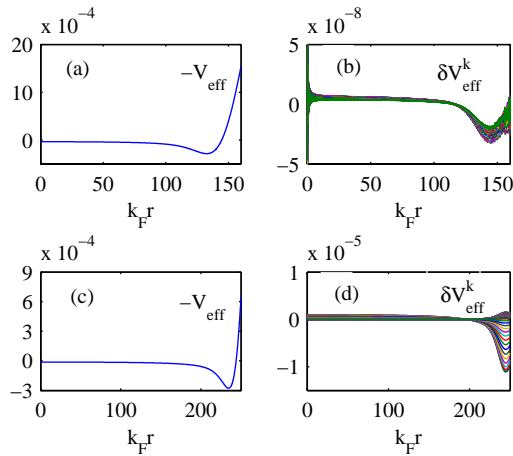


Fig. 3 – The shapes of the effective potential $-V_{eff}$ and the potential difference $\delta V_{eff}^k = V_{eff}^k - V_{eff}$ (both in the unit of E_F) at the field detuning $B - B_0 = -268$ G (a), (b) and -107 G (c), (d), respectively. Panels (b) and (d) each have twenty curves corresponding to the wave vector $|\mathbf{k}|$ evenly distributed in the range of 0 to $10k_F$.

of $|V_{eff}(\mathbf{r})|$ for different values of \mathbf{k} when the atom chemical potential $\mu \leq 0$, which justifies the approximation $V_{eff}^{\mathbf{k}}(\mathbf{r}, t) \simeq V_{eff}(\mathbf{r}, t)$ in that region. One can also see that the relative error $\left|V_{eff}(\mathbf{r}) - V_{eff}^{\mathbf{k}}(\mathbf{r})\right| / |V_{eff}(\mathbf{r})|$ goes up significantly (from roughly 10^{-4} to 10^{-1}) when one goes from the field detuning -268 G to -107 G. If one goes further to the resonance point, this approximation eventually breaks down, and one needs to use the basic equations (5), (6) instead of the reduced equation (9).

In summary, we have derived a set of dynamical mean-field equations for the evolution of strongly interacting fermionic atoms in any slowly varying potential traps, and discussed methods to solve these equations. We show that on the BEC side of the Feshbach resonance, this set of equations are reduced to a generalized dynamical GP equation. As an illustrating example, we solve the reduced equations in the case of a harmonic trap, which self-consistently verifies the approximations made in our derivation.

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This work was supported by the NSF award (0431476), the ARDA under ARO contracts, and the A. P. Sloan Fellowship.

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