Title
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Publication Date
1976-04-01

Submitted to Nuclear Physics A

LBL-5016
Preprint C. 1

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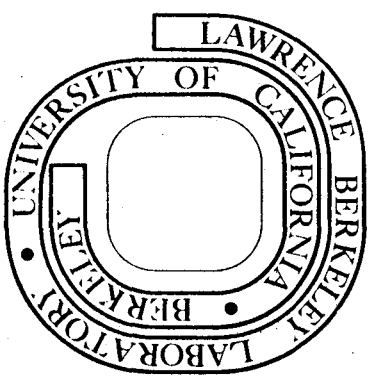
April 1976

Prepared for the U. S. Energy Research and
Development Administration under Contract W-7405-ENG-48



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LBL-5016

SIMPLE DYNAMICAL MODELS INCLUDING PAIRING RESIDUAL INTERACTION†

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ABSTRACT

Two simple models including pairing in the dynamical equations governing the motion of the nucleus are presented. They correspond to the constant pairing strength and the constant gap approximations. Their relation to the Landau-Zener type of coupling is investigated. The qualitative differences between the two pairing couplings have been studied in the particular case of the two crossing levels.

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†This report was done with support from the U. S. Energy Research and Development Administration. Any conclusions or opinions expressed in this report represent solely those of the authors and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the U. S. Energy Research and Development Administration.

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1. Introduction

The microscopic description of the dynamics of a many nucleon system has been extensively investigated during recent years.[1] Significant progress has been achieved recently with the time dependent Hartree-Fock (T.D.H.F.) method that allows for a self-consistent description of the dynamics of the nucleus.[2-4] However, in this method, the residual interactions are neglected. This together with the symmetries imposed in the calculations, leads to the unpleasant feature that a system even moving infinitely slowly could not end up in its ground state. This will appear each time two single particle levels with different quantum numbers (and, therefore, no possibility of transition between them) cross. Such a limitation of the T.D.H.F. method could for example decrease noticeably the calculated cross section of the compound nucleus formation in heavy ion collisions and it is likely to have a more serious effect for a slower collective motion like the one undergone by the nucleus during the fission process.

In order to avoid all these difficulties one could either lift all the symmetries imposed on the system which leads to a big computational problem or introduce in a way as simple as possible a residual interaction that allows for transitions between levels with different quantum numbers.

It is the aim of this paper to show that the second alternative can be achieved by using the pairing residual interaction. In the following section we use a variational principle to derive sets of coupled equations which contain the T.D.H.F. equations as a particular case plus simple equations governing the occupation probabilities of

each single particle level. In Section 3 we apply these equations to the particular case of the two level model, we discuss the solutions and we make a comparison with a Landau-Zener[5-7] type coupling. Section 4 contains our conclusions. Finally, in Appendix A, we present a suggestion for a numerical treatment of the equations derived in Section 2.

2. Derivation of the Equations

2.1. Choice of the Wave Function and Lagrangian

We assume that at all times the wave function of the nucleus can be described by a Bogoliubov state $|\phi\rangle$, which in the canonical representation[8] can be written* as

$$|\phi\rangle = \prod_{k>0} \left(u_k + v_k d_k^+ d_{\bar{k}}^+\right) |0\rangle \tag{1}$$

where $|0\rangle$ denotes the vacuum state, d_k^+ and $d_{\bar{k}}^+$ are the creation operators of the coupled states k and $\bar{k}$ and u_k and v_k satisfy the relation

$$|v_k|^2 + u_k^2 = 1 \quad . \tag{2}$$

Writing formula (2) we made use of the well known fact that only the relative phase between u_k and v_k matters and decided to take u_k as a real quantity. In the rest of this paper we shall also use the following standard notation

$$\rho_k = |v_k|^2 \tag{3a}$$

$$K_k = u_k v_k \tag{3b}$$

$$\phi_k(\bar{r}) = \langle \bar{r} | d_k^+ | 0 \rangle \tag{3c}$$

We shall start from the variational principle[9]

$$\delta I = 0 \quad \text{with} \quad I = \int_{t_1}^{t_2} \mathcal{L} dt \tag{4}$$

*The notation $k > 0$ means that only one of the coupled states k and $\bar{k}$ is involved.

and take as a Lagrangian $\mathcal{L}$

$$\mathcal{L} = E - i\hbar \langle \phi | \frac{\partial}{\partial t} | \phi \rangle = \langle \phi | H - i\hbar \frac{\partial}{\partial t} | \phi \rangle \tag{5}$$

In the equations (4) and (5) the v_k, v_k^*, ϕ_k, ϕ_k^*, $\phi_{\bar{k}}$ and $\phi_{\bar{k}}^*$ are the independent variational quantities and H the many body Hamiltonian.

From definition (1) the term $\langle \phi | \frac{\partial}{\partial t} | \phi \rangle$ in expression (5) can easily be calculated. One obtains

$$\langle \phi | \frac{\partial}{\partial t} | \phi \rangle = \sum_{\ell>0} \left[\frac{1}{2} \left(v_\ell^* \dot{v}_\ell - \dot{v}_\ell^* v_\ell \right) + |v_\ell|^2 \int d_3 r \left(\phi_\ell^* \dot{\phi}_\ell + \phi_{\bar{\ell}}^* \dot{\phi}_{\bar{\ell}} \right) \right] \tag{6}$$

The dots in Eq. (6) denote as usual the time derivatives.

The energy $E = \langle \phi | H | \phi \rangle$ is separated into two parts: The field part E_F and the pairing one E_p:

(i) The field energy E_F is the part of the total energy E that is associated with the contractions of the type $\overline{d^+ d}$ and $\overline{d^+ d}\ \overline{d^+ d}$ when one makes use of the Wick theorem. When the wave function $|\phi\rangle$ reduces to a Slater determinant, E_F becomes equal to E. The equations of motion, which shall be presented in Section 2.3 are valid for a field energy E_F derived for any two body interaction. However, we shall consider field energies of the following local functional type:

$$E_F = \int d_3 r\ \mathcal{H}(\rho, T) \tag{7}$$

where $\mathcal{H}$ is a functional of the density ρ and kinetic energy density T

$$\rho(\bar{r}) = \sum_{\ell>0} \rho_\ell \left(|\phi_\ell(\bar{r})|^2 + |\phi_{\bar{\ell}}(\bar{r})|^2 \right) \tag{8a}$$

$$T(\bar{r}) = \sum_{\ell>0} \rho_\ell \left| \bar{\nabla}\phi_\ell(\bar{r}) \right|^2 + \left| \bar{\nabla}\phi_{\bar{\ell}}(\bar{r}) \right|^2 \qquad (8b)$$

Such field energies are typical for the Skyrme or Skyrme-like[10] type effective interactions, and the success of these interactions in reproducing the nuclear ground state properties indicates that the restriction implied by formula (7) is not very serious. Anyway as mentioned before the equations of motion will not depend on this restriction, which is used here only to simplify our presentation.

(ii) The pairing energy E_p is the part of the total energy E associated with the contractions of the type $\overbrace{d^+ d^+}$ $\overbrace{dd}$. The aim of this paper is to investigate the qualitative dynamic properties of the coupling between nucleons introduced by the pairing interaction. Such an investigation can be more easily done with a schematic model rather than with the more general form of the pairing energy E_p. We have selected two models, which have been of great use in the static calculations including pairing: the constant gap Δ model and the constant pairing strength G model. Different pairing energies E_p correspond to each of these models: the constant gap pairing model leads to the pairing energy

$$E_{p_1} = -\Delta \sum_{\ell>0} \left(K_\ell + K_\ell^* \right) \qquad (9)$$

and the constant pairing strength model to

$$E_{p_2} = -G \left| \sum_{\ell>0} K_\ell \right|^2 \qquad (10)$$

In the formulas (9) and (10), Δ and G are real constants. In the following sections we shall study the differences between these two types of pairing coupling.

2.2. Constraints

Before performing the variation of the Lagrangian $\mathcal{L}$, we shall add to it two Lagrange constraints C_1 and C_2. The first constraint will be on the total number of particles

$$C_1 = -\lambda N \tag{11}$$

with

$$N = 2 \sum_{\ell>0} \rho_\ell = \text{const} \quad . \tag{12}$$

The second constraint ensures the conservation of the norm of the particle wave functions

$$C_2 = \sum_{\ell>0} \mu_\ell (n_\ell + n_{\bar{\ell}}) \tag{13}$$

with

$$n_\ell = \int d_3 r |\phi_\ell(\bar{r})|^2 = 1 \tag{14}$$

The μ_ℓ and λ are the Lagrange parameters.

2.3. Equations of Motion

In this subsection we shall present and discuss the general features of the Euler-Lagrange equations applied to $\mathcal{L} + C_1 + C_2$ for the two different pairing energies E_{p_1} and E_{p_2}.

2.3.1. Constant pairing strength (G) interaction

The Euler-Lagrange equations in this case are:

$$i\hbar\dot{\phi}_\ell = (\hat{\mathcal{H}}(\rho) - \varepsilon_\ell)\ \phi_\ell \tag{15a}$$

$$i\hbar\dot{\rho}_\ell = \Delta^* K_\ell - \Delta K_\ell^* \tag{15b}$$

$$i\hbar\dot{K}_\ell = 2K_\ell(\varepsilon_\ell - \lambda) + \Delta(2\rho_\ell - 1) \tag{15c}$$

$$\Delta = G \sum_{\ell>0} K_\ell \tag{15d}$$

where $\hat{\mathcal{H}}(\rho)$ is the one-body Hamiltonian governing the motion of the single particle states ϕ_ℓ, and ε_ℓ is a single particle energy

$$\varepsilon_\ell = \frac{\mu_\ell}{\rho_\ell}$$

Several choices can be made for ε_ℓ. One possibility is

$$\varepsilon_\ell = \int d_3r\ \phi_\ell^*\ \hat{\mathcal{H}}\ \phi_\ell \tag{16}$$

The one body Hamiltonian $\hat{\mathcal{H}}$ has the same physical meaning as the Hartree-Fock one body Hamiltonian. The equation (15a) appears then as a direct generalization of the usual TDHF equations. It is only coupled to the equations (15b)-(15d) through the dependence of ρ and T on ρ_ℓ (equation 8). Definition (16) of the energy ε_ℓ ensures not only the conservation of the norm n_ℓ but also the more strict condition

$$\int \phi_\ell^* \dot{\phi}_\ell\ d_3r = 0 \tag{17}$$

This property does not bear any physical information and simply means that we have made a particular choice for the phase factor in the wave functions ϕ_ℓ.

The equations (15b)-(15d) are the dynamical pairing equations (they were already derived in Ref. 1, except for an additional term in equation (15c)). They are coupled to equation (15a) only through the single particle energies ε_ℓ. Let us now study their properties:

(i) The summation over the index ℓ in equation (15b) gives

$$2 \sum_{\ell>0} \dot{\rho}_\ell = \dot{N} = 0 \tag{18}$$

which shows that the number of particles is conserved.

(ii) There is no equation to determine the time evolution of the Lagrange parameter λ. In fact, the analysis of equation (15c) shows that adding to λ any arbitrary function of the time simply amounts to a change of the K_ℓ (and thus the v_ℓ) by an overall phase factor, without any physical change. Therefore, one can use the freedom in the choice of λ to simplify the equations, as we shall do in the next section.

(iii) The time derivative of the total energy E is:

$$\dot{E} = \sum_{\ell>0} \left[2|v_\ell|^2 \int d_3 r \left(\dot{\phi}_\ell^* \hat{\mathcal{H}} \phi_\ell + \phi_\ell^* \hat{\mathcal{H}} \dot{\phi}_\ell \right) + \left(2\varepsilon_\ell \dot{\rho}_\ell - \Delta \dot{K}_\ell^* - \Delta^* \dot{K}_\ell \right) \right] \tag{19}$$

Equation (15a) ensures that the first term in equation (19) is equal to zero. Using the equations (15b)-(15d) one obtains:

$$\dot{E} = \lambda \dot{N} \tag{20}$$

which, because of equation (18) ensures the conservation of the energy.

2.3.2. Constant gap (Δ) pairing interaction

The gap Δ is chosen to be a real constant. Then the Euler-Lagrange equations become

$$i\hbar \dot{\phi}_\ell = (\hat{\mathcal{H}}(\rho) - \varepsilon_\ell)\, \phi_\ell \tag{21a}$$

$$i\hbar \dot{\rho}_\ell = \Delta(K_\ell - K_\ell^*) \tag{21b}$$

$$i\hbar \dot{K}_\ell = 2K_\ell(\varepsilon_\ell - \lambda) + \Delta(2\rho_\ell - 1) \tag{21c}$$

Formally these equations are very similar to the equations (15a)-(15d), the only difference is that now Δ is not determined self consistently as it was before (equation 15d). The fact that Δ is now a real

constant has several consequences. The most important one is that the conservation of the number of particles is not automatically ensured by eq. (21b). Therefore, one should choose λ in a way to keep the number of particles constant. Since one can again prove the relation (20), the conservation of the energy will be a direct consequence of the conservation of the number of particles.

It is also possible to write the equations (21a)-(21c) in a different way by introducing the following three real variables:

$$\begin{aligned} M_\ell &= \rho_\ell - \frac{1}{2} \\ K_\ell^R &= \frac{1}{2}\left(K_\ell + K_\ell^*\right) \\ K_\ell^i &= -\frac{i}{2}\left(K_\ell - K_\ell^*\right) \quad , \end{aligned} \tag{22}$$

which satisfy the relation

$$M_\ell^2 + K_\ell^{R^2} + K_\ell^{i^2} = \frac{1}{4} \tag{23}$$

and

$$i\hbar \begin{pmatrix} \dot{M}_\ell \\ \dot{K}_\ell^R \\ \dot{K}_\ell^i \end{pmatrix} = \tilde{\mathcal{H}}_\ell \begin{pmatrix} M_\ell \\ K_\ell^R \\ K_\ell^i \end{pmatrix} \tag{24}$$

with

$$\tilde{\mathcal{H}}_\ell = i \begin{pmatrix} 0 & 0 & 2\Delta \\ 0 & 0 & 2(\varepsilon_\ell - \lambda) \\ -2\Delta & -2(\varepsilon_\ell - \lambda) & 0 \end{pmatrix} \tag{25}$$

It is shown in Appendix A that the numerical treatment of the time dependent equations (21b) and (21c) is noticeably simplified by switching to the equivalent formulation (23)-(25).

The only remaining problem is to choose λ, so that the number of particles is conserved. To realize this we must have

$$\sum_{\ell>0} K_\ell^i = 0 \tag{26}$$

since we shall assume that at the initial time this condition is fulfilled we need only to impose

$$\sum_{\ell>0} \dot{K}_\ell^i = 0 \tag{27}$$

If D is the dimension of the space

$$D = 2 \sum_{\ell>0} 1 \tag{28}$$

one finds that λ must satisfy

$$\lambda = \frac{2\left(\sum_{\ell>0} \varepsilon_\ell K_\ell^R\right) + \Delta\left(N - \frac{D}{2}\right)}{2\sum_{\ell>0} K_\ell^R} \tag{29}$$

It should be noted that the equations (15b)-(15d) can be put into a form similar to eqs. (23)-(25). Indeed we can take advantage of the freedom we have in the choice of the Lagrange parameter λ to ensure that Δ (eq. (15d)) is a real quantity. One then finds that λ satisfies equation (29) with the only difference that Δ is not a constant but equal to:

$$\Delta = G \sum_{\ell>0} K_\ell^R \tag{30}$$

It is then possible to reformulate the complex equations (15b)-(15d) into the set of real equations (23)-(25), but now the matrix elements of $\tilde{\mathcal{H}}$ proportional to Δ are calculated according to eq. (30). The numerical technique described in the Appendix A could thus also be applied to the equations of motion corresponding to a constant pairing strength interaction.

2.4. Relation with the TDHF Equations

The sets of equations (15a)-(15d) and (21a)-(21c) contain as a particular case the TDHF equations. However, in the case of constant pairing strength G the TDHF equations are solutions of the system (15a)-(15d) for any value of G*, while one has to set $\Delta = 0$ to reduce the system (21a)-(21c) to TDHF equations. Indeed, if the starting conditions for the system (15a)-(15d) are such that the Bogoliubov state degenerates into a Slater determinant ($K_\ell \equiv 0$), the solution will always remain a Slater determinant no matter how large G is. This is because a Slater determinant is always solution of the static pairing equations with a constant pairing strength. On the other hand, if the constant gap Δ is different from zero, there does not exist any time dependent Hartree-Fock solution that can satisfy the set of equations (21a)-(21c).

*It is true even if one uses a more general pairing interaction.

3. Two Levels Model

In order to investigate the qualitative effects of the pairing coupling we apply the equations (15) and (21) to the particular case of the two levels model. One can question the validity of using constant G interaction in such a simplified system since pairing is a collective phenomenon. However, the situation in nuclear physics is not quite comparable to that in solid state physics. Indeed, the number of nucleons that contribute significantly to the pairing is always small (and not much larger than two) as compared to the total number of nucleons. As we shall see in this section the main difference between the cases Δ = constant and G = constant comes from the fact that in the latter case the gap is dependent on the relative phase between the coefficients v_i. This dependence is probably more pronounced in the two levels model with constant G (making in this way the difference with the constant Δ case even more clear), as compared to the more realistic case studied in Ref. 1, where pairing effects were created essentially by a dozen interacting levels. It is likely, however, that many qualitative features will remain the same. In this section we also investigate the relation between the coupling introduced by the pairing interaction and the Landau-Zener one.

The one-nucleon two levels model, that we shall study is in fact a four levels model with one pair of nucleons, where one takes into account the fact that the energies of paired levels are equal. From now on, we shall work only with one of each pair of levels. The difference between the energies of two distinct levels will be a function of time, and in the two cases we shall study, this function

is either a constant or linearly dependent on time.

3.1. Equations with the Constant Gap

In the two levels model the quantities defined by (22) satisfy:

$$M_2 = -M_1 \ , \ K_1^R = K_2^R \ , \ K_1^i = -K_2^i \tag{31}$$

where the indices 1 and 2 refer to the two distinct levels, and equation (29) reduces to:

$$\lambda = \frac{\varepsilon_1 + \varepsilon_2}{2} \tag{32}$$

where ε_1 and ε_2 are the energies of these two levels. Therefore, the equations (24) and (25) which in principle should be written for the indices 1 and 2, lead to one independent set of coupled equations:

$$i\hbar \frac{d}{dt} \begin{pmatrix} M_1 \\ K_1^R \\ K_1^i \end{pmatrix} = \begin{pmatrix} 0 & 0 & 2\Delta \\ 0 & 0 & -\delta\varepsilon \\ -2\Delta & \delta\varepsilon & 0 \end{pmatrix} \begin{pmatrix} M_1 \\ K_1^R \\ K_1^i \end{pmatrix} \tag{33}$$

with

$$\delta\varepsilon = \varepsilon_2 - \varepsilon_1 \tag{34}$$

The problem of solving these equations can be greatly simplified by noting their analogy with the Landau-Zener type of coupling, where the equations for the time evolution of the coefficients of expansion C_1 and C_2 of a state on the two unperturbed levels satisfy:

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} \varepsilon_1 & H \\ H & \varepsilon_2 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \ . \tag{35}$$

Here H is the coupling matrix element.* By making the correspondence

$$\begin{aligned} M_1 &\leftrightarrow |C_1|^2 - \frac{1}{2} \\ K_1^R &\leftrightarrow \mathrm{Re}\left(C_2^* C_1\right) \\ K_1^i &\leftrightarrow \mathrm{Im}\left(C_2^* C_1\right) \\ \Delta &\leftrightarrow -H \end{aligned} \tag{36}$$

one obtains exactly equation (33). This correspondence shows that the gap is the analogue of the coupling coefficient H. This is not too surprising since in a microscopic calculation using a two body interaction, H has the meaning of a matrix element of the Hartree-Fock field, namely the convolution of the two-body interaction with the one body density, while Δ results from the convolution of the interaction with the pairing tensor.

In fact the analogy between the pairing equations (24) and (25) and the Landau-Zener equations can be slightly extended. Indeed one can interpret the equations (24) and (25) in the case of a many levels problem by saying that each level with energy ε_ℓ undergoes a Landau-Zener transition (with coupling strength Δ) to a fictitious level with an energy ε'_ℓ satisfying

$$\lambda = (\varepsilon_\ell + \varepsilon'_\ell)/2 \quad .$$

This is because the only coupling between the equations (24) for

*We call (35) the Landau-Zener equation for the two types of variation $\delta\varepsilon$ with time, although generally this name is used only when $\delta\varepsilon$ depends linearly on time.

different levels is due to λ and the analogue of what we call $\delta\varepsilon$ in eq. (34) is $2(\lambda - \varepsilon_i)$.

Because of the identity between the constant gap two levels model equations and Landau-Zener equations, we can immediately obtain the solutions for the two time dependences of $\delta\varepsilon$ considered here.

When $\delta\varepsilon$ does not depend on time one finds that the probability of the level occupation $\rho_1 = |v_1|^2$ oscillates as a sine (or cosine) function with a period

$$T = \frac{2\pi\hbar}{(4\Delta^2 + \delta\varepsilon^2)^{1/2}} \tag{37}$$

If one chooses the initial time such that $\dot{\rho}_1$ is equal to zero and $\rho_1 = \frac{1}{2} + M_o \equiv \rho_o$, the amplitude of the oscillations is

$$\delta\rho = \left| \frac{8\Delta^2 M_o - 2\cdot\delta\varepsilon\cdot\Delta\left(1 - 4M_o^2\right)^{1/2}}{4\Delta^2 + \delta\varepsilon^2} \right| \tag{38}$$

From eq. (37) one can see that the period of oscillation depends only on Δ and $\delta\varepsilon$ and not on the initial density ρ_o. Equation (38) shows that the amplitude of the oscillations is zero only when the initial density is equal to its static equilibrium value

$$\rho_1^{st} = \frac{1}{2}\left(1 + \frac{\delta\varepsilon}{(4\Delta^2 + \delta\varepsilon^2)^{1/2}}\right) \tag{39}$$

One can also notice that the amplitude of oscillations $\delta\rho$ is exactly the same whether the initial density is zero or one.

The case when $\delta\varepsilon$ is a linear function of time has been investigated by Landau and Zener.[5-7] We shall assume the following variation for $\delta\varepsilon$.*

$$\delta\varepsilon = -2at \tag{40}$$

Applying the Landau-Zener results to the case Δ = constant, one can compute the final density $\rho_f \equiv \rho_1(t = +\infty)$ for the unperturbed first level, knowing the initial density $\rho_i \equiv \rho_1(t = -\infty)$ for this level. The result is generally dependent on the initial relative phase between u_1 and v_1 (phase of K_1). The only two exceptions are when the level is either totally filled or totally empty at $t = -\infty$. The results can be summarized in the following way. The average final density $\bar{\rho}_f$ is equal to

$$\bar{\rho}_f = \rho_i(1 - 2w) + w \tag{41}$$

and the dispersion σ of the values of ρ_f is given by

$$\sigma^2 = \overline{(\rho_f - \bar{\rho}_f)^2} = 2\rho_i(1 - \rho_i)\, w(1 - w) \tag{42}$$

where w is the well known Landau-Zener probability of transition

$$w = 1 - \exp\left(-\frac{\pi\Delta^2}{\hbar a}\right) \tag{43}$$

These results exhibit a symmetry under the transformation $\rho_i \leftrightarrow 1 - \rho_i$. Indeed, eq. (42) is evidently invariant under this transformation, as well as the absolute value of the transition amplitude $|\bar{\rho}_f - \rho_i|$. This

*From now on we shall call a - velocity, although it has a dimension $\text{MeV}\cdot\text{sec}^{-1}$.

symmetry is commonly expressed by saying that the probability of jump from one unperturbed level to the other one is identical whether it is the upper or lower level which is occupied at minus infinity. In other words, the Landau-Zener coupling does not take into account the fact that once the perturbation is introduced one of the static perturbed levels is always more bound than the other one.

Before going to the next section we shall present two different ways of formulating eq. (33) only for the purpose of comparison with the constant G interaction. By calling Θ the phase between u_1 and v_1, eq. (33) can be replaced by the first order differential system

$$\begin{aligned} \hbar\dot{M}_1 &= \Delta\left(1 - 4M_1^2\right)^{1/2} \sin\Theta \\ \hbar\dot{\Theta} &= \delta\varepsilon - 4\Delta\left(\frac{M_1}{\left(1 - 4M_1^2\right)^{1/2}}\right) \cos\Theta \end{aligned} \tag{44}$$

or a second order differential equation

$$\dot{M}_1\delta\varepsilon = \left(\Delta^2\left(1 - 4M_1^2\right) - \left(\hbar\dot{M}_1\right)^2\right)^{1/2} . \tag{45}$$

3.2. Equations with the Constant G Interaction

Formally most of the results that have been obtained in the case Δ = constant remain valid. Indeed if one wants the gap Δ to remain real, the Fermi level λ should satisfy equation (32). The relations (31) and eq. (33) are still valid. The only difference is that now the gap Δ should be calculated selfconsistently as

$$\Delta = 2GK_1^R = G\left(1 - 4M_1^2\right)^{1/2} \cos\Theta \tag{46}$$

Θ represents here, as in eq. (44) the phase of K_1. The already noted analogy between the eq. (33) and the Landau-Zener equations shows again that the quantity corresponding to the Landau-Zener coupling parameter H is the gap Δ.

We shall now see how the self-consistency (or nonlinearity) introduced by the formula (46) modifies the results obtained in section 3.1. In the particular case of the two levels model it appeared to be easier not to solve the equations of motion in the form indicated by formula (33) but rather to use the first order differential system.

$$\begin{aligned} \hbar \dot{M}_1 &= \frac{G}{2}\left(1 - 4M_1^2\right) \sin 2\Theta \\ \hbar \dot{\Theta} &= \delta\varepsilon - 4GM_1 \cos^2\Theta \end{aligned} \tag{47}$$

which corresponds to the system (44). In fact one can note that eq. (47) can be obtained from eq. (44) by simply inserting expression (46) for Δ. The analogue of the second order differential equation (45) is:

$$\dot{M}_1(8GM_1 - 4\delta\varepsilon) = \left(G^2\left(1 - 4M_1^2\right)^{\cdot 2} - 4(\hbar\dot{M}_1)^2\right)^{1/2} \tag{48}$$

3.3. Results and Comparison of the Two Models

When the difference between energies of the two levels $\delta\varepsilon$ does not depend on time, equation (48) can be easily integrated. We shall study the solutions, which at time t = 0 satisfy $\dot{\rho}_1 = 0$ and $\rho_1 = 1/2 + M_o \equiv \rho_o$. Equation (48) leads to the following first order differential equation for M_1

$$\dot{M}_1^2 = \frac{8G\delta\varepsilon}{\hbar^2} M_1(M_1 - a_1)(M_1 - a_2) \tag{49}$$

with

$$a_1 = \left(\frac{\delta\varepsilon}{2G} - 2M_o\right) \quad , \quad a_2 = \frac{G}{2\delta\varepsilon}\left(1 - 4M_o^2\right) \quad . \tag{50}$$

The solution of equation (49) can be expressed in terms of the elliptic functions and the results are summarized in Table 1.

In Fig. 1 we show the results for the period an amplitude of the motion for the two cases: $\delta\varepsilon$ = 1.5 MeV and $\delta\varepsilon$ = 3 MeV, as a function of the initial occupation $\rho_o \equiv 1/2 + M_o$ at t = 0. The first case ($\delta\varepsilon$ = 1.5 MeV) is an example of the situation where a static pairing solution exists ($|\delta\varepsilon| \leqslant 2G$). One can notice the strong dependence of the period on ρ_o to be compared with the constant Δ case, where period is completely independent of ρ_o. When $\delta\varepsilon$ becomes larger than 2G (case: $\delta\varepsilon$ = 3 MeV) there does not exist any static pairing solution. From the results shown in Fig. 1b, one can see that then the period varies smoothly with ρ_o. In this case the amplitude (shown in the lower part of Fig. 1) is a symmetric function of ρ_o, going to zero when ρ_o goes to zero or one. However, when $\delta\varepsilon$ becomes smaller than 2G (Fig. 1a) one can see, that the amplitude still goes to zero with ρ_o, but has a nonzero value at ρ_o equal one. Finally, one can note that when ρ_o is exactly zero or one there is no motion at all either because the amplitude of oscillations is zero or the period is infinite.

We shall see how these results can help us to understand some of the features appearing in the situation when two levels cross.

In the case of two crossing levels, which is of much more interest, we were not able to solve the equations analytically. Therefore, we solved the system (47) by using the fourth order Runge-Kutta method.[12]

As a check the Adams-Moulton-Bashforth[13] predictor corrector method was used too. In Figs. 2 and 3 some of the results are presented and compared with the results obtained in the constant Δ calculations. To make a reasonable comparison between the constant G and Δ calculations it seemed to us necessary to ensure that in both cases the average value of the gap is the same. Indeed our comparison with the Landau-Zener case showed that the gap is the quantity responsible for the transition. According to formula (46) when G is constant the average value of Δ^2 is $G^2/4$. Therefore, we choose a value of G twice as large as the value of the constant Δ. Finally we choose Δ equal to 0.5 MeV, which is a reasonable value for real nuclei and, therefore, should give us a good idea about what the transition would be in realistic situations.

In Fig. 2, we plot for a given velocity $a = 0.4 \cdot 10^{22} \frac{\text{MeV}}{\text{sec}}$ (see formula (40)) the final density ρ_f $(t = +\infty)$ for the unperturbed level 1 as a function of the initial density ρ_i $(t = -\infty)$ for the same level. According to our definitions when a is positive, the unperturbed level 1 is close to the lower perturbed level at minus infinity and close to the upper one at plus infinity.

One can see that with a constant G interaction there is no transition when the initial filling is zero or one. Again this is due to the fact that the Hartree-Fock solution is always a solution of the pairing equation. We assume that some kind of measure of the strength of the transition is given by the deviation of the average curve $\bar{\rho}_f$ from the diagonal indicated by a dashed line in Fig. 2(a) or 2(b). These diagonals correspond to the infinite-velocity case. Now one can

see that the absolute value of the deviation is on the average larger in the constant Δ case.

In Fig. 3 we present the probability of the transitions as a function of the velocity a. The quantity $\bar{\rho}_f$ that we plot is in fact the average occupation of the upper perturbed level at plus infinity. For the constant Δ case we present the results when the occupation probabilities of the lower perturbed level at minus infinity equal zero or one. According to formula (41) the sum of two curves is equal one for any value of the velocity. In the constant G coupling there is no point to studying the cases when initial filling is zero or one, because as it was noted in section 2.4 there is no transition for these fillings. So, we made calculations for the initial fillings which are close, but not equal to zero and one, namely 0.01 and 0.99. The comparison with the constant gap case shows that for a given velocity the strength of the transition in the G coupling is much less. One can also note a difference in the behavior of the two curves with initial fillings $\rho_i = 0.99$ and 0.01. This difference is particularly important for the lowest velocities that we have studied ($\log(a) < -1.5$). For these velocities we find an almost complete transition when the initial filling of the lower level is equal 0.99 (Fig. 3b). This means that after the crossing the probability of occupation of the lower perturbed level is close to 1. But when the lower level is almost empty at $t = -\infty$ the probability of occupation of the lower perturbed level after crossing is larger than 0.5 (Fig. 3a). Therefore, one can say, that the constant G coupling takes into account the fact that one of the perturbed levels is more bound than the other

one and on the average it is more filled after crossing. This "asymmetry" between the results for the initial fillings 0.01 and 0.99 can be understood from static results. Assuming that the velocity is sufficiently small, so that one can extract some information from the results with constant $\delta\varepsilon$, it comes out (Fig. 1) that when the initial filling is close to zero the amplitude of the oscillations will remain very small until $\delta\varepsilon$ becomes negative. Therefore, during half of the crossing time no transition can occur. On the contrary when the initial filling is close to 1, as soon as $\delta\varepsilon$ becomes less than 2G the amplitude of the oscillations is increasing very fast and, therefore, the overall time available for the transition is much larger than in the previous case.

4. Conclusions

In this paper we have presented two different sets of equations which lead to a simple self consistent model for a dynamical description including the pairing residual interaction. These two sets correspond to the constant gap and constant pairing strength approximation models. The TDHF equations are always contained as a particular case of the complete sets and we have shown that the pure TDHF solutions are always solutions of the complete set of equations with constant G no matter how large G is.

By applying the equations to a simple two levels model it was possible to show the connection with the Landau-Zener theory. Going to the many levels problem we have shown that each level undergoes a Landau-Zener type transition to a fictitious level symmetric with respect to the Fermi level and with a coupling strength determined by the magnitude of the gap. Formally, the only difference between the two pairing models lies in the fact that the gap is calculated self consistently from the pairing tensor solution when one is working with the constant G interaction.

From the solutions of the two levels model it was also possible to extract the qualitative features of the transitions induced by the two pairing models. It has been shown that using the constant G interaction the transition between two unperturbed levels is weaker (it requires a slower motion) and also that it is easier to populate the lower perturbed level contrary to the Landau-Zener type (and constant gap) coupling which gives equal probabilities of a jump from either perturbed level to the other one.

Both pairing residual interaction models can be used as a phenomenological way to allow for the interactions between levels with different quantum numbers; however, the constant gap formulation is much simpler. In this case the gap should be partly interpreted as a symmetry breaking matrix element of the field.

Acknowledgements

We would like to thank S. Koonin, J. R. Nix, H. J. Mang and W. J. Swiatecki for useful discussions and suggestions. Thanks are also due to M. Redlich for reading the manuscript and any valuable comments. We would also like to thank K. N. Glendenning for the hospitatility of the Nuclear Theory Group.

Appendix A. Numerical Treatment of the Pairing Time Evolution Equations

According to the definitions[22,25] and the equations (23) and (24) the time evolution of the occupation probabilities and of the pairing tensor for a D/2 level system is equivalent to the evolution of a set of D/2 three dimensional normalized vectors. The evolution of each vector is determined by the Hamiltonian operator $\tilde{\mathcal{H}}_\ell$ defined by formula (25). The vectors are coupled only through the Fermi level λ. A well known numerical method which preserves exactly the norm of a vector in a calculation with a finite time step consists in using the Crank Nicholson unitary propagator

$$\begin{pmatrix} M_\ell \\ K_\ell^R \\ K_\ell^i \end{pmatrix}^{(n+1)} = \frac{1 - \frac{i}{2}\frac{dt}{\hbar}\tilde{\mathcal{H}}_\ell}{1 + \frac{i}{2}\frac{dt}{\hbar}\tilde{\mathcal{H}}_\ell} \begin{pmatrix} M_\ell \\ K_\ell^R \\ K_\ell^i \end{pmatrix}^{(n)} \qquad (A.1)$$

In the above equation (n) refers to a given time step and dt is the magnitude of the time step. Due to the simplicity of the operator $\tilde{\mathcal{H}}_\ell$ the propagator can be written in a closed form and one obtains

$$\begin{pmatrix} M_\ell \\ K_\ell^R \\ K_\ell^i \end{pmatrix}^{(n+1)} = \left(1+a^2+b_\ell^2\right)^{-1} \begin{pmatrix} 1+b_\ell^2-a^2 & -2ab_\ell & 2a \\ -2ab_\ell & 1+a^2-b_\ell^2 & 2b_\ell \\ -2a & -2b_\ell & 1-a^2-b_\ell^2 \end{pmatrix} \begin{pmatrix} M_\ell \\ K_\ell^R \\ K_\ell^i \end{pmatrix}^{(n)} \qquad (A.2)$$

where

$$a = \frac{dt}{\hbar}\Delta \quad \text{and} \quad b_\ell = \frac{dt}{\hbar}(\varepsilon_\ell - \lambda) \qquad (A.3)$$

The only remaining problem is to ensure the exact conservation of the particle number. This is done by choosing the Fermi level λ such that the quantity

$$A(\lambda) = \sum_{\ell>0} \left(1 + a^2 + b_\ell^2\right)^{-1} \left(aM_\ell^{(n)} + b_\ell K_\ell^{R(n)} - K_\ell^{i(n)}\right) \qquad (A.4)$$

vanishes. The zero of $A(\lambda)$ is easily obtained by using a Newton-Raphson method. Indeed the derivative of $A(\lambda)$ can be calculated in a closed form and one knows a good approximation of the solution

$$\lambda \simeq \frac{\sum_{\ell>0} \left(\Delta \cdot M_\ell^{(n)} + \varepsilon_\ell K^{R(n)}\right)}{\sum_{\ell>0} K_\ell^{R(n)}} \qquad (A.5)$$

In a subsequent paper[14] we shall indicate how one should choose the energies ε_ℓ, the gap Δ (when one works with the constant G interaction) and the one body Hartree-Fock Hamiltonian $\hat{\mathcal{H}}(\rho)$ (formulae (15) and (21)), to ensure exact conservation of the total energy in a finite time step calculation.

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Table 1. Solutions of the constant G model for $\delta\varepsilon$ = constant.

Range of $\delta = \frac{\delta\varepsilon}{G}$	Solution for $(M_1 - M_o)^*$	m	Period T**	Amplitude of the Oscillations $\delta\rho$
$0 \leqslant \delta \leqslant 4M_o$	$\sim Sd^2\left(\pi \frac{t}{T}\right)$	$\frac{\delta(4M_o - \delta)}{1 - (2M_o - \delta)^2}$	$\frac{2\hbar}{G} \frac{K(m)}{(1 - (2M_o - \delta)^2)^{1/2}}$	$2M_o - \frac{\delta}{2}$
$4M_o \leqslant \delta < 1 + 2M_o$	$\sim Sn^2\left(\pi \frac{t}{T}\right)$	$\frac{\delta(\delta - 4M_o)}{1 - 4M_o^2}$	$\frac{2\hbar}{G} \frac{K(m)}{\left(1 - 4M_o^2\right)^{1/2}}$	$\frac{\delta}{2} - 2M_o$
$\delta = 1 + 2M_o$	$\left(\frac{1}{2} - M_o\right) th^2\left(\frac{G}{\hbar}\left(1 - 4M_o^2\right)^{1/2} t\right)$	1	aperiodic motion	$\frac{1}{2} - M_o$
$\delta > 1 + 2M_o$	$\sim Sn^2\left(\pi \frac{t}{T}\right)$	$\frac{1 - 4M_o^2}{\delta(\delta - 4M_o)}$	$\frac{2\hbar}{G} \frac{K(m)}{(\delta(\delta - 4M_o))^{1/2}}$	$\frac{1 - 4M_o^2}{2\delta}$

*For the definitions of the functions Sd and Sn see Ref. 11. The solutions are only given for the positive values of δ since the results for the couples of parameters (δ, M_o) and $(-\delta, -M_o)$ are identical (interchange of the role of levels 1 and 2).

**The quantity K(m) is the complete elliptic integral of the first kind $K(m) = \int_0^{\pi/2} (1 - m \cdot \sin^2\Theta)^{-1/2} \, d\Theta$.

Figure Captions

Fig. 1. The dependence of the period T (in 10^{-22} sec) and the amplitude of oscillations $\delta\rho$ on the initial filling ρ_o in the case of two parallel levels distant by: δE = 1.5 MeV (case a) and δE = 3 MeV (case b). The solid lines correspond to the constant G = 1 MeV coupling. The dashed lines to the constant Δ = 1 MeV coupling.

Fig. 2. The dependence of the final filling ρ_f on the initial one ρ_i for two considered couplings: constant Δ = 0.5 MeV (case a) and constant G = 1 MeV (case b). The velocity in both cases is equal a = $0.4 \cdot 10^{22}$ MeV sec^{-1}. The hatched areas correspond to the dispersion zones: $\bar{\rho}_f \pm \sigma$. The solid lines correspond to the average values $\bar{\rho}_f$.

Fig. 3. The dependence of the final filling ρ_f on the velocity a for constant G = 1 MeV coupling (solid lines) and constant Δ = 0.5 MeV coupling (dashed lines). The initial fillings ρ_i are: 0.01 in G coupling and 0 in Δ coupling (case a) and correspondingly 0.99 and 1 (case b). The dots indicate the average values $\bar{\rho}_f$ and the error bars the dispersion $\pm\sigma$.

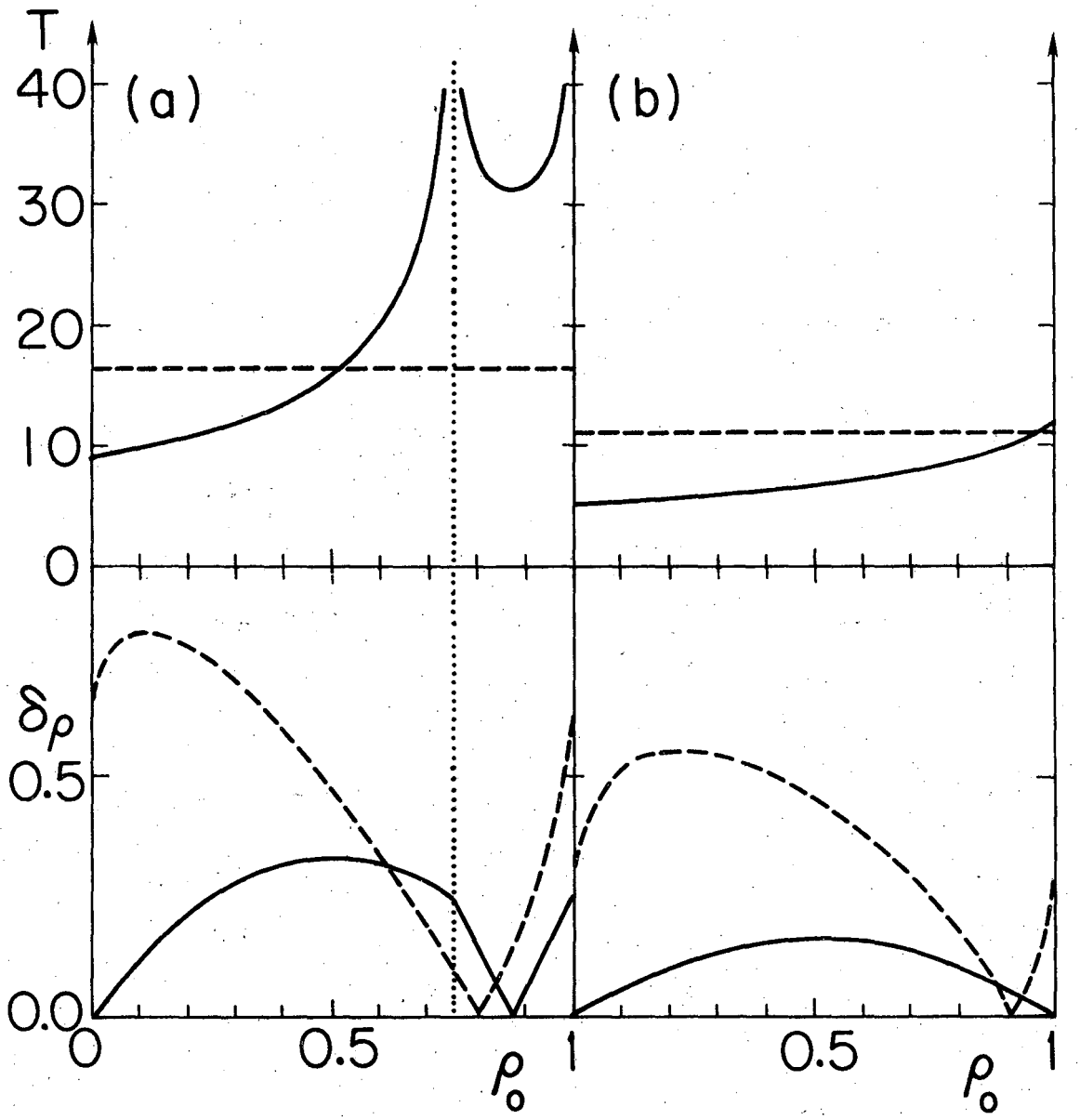

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Fig. 1

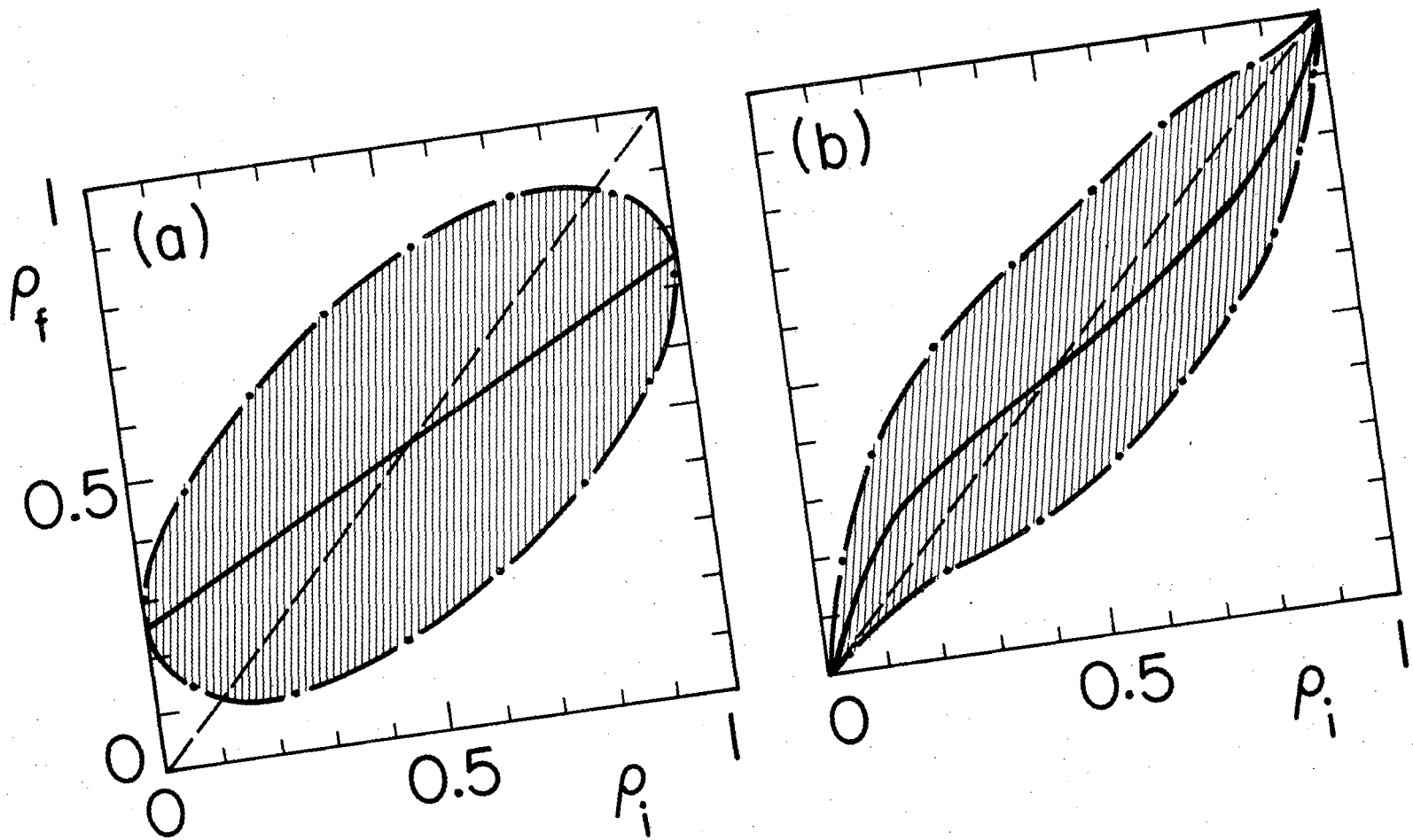

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Fig. 2

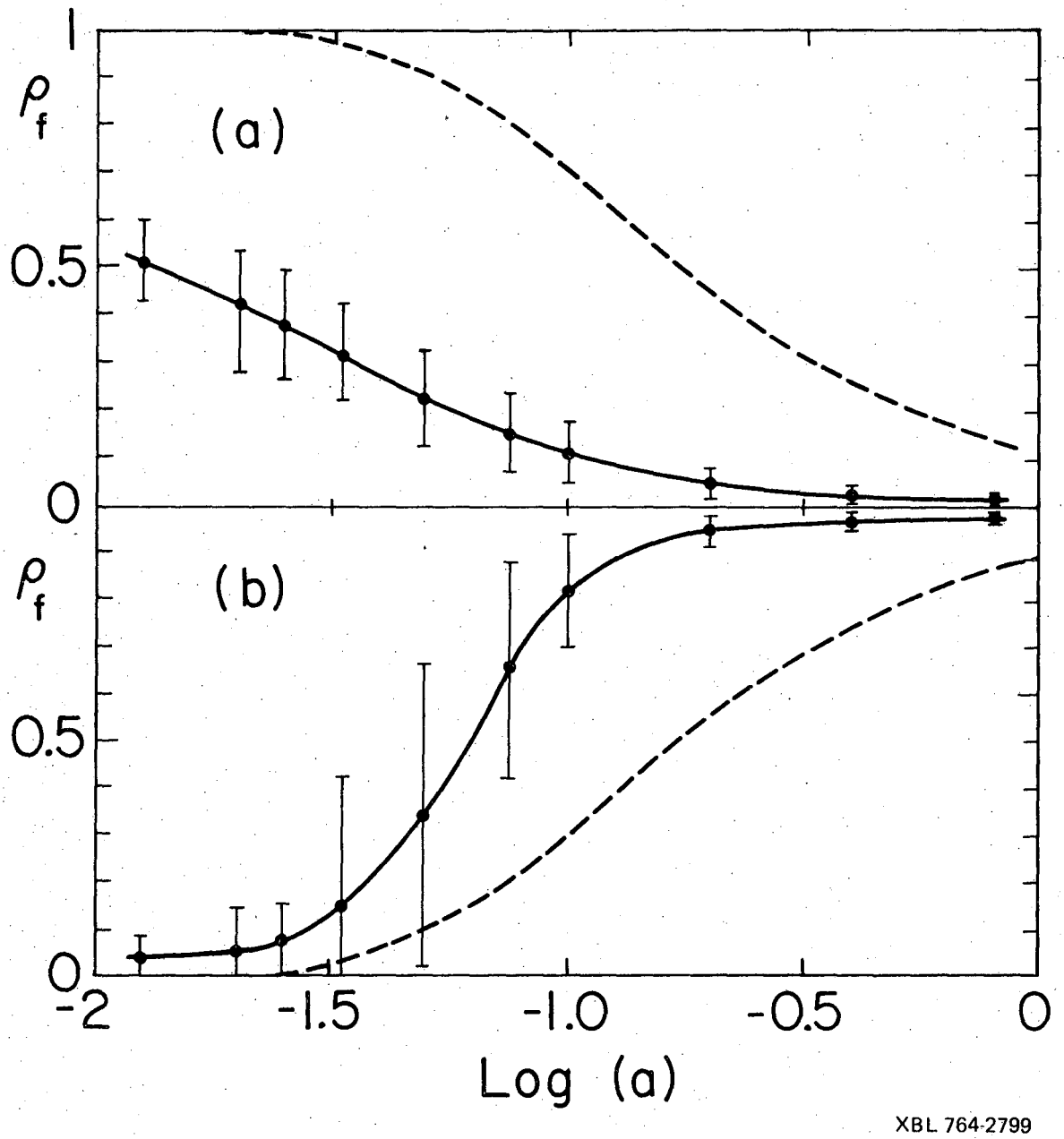

Fig. 3

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