Cooper Pairing in "Exotic" Fermi Superfluids: An Alternative Approach

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Lecture 3

In lecture 2 we saw that for any "completely paired" N (= even) -- particles GS

$$\Psi_{No} = \mathcal{N}\left(\sum_n c_n a_n^+ a_{\bar{n}}^+\right)^{N/2} |vac\rangle$$

$\rightarrow$ MF Hamiltonian $\rightarrow$ BdG equations.

$\rightarrow$ (simplest) $N+1$ (= odd) particle energy eigenstates in form $\gamma_i^\dagger|\Psi_{No}\rangle$.

So, BdG equations tell us (directly) about neither the even-parity nor the odd-parity states, but about the relation between even- and odd-parity states. Does the converse hold, *i.e.* is an arbitrary set of solutions to the BdG equations (with Δ_{ij} self-consistently determined) guaranteed to correspond to a possible Ψ_{No}? Delicate point, for the moment assume yes.

Majorana fermions (MF's) (within textbook approach)

Definition: A MF is a solution $\gamma_o^\dagger$ of the BdG equations for $\hat{H}_{MF}$ ← mean-field

which has

(a) $E = 0$

(b) $u_0(r) = v_0^*(r)$ and thus $\gamma_0^\dagger \equiv \gamma_0$

(c) $u(r), v(r)$ localized in space

Notes:

(1) $(b) \Longrightarrow (a)$, since if $\begin{pmatrix} u \\ v \end{pmatrix}$ is a solution of the BdG equations with eigenvalue ϵ.

then * $\begin{pmatrix} v^* \\ u^* \end{pmatrix}$ is a solution with eigenvalue $-\epsilon$.

(2) The condition (c) excludes *e.g.* excitations exactly at the nodes of the gap in a d-wave superconductor.

(3) The condition (a) is equivalent to

$$[\hat{H} - \mu\hat{N}, \gamma_0^\dagger] = E\gamma_0^\dagger = 0$$

* We derive this for $\begin{pmatrix} -v * \\ u * \end{pmatrix}$ but the overall phase of v can be arbitrarily changed by π by a similar change in Δ (which has no physical consequences).

What is a Majorana fermion? Let's suppose it is a regular fermion, that is, it creates (in the standard approach) a zero-energy eigenstate of the odd-parity system. In that case it must be expressible as a linear combination of the α_m^+'s and $\alpha_{\bar{m}}^+$'s of lecture 2:

$$\gamma_o^\dagger = \sum_m (c_{mo}\alpha_m^+ + d_{mo}\alpha_{\bar{m}}^+)$$

where (in the PC representation)

$$\alpha_m^+ \equiv u_m a_m^+ - v_m^* a_{\bar{m}} \,, \quad \alpha_{\bar{m}}^+ \equiv u_m a_{\bar{m}}^+ + v_m^* a_m$$

Writing $\gamma_o^\dagger = \gamma_o$ and equating coefficients of the linearly independent operators a_m^+, $a_{\bar{m}}^+$, we find for each m

$$c_{mo}u_m = d_{mo}^* v_m^*, \quad c_{mo}v_m^* = -d_{mo}^* u_m$$

which have no solution. Thus, $\gamma_o^\dagger$ cannot create a pure zero-energy odd-parity state. (Also follows from $\gamma_o^2 = 1$ not 0)

However, at this point we realize the condition

$$[H - \mu N, \gamma_o^\dagger] = o$$

has two possible interpretations:

1. $\gamma_o^\dagger$ creates a fermionic excitation with zero energy

2. $\gamma_o^\dagger$ is a pure annihilator, $\gamma_o^\dagger|\Psi_N\rangle = 0$

We have just seen that (1) by itself is impossible, and a similar argument shows that (2) by itself is impossible. But a superposition of (1) and (2) is perfectlypossible!

Thus,

the Majorana fermion is simply a quantum superposition of the creation operator for a zero-energy fermion and a pure annihilator.

In the literature this statement is more familiar in the inverted form: given two M.F.'s γ_1, γ_2, one can always combine them in the form $\frac{1}{2}(\gamma_1 + i\gamma_2) \equiv d_o^+$ to form a zero-energy fermion creation operator ($d_o \equiv \frac{1}{2}(\gamma_1 - i\gamma_2)$ is a pure annihilator). And, fortunately, M.F.'s are guaranteed to always occur in pairs...

How much of this follows in a PC approach? We can still define zero-energy fermions $\left(\alpha_o^+ = \sum_m c_{mo} a_m^+ + d_{mo} a_{\bar{m}} \hat{C}^\dagger\right)$ and the corresponding PA's, but the Majoranas are now no longer self-conjugate $\left(\gamma^\dagger \sim \int u_o(r)\psi^\dagger(r) + v_o(r)\psi(r)\,\hat{C}^\dagger\right) \neq \gamma_o$. Hence some "intuitive" features may not be preserved...

Illustration: an (ultra-)toy model

Consider N (= even) spinless fermions which can occupy

a) a "bath" of states which need not be specified in detail, or

b) two specific sites 0, 1 ("system").

We use a notational convention such that wherever the number of particles in the "system" changes by +2 (–2), the operator C ($C^{\dagger}$) is applied to the bath so as to conserve particle number. Then the effect of the bath is to supply to the effective (BdG-type) Hamiltonian of the system a term of the form

$$\Delta a_0^{\dagger} a_1^{\dagger} + \mathrm{H.C.}$$

There will also be in general a "tunneling" term, of the form

$$t a_0^{\dagger} a_1^{\dagger} + \mathrm{H.C.}$$

and a term of the form $U_0 a_0^{\dagger} a_0 + U_1 a_1^{\dagger} a_1$, which we will set = 0. Let's make the special choice

$$\Delta = it$$

and measure energies in units of t. Then

$$\hat{H}_{BdG} = \left(a_1^{\dagger} a_0 - i a_1^{\dagger} a_0^{\dagger} \right) + \mathrm{H.C.}$$

The GS is easily found to be

$$\psi_{\circ} = \tfrac{1}{\sqrt{2}} \left(1 + i a_1^{\dagger} a_0^{\dagger} \right) \left| vac \right\rangle$$

or more accurately

$$\psi_{\circ} = \tfrac{1}{\sqrt{2}} \left(1 + i a_1^{\dagger} a_0^{\dagger} \hat{C} \right) \left| vac \right\rangle$$

where (vac) = (no particles in system, N in bath).

Illustration: an (ultra-)toy model (cont.)

Consider now the linear combinations of the operators

$$a_0^\dagger, a_1^\dagger, a_0, a_1$$

The operators

$$\hat{\Omega}_1 \equiv \tfrac{1}{\sqrt{2}}\left(a_1^\dagger - ia_0\right), \hat{\Omega}_2 \equiv \left(a_0^\dagger + ia_1\right)$$

are pure annihilators. The operator

$$\hat{\Pi}_1 \equiv \tfrac{1}{2}\left(a_1^\dagger + ia_0 - a_0^\dagger + ia_1\right)$$

when acting on ψ_o creates the "+" state $\psi_+ = \tfrac{1}{\sqrt{2}}\left(a_1^\dagger + a_0^\dagger\right)\left|vac\right\rangle$ with energy 1 and the operator

$$\hat{\Pi}_2 \equiv \tfrac{1}{2}\left(a_1^\dagger + ia_0 - a_0^\dagger + ia_1\right)$$

creates the "–" state $\psi_- = \tfrac{1}{\sqrt{2}}\left(a_1^\dagger - a_2^\dagger\right)\left|vac\right\rangle$ The state ψ_- has zero energy relative to the GS.

The 2 MF's are linear combinations of the pure annihilators and the zero-energy DB fermion state ψ_-:

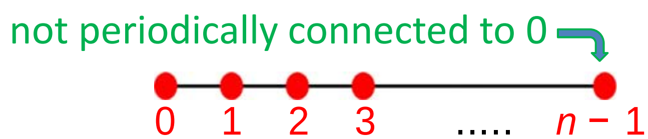
$$\hat{M}_0 \equiv -\hat{\Pi}_- + \hat{\Omega}_1 + \hat{\Omega}_2 = a_0^\dagger - ia_0$$

$$\hat{M}_1 \equiv +\hat{\Pi}_- + \hat{\Omega}_1 + \hat{\Omega}_2 = a_1^\dagger + ia_1$$

and are each localized on a single site.

Slightly less trivial model (Kitaev 1D quantum wire)

Consider a linear array of n sites (the "system") coupled to a large superfluid "bath", so that there are N ($> n$) particles in total. In the mean-field approximation the most general Hamiltonian of the system has the form, for nearest-neighbour coupling only.



$$\hat{H} = \sum_{i=0}^{n-1} U_i a_i^\dagger a_i - \sum_{i=1}^{n-1}\left(t_i a_{i-1}^\dagger a_i + \text{H.C.}\right) + \sum_{i=1}^{n-1}\left(\Delta_i a_{i-1}^\dagger a_i^\dagger + \text{H.C.}\right)$$

↳ can contain μ ↳ $\times\hat{C}$

Let us make the very special choice

$$U_i = 0, \Delta_i = -it_i \leftarrow \equiv -iX_i$$

Then the Hamiltonian becomes

$$\hat{H} = -\sum_{i=1}^{n-1} X_i \hat{K}_i$$

where

$$\hat{K}_i \equiv \left(a_{i-1}^\dagger + ia_{i-1}\right)\left(a_i + ia_i^\dagger\right)$$

Note:

a) $\hat{K}_i$ Hermitian

b) $\hat{K}_i^2 = 1$

c) $\hat{K}_i$'s mutually commuting

d) $\prod_{i=0}^{n-1}\hat{K}_i$ = number parity

$\Rightarrow$ GS must satisfy $\hat{K}_i|\psi_\circ\rangle = |\psi_\circ\rangle, i = 1, 2, \ldots, n-1$

$$E_\circ = -\sum_{i=1}^{n-1} X_i$$

Slightly less trivial model (cont.)

Explicit form of GSWF is

$$\left|\psi_\circ\right\rangle = \mathcal{N}\cdot\prod_{i=1}^{n-1}\left(1+\hat{K}_i\right)\left|\text{vac}\right\rangle$$

e.g. for *n* = 4,

$$\left|\psi_\circ\right\rangle = N\cdot\left\{\begin{aligned}&1+i\left(a_0^\dagger a_1^\dagger + a_1^\dagger a_2^\dagger + a_2^\dagger a_3^\dagger - a_0^\dagger a_2^\dagger - a_1^\dagger a_3^\dagger + a_0^\dagger a_3^\dagger\right)\left(\times\hat{C}\right)\\&-a_0^\dagger a_1^\dagger a_2^\dagger a_3^\dagger\left(\times\hat{C}^2\right)\end{aligned}\right\}\left|\text{vac}\right\rangle$$

Note entanglement without interaction!

Note: The GSWF of the whole "universe" (system + bath) can be written in the form $\Psi_\circ = \left(\hat{\Lambda}+\hat{C}\right)^{N/2}$ where $\hat{\Lambda} \equiv \Sigma_{l=1}^{n/2} c_l \alpha_l^\dagger \alpha_{\bar{l}}^\dagger$ $\left(\alpha_l^\dagger \equiv \Sigma_i q_{li} a_i^\dagger\right)$ but it is not entirely trivial to determine the constants* c_l and q_{lj}.

*For *n* = 4 the solution is

$$\alpha_1^\dagger = \tfrac{1}{2}\sum_{j=0}^{3} e^{ij\pi/4} a_j^\dagger,\ \alpha_{\bar{1}}^\dagger = \tfrac{1}{2}\sum_{j=0}^{3} e^{-ij\pi/4} a^\dagger,\ \alpha_2^\dagger = \tfrac{1}{2}\sum_{j=0}^{3} e^{3ij\pi/4} a_j^\dagger,$$

$$\alpha_{\bar{2}}^\dagger = \tfrac{1}{2}\sum_{j=0}^{3} e^{-3ij\pi/4} a^\dagger,\ c_1 = i\left(1-\sqrt{2}\right),\ c_2 = -i\left(1+\sqrt{2}\right)$$

Slightly less trivial model (cont.)

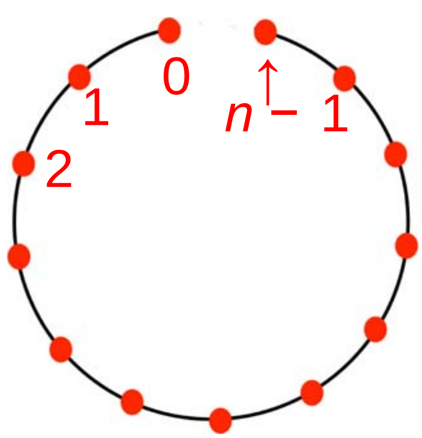
However, we are still missing one DB creation operator and one pure annihilator. Clearly these have to be associated with the “missing” link $(n-1)$–0. In fact, consider

$$\hat{\Pi}_\circ \equiv \tfrac{1}{2}\left[\left(a_{n-1}^\dagger + ia_{n-1}\right) + \left(a_0^\dagger - ia_0\right)\right]$$

This may be verified explicitly to create an $(N+1)$-particle energy eigenstate which is degenerate with the groundstate.

$$\hat{M}_\circ \equiv \tfrac{1}{\sqrt{2}}\left(\hat{\Pi}_\circ + \hat{\Omega}\right) = \tfrac{1}{\sqrt{2}}\left(a_{n-1}^\dagger + ia_{n-1}\right)$$

The corresponding pure annihilator is



$$\hat{\Omega}_\circ \equiv \tfrac{1}{2}\left[\left(a_{n-1}^\dagger + ia_{n-1}\right) - a_0^\dagger - ia_0\right].$$

If now we consider the operators

$$\hat{M}_\circ \equiv \tfrac{1}{\sqrt{2}}\left(\hat{\Pi}_\circ + \hat{\Omega}\right) = \tfrac{1}{\sqrt{2}}\left(a_{n-1}^\dagger + ia_{n-1}\right)$$

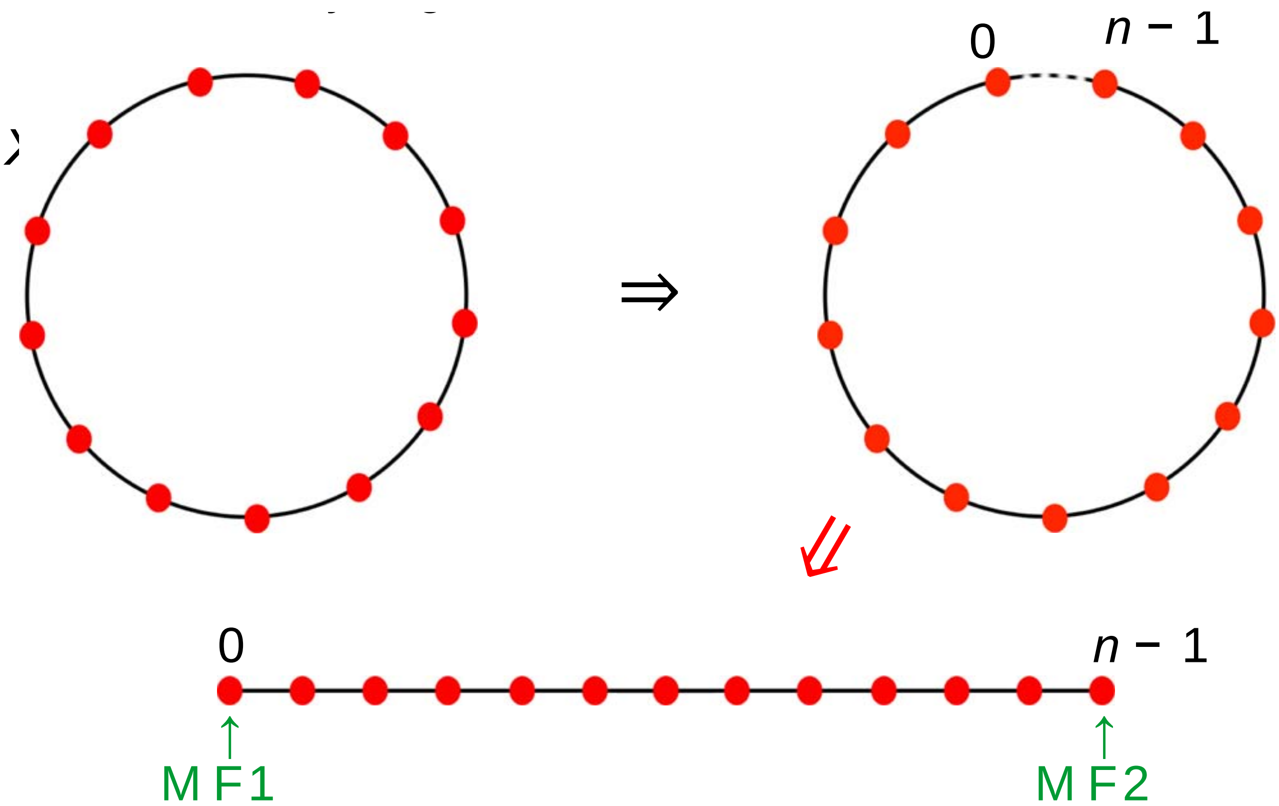
$$\hat{M}_n \equiv \tfrac{1}{\sqrt{2}}\left(\hat{\Pi}_\circ - \hat{\Omega}\right) = \tfrac{1}{\sqrt{2}}\left(a_0^\dagger - ia_0\right)$$

these generate Majorana fermions localized on sites $n-1$ and 0 separately.

Slightly less trivial model (cont.)

An intuitive way of generating MF's in the KQW:

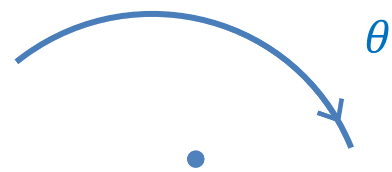
Kitaev quantum wire



[Variations on KQW – *T*-junctions etc.]

A more realistic example: vortex in a $p + ip$ superfluid

Consider the fermionic states in the case of an Abrikosov vortex, $r \ll \lambda$ but $\sim\xi$ (so magnetic effects negligible $\Rightarrow$ equivalent to neutral superfluid).



(1) For the s-wave case

$$\widehat{\mathrm{H}_0} u(r) + \Delta(r) v(r) = E u(r) \quad \text{(etc.)}$$

with

$$\Delta(r) \sim \exp i\theta$$

Hence if $u(r) \sim \exp i\ell_u\theta$ and $v(r) \sim \exp i\ell_{\mathrm{v}}\theta$,

$$\ell_u - \ell_v = 1$$

So u and v cannot be complex conjugates $\Longrightarrow$ no Majoranas (all E nonzero, Caroli et al. 1964)

(2) For $p + ip$ case

$$\hat{H}_o u(r) + \int \Delta(r, r')v(r')dr' = Eu(r) \qquad \text{(etc.)}$$

but $\Delta(r, r'\,) = \exp i\varphi_R\,(x \pm iy)_\rho \quad (\boldsymbol{R} \equiv \text{COM}, \boldsymbol{\rho} \equiv \text{rel.})$

So $v -$ term is $\cong$

$$\exp - i\varphi(r)\big(\partial_x \pm i\partial_y\big)v(r)$$

but $\partial_x - i\partial_y \equiv e^{-i\theta}\left(\frac{\partial}{\partial r} + \frac{i}{r}\frac{\partial}{\partial \theta}\right)$,

so "effective" $\ell_\Delta = 0$ or 2

$\Rightarrow$ in either case,

$$\ell_u - \ell_v = \text{even}$$

$\Rightarrow \ell_u = -\ell_v$ is allowed $\Rightarrow u$ and v can be complex conjugates

$\Rightarrow$ Majoranas can (and must*) exist

Now $\exists$ a topological theorem: in a $p + ip$ superfluid, either number of vortices is even or $\exists$ a "Majorana-hosting" singularity on boundary. Hence $(p + ip)$ system with $2n$ vortices tolerates n zero-energy fermions.

*Kopnin & Salomaa 1991

Reminders on (Abelian) Berry phases

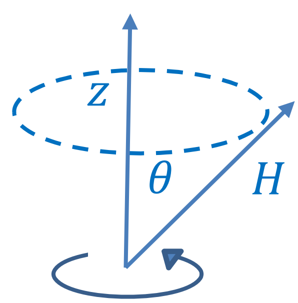
Suppose the wave function Ψ (single-particle/MB) is a junction of some control parameter, $\Psi = \Psi(\lambda)$, and λ is swept adiabatically around a closed loop and returned to its original value.

Then

$$\varphi_B \equiv i \oint \Psi^*(\lambda) \frac{d\Psi}{d\lambda} d\lambda$$

($\equiv Im \oint \Psi^*(\lambda)\, d\Psi(\lambda)/d\lambda$, since $\Psi(\lambda)$ normalized)

Standard textbook example: particle of spin ½ in tilted magnetic field which is rotated around z-axis.



We need to choose an appropriate form of spinor wave function $\binom{\alpha}{\beta}$, $\alpha, \beta \equiv f(\theta, \varphi)$, $|\alpha|^2 + |\beta|^2 = 1$. The unique criterion for a correct choice is that it gets e.v.'s $\langle\sigma_z\rangle = \cos\theta$, $\langle\sigma_x\rangle = \sin\theta\cos\varphi$, $\langle\sigma_y\rangle = \sin\theta\sin\varphi$ correct. One standard choice is $\alpha = \left(\cos\frac{\theta}{2}\right) e^{i\varphi/2}$, $\beta = \left(\sin\frac{\theta}{2}\right) e^{-i\varphi/2}$, but it is clear that multiplication by any overall factor $\exp i\zeta(\varphi)$, $\zeta(\varphi)$ real, will leave the e.v.'s unchanged, so convenient to require α and β to be single-valued functions of φ ("monodromy"). Thus

$$\alpha = \cos\theta/2$$
$$\beta = \sin\theta/2 \exp - i\varphi$$

Note singularity on negative z-axis

Then

$$\varphi_B = i\int_{o}^{2\pi} d\varphi\left\{\alpha^*(\varphi)\frac{d\alpha}{d\varphi} + \beta^*(\varphi)\frac{d\beta}{d\varphi}\right\} = \int_{o}^{-2\pi} \sin^2\frac{\theta}{2}\,d\varphi$$

↑ O

$$= \pi(\cos\theta - 1)$$

$$\left(= -\frac{1}{2}\left(\equiv \frac{1}{2}\text{area on unit sphere "swept out" by } H\right)\right)$$

Note:

(a) for $\theta = \pi/2$ reproduces sign change of spinor wave function under 2π rotation

(b) had we taken a different "monodromic" choice, $\alpha = \cos\theta/2\exp i\varphi$, $\beta = \sin\theta/2$, we would have got

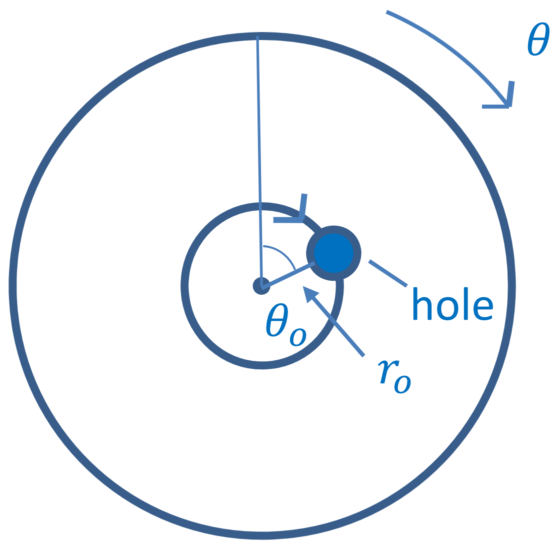
$$\varphi'_B = \pi(1 + \cos\theta) \equiv \varphi_B + 2\pi \sim \varphi_B$$

(c) had we taken an arbitrary $\zeta(\varphi)$, we would have got an extra term

$$i\int \exp - i\zeta(\varphi)\frac{d}{d\varphi}\exp i\zeta(\varphi)d\varphi = \zeta(2\pi) - \zeta(0)$$

But must then subtract out an equal and opposite term ("monodromy phase")

Another example, this time involving orbital wave function: single (Schrödinger) particle moving in potential $V(r)$ which is cylindrically symmetric except for "hole" at distance r_o from origin. Hole is moved adiabatically so as to "encircle" origin.



What Berry phase (if any) is picked up?

Crucial point: $\psi(|r|, \theta : \theta_o) = \psi(|r| : \theta - \theta_o)$. Hence,

$$\varphi_\beta \equiv i \int_o^{2\pi} \left(\psi(\theta_o) \frac{d\psi}{d\theta_o} d\theta_o = \int_o^{2\pi} \left(\psi(\theta_o), -i \frac{d}{d\theta} \psi\,(\theta_o)\right) d\theta_o \equiv 2\pi \langle L_z \rangle\right.$$

$\uparrow$ $\hat{L}_z \psi$

Hence, if particle is not in eigenstate of $\hat{L}_z$, *e.g.*

$$\psi = a\psi_s + b\psi_p$$

then

$$\varphi_\beta = 2\pi |b|^2$$

nontrivial!

Note: surprisingly, result is independent both of "strength" of potential and of r_o, provided both are nonzero.