特別演習B B23

調和型二次元量子ドットに閉じ込められた少数電子系のスピン多重度不安定性

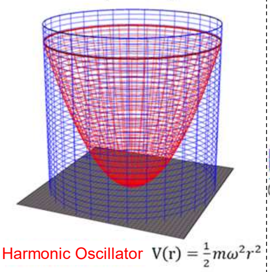
Instability in spin multiplicity for few electrons confined in the two-dimensional harmonic system

量子材料学研究（武田京三郎研究室）藤原大地 (Fujiwara Daichi)

Waseda University

Introduction

Two-dimensional GaAs quantum dot (2DQD)

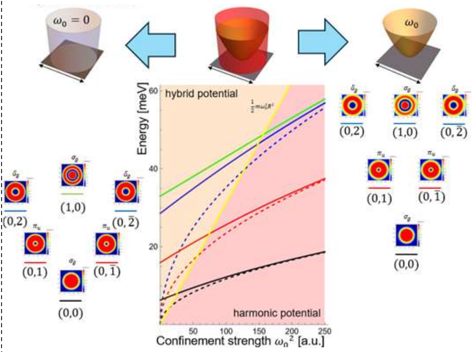


Harmonic Oscillator $V(r)=\frac{1}{2}m\omega^2r^2$

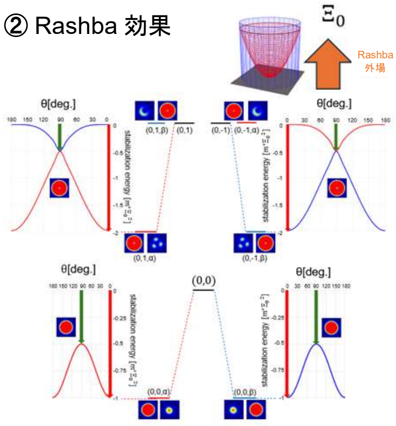
+

Hard Wall

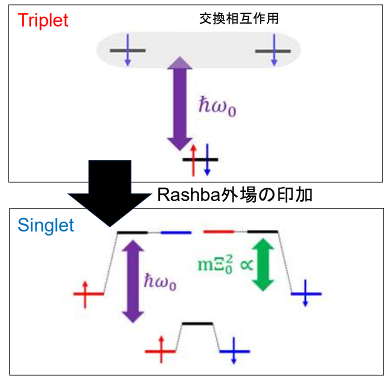
① 閉じ込め強度



② Rashba 効果



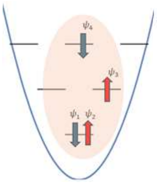
③ Singlet-Triplet 不安定性



Theoretical treatment

① Generalized UHF

Slater



$$\Psi(\tau_1,\ldots,\tau_4)=\frac{1}{\sqrt{4!}}\begin{vmatrix}\psi_1(\tau_1) & \psi_1(\tau_2) & \psi_1(\tau_1) & \psi_1(\tau_4)\\ \psi_2(\tau_1) & \psi_2(\tau_2) & \psi_2(\tau_1) & \psi_2(\tau_4)\\ \psi_3(\tau_1) & \psi_3(\tau_2) & \psi_3(\tau_3) & \psi_3(\tau_4)\\ \psi_4(\tau_1) & \psi_4(\tau_2) & \psi_4(\tau_3) & \psi_4(\tau_4)\end{vmatrix}$$

UHF

$$\mathscr{H}=\sum_i^4\mathscr{H}_0(r_i)+\sum_j^4\sum_{i>j}^4\frac{1}{r_{ij}}$$

$$\psi_i(\tau_j)=\phi_i(r_j)\alpha(\sigma_j)\quad or\quad \phi_i(r_j)\beta(\sigma_j)$$

Rashba スピン軌道相互作用

スピン混成

GUHF

$$\mathscr{H}=\sum_i^4\mathscr{H}_0(r_i)+\sum_j^4\sum_{i>j}^4\frac{1}{r_{ij}}+\sum_i^4\mathscr{H}_R(r_i)$$

スピノル表示

$$\psi_i(\tau_j)=\phi_i^\alpha(r_j)\alpha(\sigma_j)+\phi_i^\beta(r_j)\beta(\sigma_j)$$

全エネルギー

$$\langle E\rangle=\left\langle\Psi\middle|\hat{\mathscr{H}}\middle|\Psi\right\rangle=I+R+J-K$$

$$I=\sum_i^4\left\langle\psi_i(r_i)\middle|\hat{\mathscr{H}_0}(r_i)\middle|\psi_i(r_i)\right\rangle$$ 運動およびポテンシャルエネルギー $\propto \omega_0$

$$R=\sum_i^4\left\langle\psi_i(r_i)\middle|\hat{\mathscr{H}_R}(r_i)\middle|\psi_i(r_i)\right\rangle$$ Rashba効果 $\propto \Xi_0^2$

$$J=\sum_i^4\sum_{j>i}^4\left\langle\phi_i(\tau_1)\phi_j(\tau_2)\middle|\frac{1}{r_{12}}\middle|\phi_i(\tau_1)\phi_j(\tau_2)\right\rangle$$ クーロン相互作用 $\propto\sqrt{\omega_0}$

$$K=\sum_i^4\sum_{j>i}^4\left\langle\phi_j(\tau_1)\phi_i(\tau_2)\middle|\frac{1}{r_{12}}\middle|\phi_i(\tau_1)\phi_j(\tau_2)\right\rangle$$ 交換相互作用 $\propto\sqrt{\omega_0}$

規格化条件

$$\langle\psi_i|\psi_j\rangle=\delta_{ij}\qquad E'=\langle E\rangle-\sum_i^N\sum_j^N\varepsilon_{ij}(\langle\psi_i|\psi_j\rangle-\delta_{ij})$$

＋ 変分原理

$$\frac{\delta E'}{\delta\psi_i}=0$$

GUHF 方程式

Fock演算子

$$\hat{F}\psi_i=\varepsilon_i\psi_i$$

$$\hat{\mathscr{H}}_0(\boldsymbol{r}_i)=-\frac{\hbar^2}{2m^*}\nabla^2_{\boldsymbol{r}_i}+\frac{1}{2}m^*\omega_0^2|\boldsymbol{r}_i|^2$$

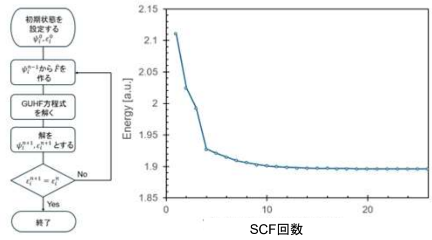
$$\hat{\mathscr{H}}_R(\boldsymbol{r}_i)=\boldsymbol{\sigma}\cdot(\boldsymbol{\Xi}_z\times\hat{\boldsymbol{p}}_i)$$

$$\hat{J}^t\phi_i^s(\tau_1)=\sum_{j=1}^N\int\phi_j^{t*}(\tau_2)\phi_j^{t}(\tau_2)\frac{1}{r_{12}}d\tau_2\phi_i^s(\tau_1)$$

$$\hat{K}^{st}\phi_i^s(\tau_1)=\sum_{j=1}^N\int\phi_j^{s*}(\tau_2)\phi_i^{s}(\tau_2)\frac{1}{r_{12}}d\tau_2\phi_j^t(\tau_1)$$

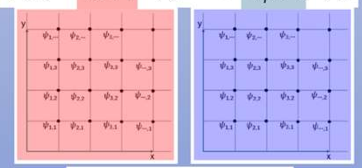
$$\begin{pmatrix}\hat{\mathscr{H}}_0+(\hat{J}^\alpha+\hat{J}^\beta-\hat{K}^{\beta\beta})+\hat{\mathscr{H}}_R^z & \hat{K}_j^{\beta\alpha}+\hat{\mathscr{H}}_R^+\\ \hat{K}_j^{\alpha\beta}+\hat{\mathscr{H}}_R^- & \hat{\mathscr{H}}_0+(\hat{J}^\alpha+\hat{J}^\beta-\hat{K}^{\beta\beta})+\hat{\mathscr{H}}_R^z\end{pmatrix}\begin{pmatrix}\phi_i^\alpha\\ \phi_i^\beta\end{pmatrix}=\varepsilon_i\begin{pmatrix}\phi_i^\alpha\\ \phi_i^\beta\end{pmatrix}$$

② SCF法



③ 実空間差分法

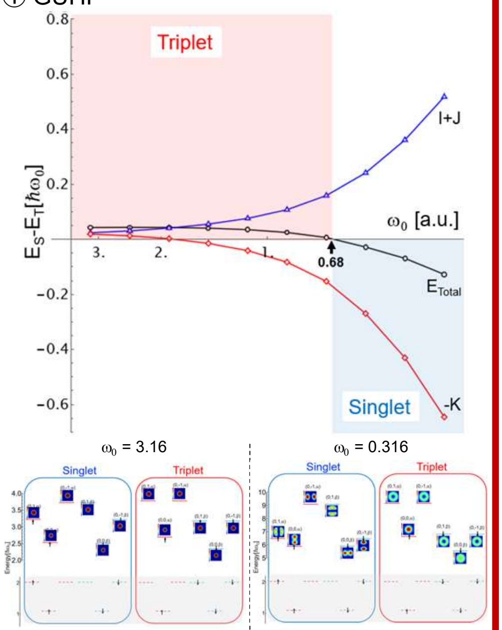
$$\psi(\tau)=\phi_\alpha(r)\alpha(s)\;+\;\phi_\beta(r)\beta(s)$$



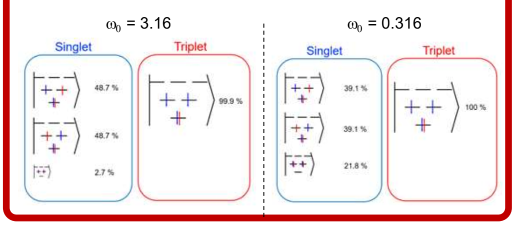
$$\frac{d^2}{dx^2}f(x)=\frac{f(x+\Delta x)+f(x-\Delta x)-2f(x)}{\Delta x^2}$$

閉じ込め強度依存性

① GUHF

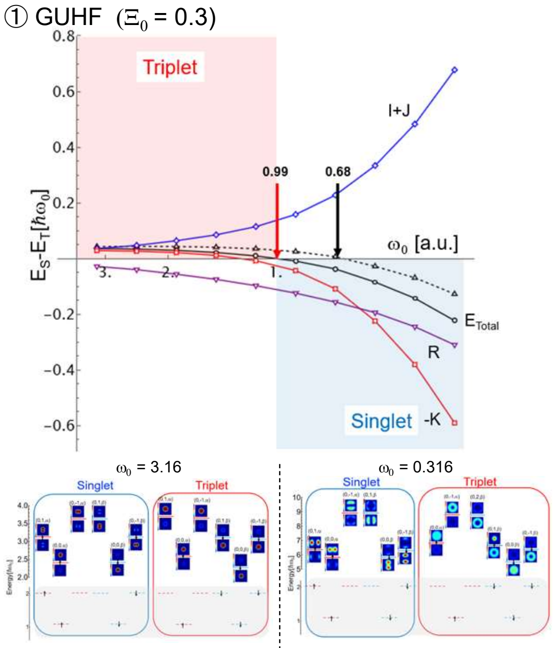


② Heitler・London法



Rashba外場印加

① GUHF (Ξ_0 = 0.3)



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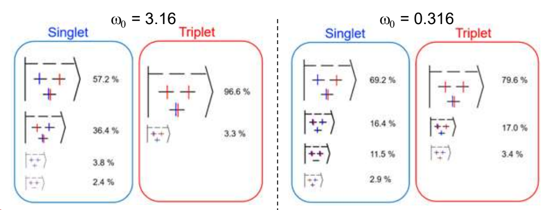

③ 無次元化 GUHF

$$\hat{F}(\boldsymbol{r})=\hat{\mathscr{H}}_0(\boldsymbol{r})+\sum_j^N(\hat{J}_j(\boldsymbol{r})-\hat{K}_j(\boldsymbol{r}))+\hat{\mathscr{H}}_R(\boldsymbol{r})$$

Normalized Fock operator

interelectron interaction: direct term, exchange term; SOI term driven by Rashba field

$$\hat{F}^{nd}(\boldsymbol{z})=\hat{\mathscr{H}}_0^{nd}(\boldsymbol{z})+\mu[J^{nd}(\boldsymbol{z})-K^{nd}(\boldsymbol{z})]+\lambda\hat{\mathscr{H}}_r^{nd}(\boldsymbol{z})$$

normalized parameters

$$\mu=\frac{1}{a_0^*}\sqrt{\frac{\hbar}{m^*\omega_0}}\qquad\lambda=\sqrt{\frac{m^*\Xi_0^2}{\hbar\omega_0}}$$

$$\mu\propto\sqrt{\frac{1}{\omega_0}}\qquad\gamma=\frac{\lambda}{\mu}\propto\Xi_0$$

generalization in material choice