Nonlinearity versus Perturbation Theory in Quantum Mechanics

the particle-particle Coulomb interaction

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There are basically two "*simple*" (i.e. with classical fields: =/= QED) ways of quantum-mechanically describing Coulomb interaction between, say, two electrons confined in the 2d parabolic potential $V(x,y) = V(r) = M\omega^2 r^2/2$ with $r^2 = x^2 + y^2$ inside the vertical slab of height H_z (*quantum-dot helium*) .

i) ***<u>either</u>*** the Coulomb solution $\Phi(\underline{x}) = e^2 \int \frac{|\Psi(\underline{x}')|^2}{|\underline{x} - \underline{x}'|} d^2 \underline{x}'$ of the *classical* differential Poisson equation $\nabla^2 \Phi = -4\pi (e^2 / H_z) |\Psi|^2$ including the **mean-field source term** $|\Psi|^2$ is explicitly present in the single-particle Schrödinger equation for Ψ in addition to *V(r)* :

$$-\frac{\hbar^2}{2M}\nabla^2\Psi(r)+\left[V(r)+e^2\int\frac{|\Psi(\underline{x}')|^2}{|\underline{x}-\underline{x}'|}d^2\underline{x}'\right]\Psi(r)=E\ \Psi(r)$$

We consider the stationary case for the sake of simplicity; e.g. two opposite-spin electrons: cf. Pauli.

Common *2d* orbital wavefunction Ψ («*orbital bosons*»). Nonlinear eigenvalue *E* : *chemical potential*.

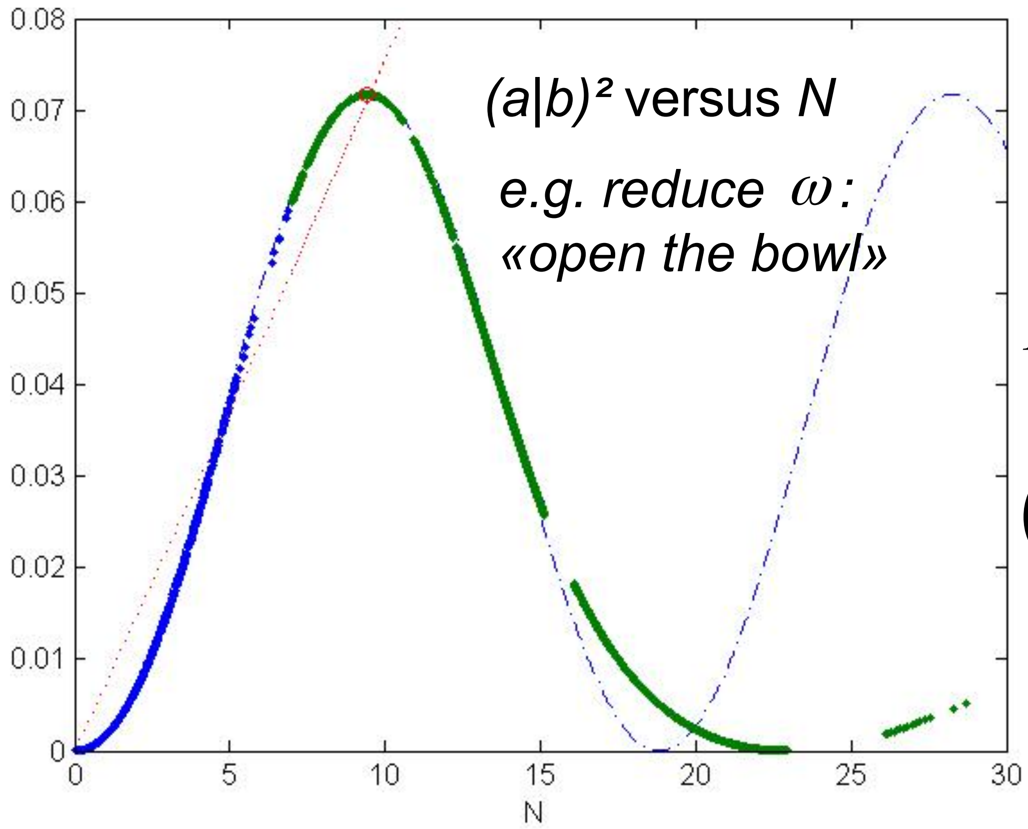
Then the resulting integrodifferential equation is **implicit**. Hence iterative perturbation series about orthogonal base elements to get an **approximate** converging definition of the Schrödinger wavefunction Ψ &/or search of the variational minimum of the corresponding energy functional.

ii) ***<u>or</u>*** the Poisson equation $\nabla^2\Phi = -4\pi(e^2/h_z)|\Psi|^2$ is (at least numerically) formally coupled to the Schrödinger equation

$$-\frac{\hbar^2}{2M}\nabla^2\Psi(r,t) + \left[V(r) + \Phi(r,t)\right]\Psi(r,t) = E\ \Psi(r)\ .$$

This nonlinear Schrödinger-Poisson (SP) <u>differential</u> system yields (though only numerically...) the **explicit** mean-field solution Ψ **without any approximation.** Moreover it also yields **excited states** (=/= case (i)).

<u>Non-orthogonality</u> of the nonlinear eigenstates, say |*a)* & |*b),* yields **<u>quantum coherence</u>** => ***interference*** between the eigenstates ***<u>without</u>*** superposition!



Nonlinearity $\propto$ N :

$$N = \frac{2e^2 / H_z}{\hbar\omega} \propto \| \, |a) \, \|^2 = \| \, |b) \, \|^2$$

$$\left(a \,|\, b\right) = \frac{1}{N}\int_0^\infty \Psi^*{}_a(r)\Psi_b(r)\; 2\pi r dr$$

<u>Dashed</u>:

$$\left(a \,|\, b\right) = -0.2678 \sin\left(\frac{N}{6}\right) ;$$

note: $\pi\sqrt{\alpha}$=0.2684 ,

α=1/137.036 .

In $S_{2d}P_{2d}$ we had $\sqrt{\pi}\sqrt{\alpha}$

vs $\pi\sqrt{\alpha}$ for $S_{2d}P_{3d}$ here.

technically…

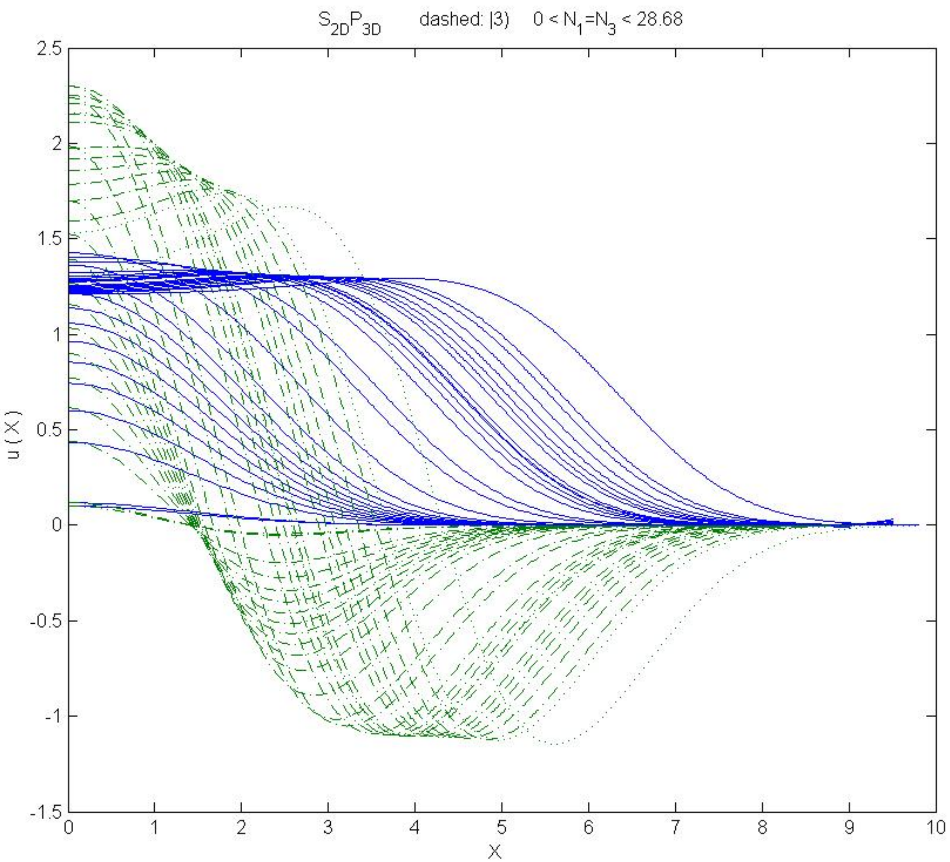
Consider the stationary SP system with two opposite-spin electrons => « orbital bosons » (cf. Pauli).

In appropriate dimensionless units (*2d* radial symmetry with angular momentum *m*), it becomes ($\tilde{E} = E/\hbar\omega$):

$$u'' + \frac{1}{X}u' + \left[\tilde{E} - \tilde{\Phi} - \frac{m^2}{X^2} - \frac{X^2}{4}\right]u = 0\ , \qquad u = \sqrt{\frac{2\pi e^2}{M\omega^2}}\ \Psi$$

$$\tilde{\Phi}'' + \frac{2}{X}\tilde{\Phi}' + u^2 = 0\ ; \qquad X = r/\sqrt{\frac{\hbar}{2M\omega}}\ ;$$

$$\int_0^\infty |\Psi|^2 2\pi r dr = 1 \Leftrightarrow \int_0^\infty u^2 X dX = \frac{2e^2/H_z}{\hbar\omega} = N\ .$$



We want eigenstate **non-**orthogonality. Therefore:

$m_a = m_b$ (selection rule).

Indeed inner product due to polar angle φ yields (radial symmetry):

$$m_a \neq m_b \Rightarrow \int_0^{2\pi} e^{i(m_b - m_a)\varphi} d\varphi = 0$$

$$\Rightarrow (a \,|\, b) = 0 \;.$$

|*a*) : ground eigenstate $n_a = 0;\; m_a = 0$ (continuous)

|*b*) : 1rst excited eigenstate $n_b = 1;\; m_b = 0$ (dashed)

$n_{a,b}$ main quantum numbers: number of nodes.

$u \propto \sqrt{N}\ \Psi$: $\mathrm{N} \to 0 \Rightarrow u << 1$: quasilinear !

cf. Poisson: $\tilde{\Phi}_E'' + \frac{2}{\mathrm{X}}\tilde{\Phi}_E' + u_E^{\,2} \approx \tilde{\Phi}_E'' + \frac{2}{\mathrm{X}}\tilde{\Phi}_E' = 0$ if $u << 1$;

Theorem (*J. Bec, OCA 2010*)

$$\left(a\,|\,b\right) = \frac{W_{ab}}{E_a - E_b} \quad \text{where} \quad W(X) = \Phi_a(X) - \Phi_b(X) \ \text{ and}$$

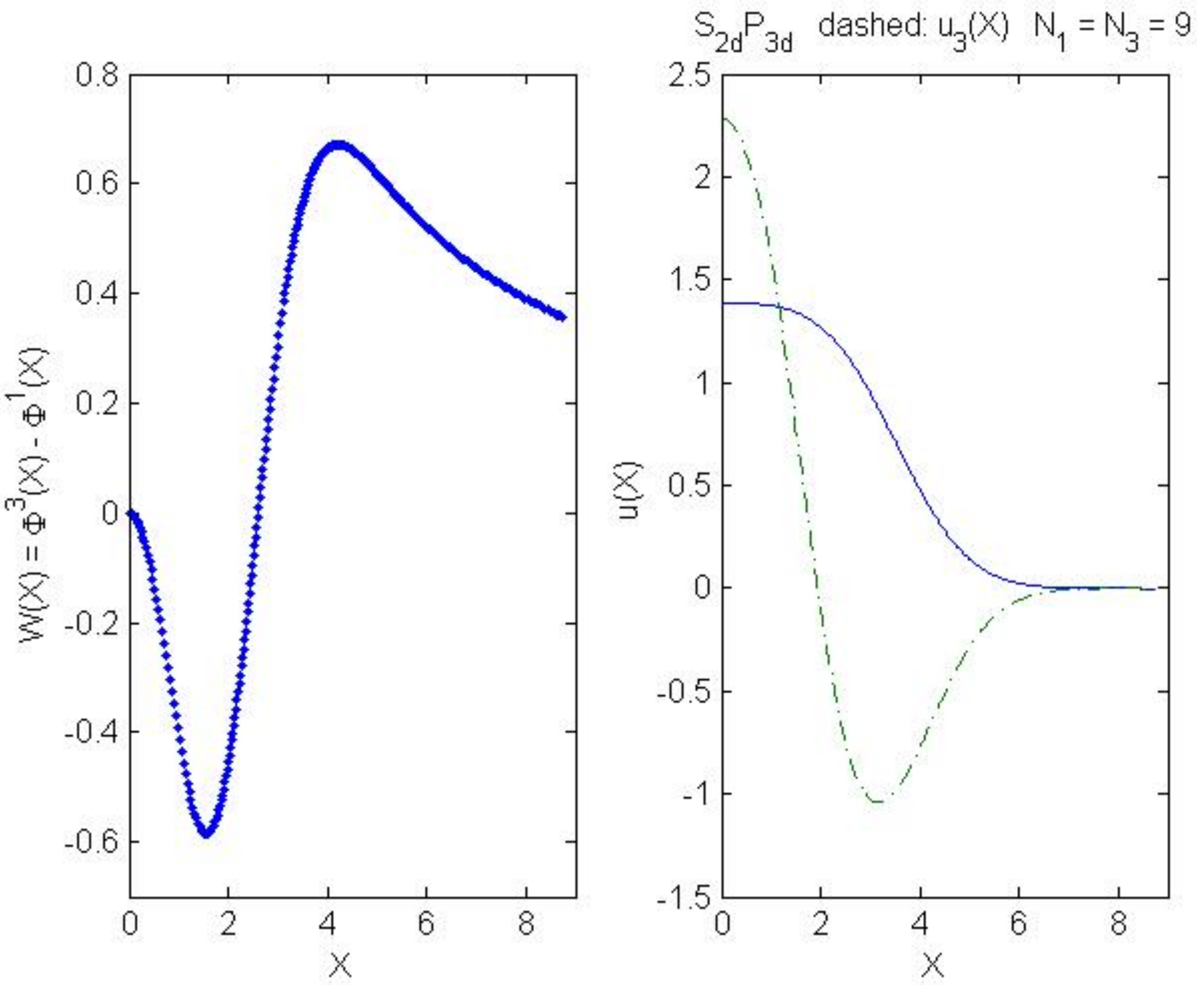
$W_{ab} = \left(a\,|\,W\,|\,b\right)$; potential $\Phi_{a,b}$ is resp. defined by ${u_{a,b}}^2$ through Poisson equation.

Consider the Schrödinger equation for *|a)* :

$$u_a'' + \frac{1}{X}u_a' + \left[\tilde{E}_a - \tilde{\Phi}_a - \frac{X^2}{4}\right]u_a = 0$$; add « perturbation » *W* :

$$u'' + \frac{1}{X}u' + \left[\tilde{E}_a - \tilde{\Phi}_a - \frac{X^2}{4} + W\right]u \;=\; u'' + \frac{1}{X}u' + \left[\tilde{E}_a - \tilde{\Phi}_b - \frac{X^2}{4}\right]u \;=\; 0\,;$$

« Perturbation » *W* exchanges the respective Coulomb potentials. Therefore *u* is no more eigenstate !



X>9 => W(X) ~ 1/X (Coulomb).

(a | b) is an invariant …

$u_f = \hat{K}_W(t_f, t_i)\, u_i \;\; ; \;\; u_i = |a) \;\; ; \;\; u_f \neq |b)$ a priori !

pb : $\left|\left(b \,|\, u_f\right)\right|$ when $W = \Phi_a - \Phi_b$?

$$i\hbar \frac{\partial}{\partial t} u = \left[\tilde{H}_{W\equiv 0} + \tilde{W}\right] u \;\;\Rightarrow\;\; i\hbar \frac{\partial}{\partial t_f} \hat{K}_W = \left[\tilde{H}_{W\equiv 0} + \tilde{W}\right] \hat{K}_W \;,$$

$$\Rightarrow \;\hat{K}_W(t_f; t_i) = \hat{K}_{W\equiv 0}(t_f; t_i) - i\hbar \int_{t_i}^{t_f} dt \left[\hat{K}_{W\equiv 0}(t_f; t)\; \tilde{W} \hat{K}_W(t; t_i)\right] \;.$$

<u>exact</u> but <u>implicit</u> !

Lowest-order in W: $\hat{K}_W \approx \hat{K}_{W\equiv 0}$ in the integral:

$$\hat{K}_W(t_f; t_i) = \hat{K}_{W\equiv 0}(t_f; t_i) - i \int_{t_i}^{t_f} dt \left[\hat{K}_{W\equiv 0}(t_f; t)\; \tilde{W} \hat{K}_{W\equiv 0}(t; t_i)\right] + o(W^2) + o(W^4) + \ldots$$

$$\hat{K}_{W\equiv 0}(t_f;t_i) = e^{-i\tilde{E}_a(t_f-t_i)} \quad ; \quad \hat{K}_{W\equiv 0}(t;t_i) = e^{-i\tilde{E}_a(t-t_i)} \quad ;$$

$$\hat{K}_{W\equiv 0}(t_f;t) = e^{-i\tilde{E}_b(t_f-t)}$$

Remind: $\hat{K}_W(t_f;t_i) = \hat{K}_{W\equiv 0}(t_f;t_i) - i\int_{t_i}^{t_f} dt \left[\hat{K}_{W\equiv 0}(t_f;t)\ \tilde{W}\hat{K}_{W\equiv 0}(t;t_i)\right] + o\left(\tilde{W}^2\right) + o\left(\tilde{W}^4\right)...$

and $\left(b\,|\,u_f\right) = \left(b\,|\,\hat{K}_W(t_f,t_i)\ u_i\right) = \left(b\,|\,\hat{K}_W(t_f,t_i)\,|\,a\right)$. Therefore, since $W \equiv W(X)$:

$$\left(b\,|\,u_f\right) = e^{-i(t_f-t_i)\tilde{E}_a}\ \left(b\,|\,a\right) - i\tilde{W}_{ab}e^{i\left(\tilde{E}_a t_i - \tilde{E}_b t_f\right)}\int_{t_i}^{t_f} dt \left[\ e^{i\left(\tilde{E}_b - \tilde{E}_a\right)t}\ \right] + o\left(\tilde{W}^2\right) + \ ...$$

Theorem: $\tilde{W}_{ab} = \left(a\,|\,b\right)\left(\tilde{E}_a - \tilde{E}_b\right)$. Defining $T = t_f - t_i$ & $\tau = \frac{1}{2}\left(\tilde{E}_b - \tilde{E}_a\right)T$:

$$\left|\left(b\,|\,u_f\right)\right| = \left|e^{-i\tilde{E}_a T}\left(1 - 2ie^{-i\tau}\sin\tau\right)\right|\ \left|\left(a\,|\,b\right)\right| + o\left(a\,|\,b\right)^2 + o\left(a\,|\,b\right)^4 + ...$$

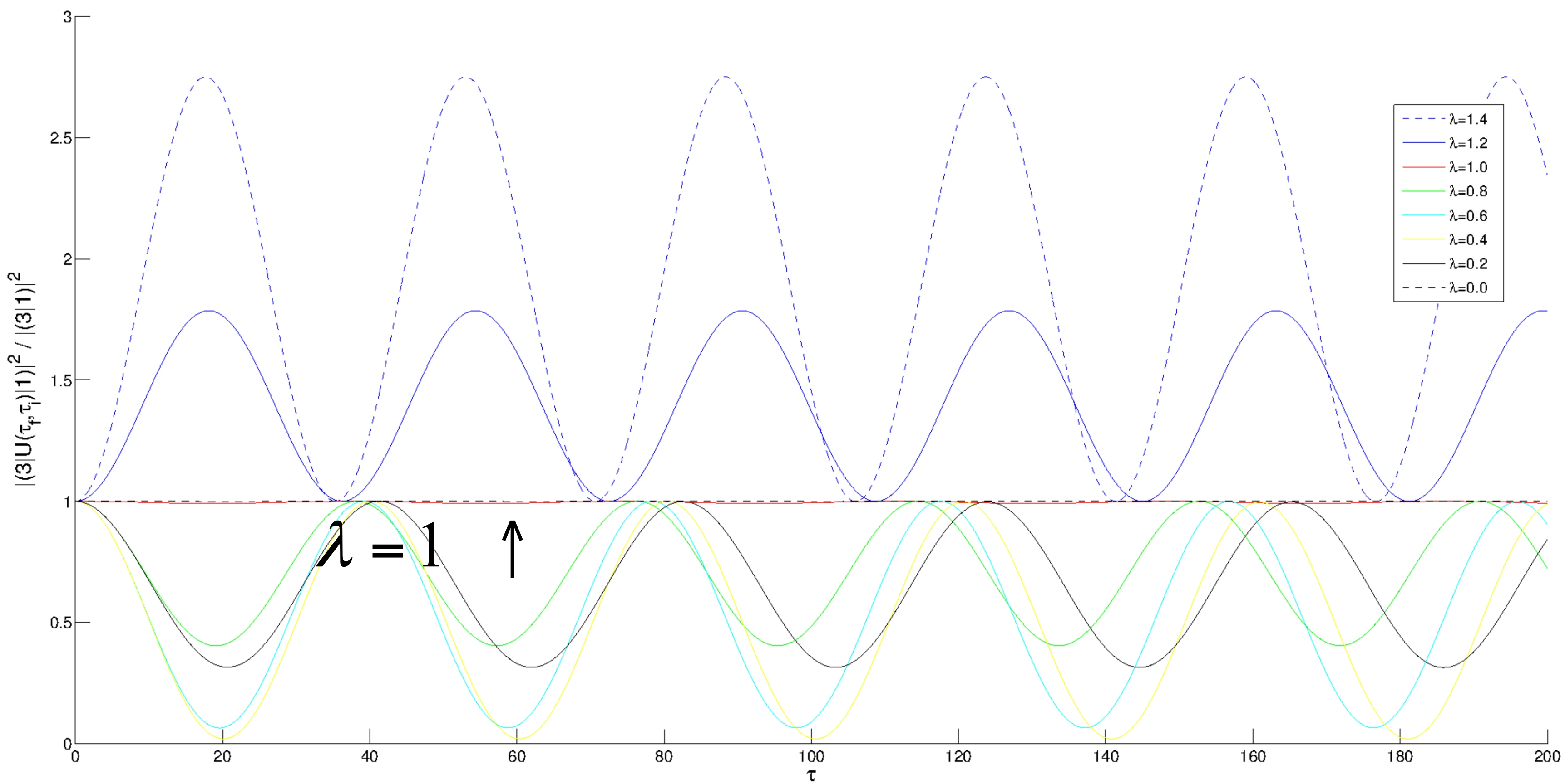
$$\left|\left(1 - 2ie^{-i\tau}\sin\tau\right)\right| \equiv 1\ ! \quad \Rightarrow \quad \left|\left(b\,|\,u_f\right)\right| = \left|\left(a\,|\,b\right)\right| + o\left(a\,|\,b\right)^2 + o\left(a\,|\,b\right)^4 + ...$$

$$\left|\left(\ b\,|\,u(\mathrm{X,t})\ \right)\right| = \left|\left(a\,|\,b\right)\right| + o\left(a\,|\,b\right)^2 + o\left(a\,|\,b\right)^4 + ...$$

$$= \mathrm{cste} + o\left(a\,|\,b\right)^2 + o\left(a\,|\,b\right)^4 + ... \neq \text{Golden Rule}$$

We plot $\left|\left(b\,|\,u(\mathrm{X},\mathrm{t})\right)\right| / \left(a\,|\,b\right)$ versus time for $\tilde{W}^0 = \lambda\left(\tilde{\Phi}_a^0 - \tilde{\Phi}_b^0\right)$:

(C. Besse & G. Dujardin: 2013 U. Lille1 & INRIA-Lille)



Probability of finding the 2-level nonlinear SP system in its excited state |b) is constant in time and equal to (a|b) if starting in g.s. |a) !

La mécanique quantique,c'est le plus bel outil que l'homme a créé pour marquer son territoire entre le zéro de la matière et l'infini de sa conscience…

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<u>Refs</u>:

G. Reinisch & V. Gudmundsson, *Eur. Phys. J. B* **84**, 699 (2011)
G. Reinisch & V. Gudmundsson, *Physica D* **241**, 902 (2012)
G. Reinisch, V. Gudmundsson & A. Manolescu, *Physics Letters A* **378**, 1566 (2014)
V. Gudmundsson, S. Hauksson, A. Johnsen, G. Reinisch, A. Manolescu, C. Besse, & G. Dujardin, *Annalen der Physik*, May 2014 (in press)