Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
**MINIWORKSHOP ON**
**QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS**
**30 JUNE - 11 JULY 1997**
and
**CONFERENCE ON**
**QUANTUM SOLIDS AND POLARIZED SYSTEMS**
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# "QMC methods for systems with complex-valued states"

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Miniworkshop on Quantum Monte Carlo

Simulations of Liquids and Solids

30 June - 11 July 1997

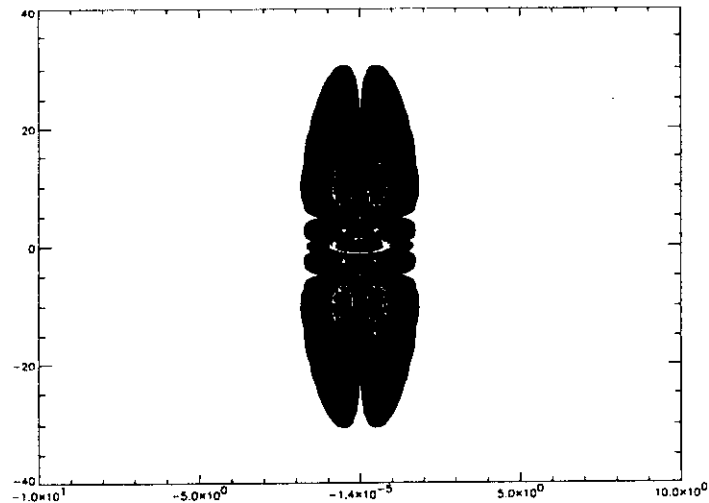International Center for Theoretical Physics

Trieste-Italy

LECTURE NOTES on

QMC methods for systems with complex-valued states

by

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Lecture I:

QUANTUM MONTE CARLO FOR COMPLEX-VALUED STATES I:
## FIXED-PHASE CONSTRAINT

Lecture II:

QUANTUM MONTE CARLO FOR COMPLEX-VALUED STATES II:
## RELEASING THE CONSTRAINT

# Astrophysical Applications

- **Some Compact Stellar Remnants Undergo Flux Compression**
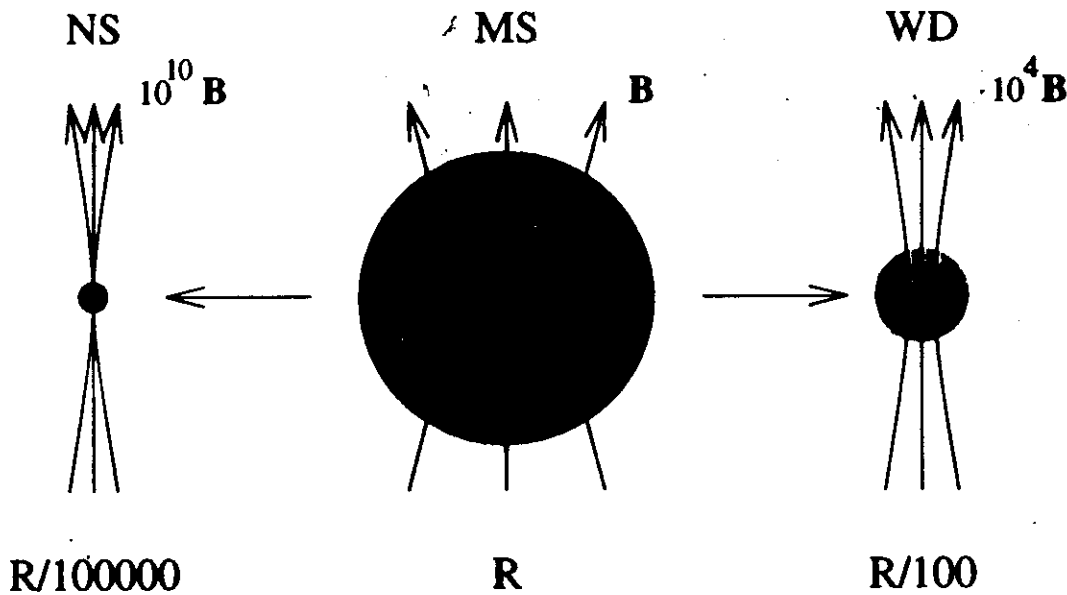


- ○ Main Sequence (MS) $R \simeq 10^{11}$ cm, $B \simeq 10^2$ G
- ○ White Dwarf (WD) $R \simeq 10^9$ cm, $B \simeq 10^6$ G
- ○ Neutron Star (NS) $R \simeq 10^6$ cm, $B \simeq 10^{12}$ G

- **Stellar High Magnetic Field Laboratories**

  - ○ Observed White Dwarf Stars with Fossil Fields $B \gtrsim 10^8$ G
  - ○ Neutron Stars with $B \gtrsim 10^{12}$ G
  - ○ Anomalous Magnetized White Dwarf Spectra (GD229)

$\beta_z = B/B_0 Z^2$

$B_0 = 4.7 \times 10^9$ G

| H⁻ | He | Li | C | System |
|---|---|---|---|---|
| 2.5 | 1.0 | 0.3 | 0.26 | $\beta_z$ |
| $(-1,+,-1)$ | $(-1,+,-1)$ | $(-1,-,-3/2)$ | $(-2,+,-3)$ | |
| 1.0 | 0.7 | 0.2 | 0.2 | |
| $(-1,+,-1)$ | $(-1,+,-1)$ | $(-1,-,-3/2)$ | $(-2,+,-3)$ | |
| 0.1 | 0.5 | 0.12 | 0.18 | |
| $(-1,+,-1)$ | $(-1,+,-1)$ | $(-1,+,-1/2)$ | $(-2,+,-2)$ | |
| 0.03 | 0.1 | 0.03 | 0.01 | |
| $(-1,+,-1)$ | $(-1,+,-1)$ | $(-1,+,-1/2)$ | $(-2,+,-2)$ | |
| 0.01 | 0.07 | 0.007 | 0.003 | |
| $(0,+,0)$ | $(0,+,0)$ | $(0,+,-1/2)$ | $(-1,-,-1)$ | |
| 0 | 0 | 0 | 0 | $\beta_z$ |
| | | | | $\rho(x,z)$ |
| $(0,+,0)$ | $(0,+,0)$ | $(0,+,-1/2)$ | $(-1,-,-1)$ | $(L_z,\pi_z,S_z)$ |

GROUND STATES

-4-
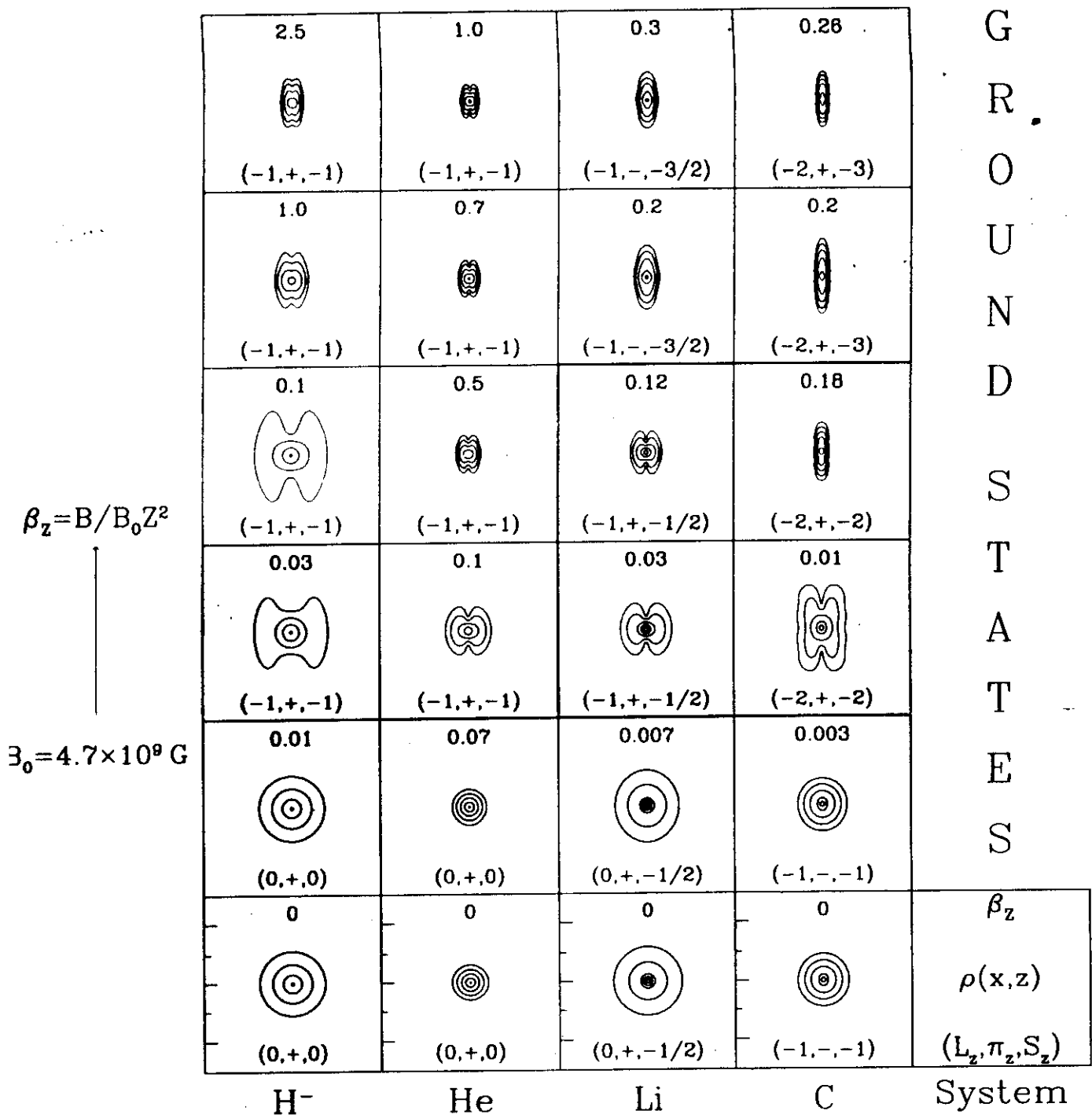
# Solid State Applications

- **Excitons in Semiconductors with Large Dielectric Constants**

$$\widehat{\mathbb{H}} = -\nabla^2 - \frac{2\mu}{m^* r} + 2\beta^* \left( \frac{m_h - m^*}{m_h + m^*} \right) L_z + \beta^{*2}(x^2 + y^2)$$

$$\mathrm{Ry}^* = (m^*/m\epsilon^2)\mathrm{Ry}, \quad \beta^* = \beta(m\epsilon/m^*)^2, \quad \beta = B/4.701 \times 10^9 \, \mathrm{G}$$

- o **Effective mass of electron, $m^*$, hole, $m_h$**
- o **For $m_h \gg m^*$, recover Hamiltonian for magnetized hydrogen**
- o **InSb: $m^* = .013m$, $\epsilon = 16$, $\beta^* = 1.5 \times 10^6 \beta$**

- **Other Systems:**

  - o **Quantum Dots**
  - o **NHMFL Initiative to Achieve Sustainable B $\geq 10^2$ T**

Lecture I

"In search of a stable stochastic solution free
from the **Fermi demon**"

## A) Statement of the problem

## B) Constraining the configuration (state) space :

— General quantum mechanical formulation

— Fermions in the euclidean continuum:

Applications:

Broken time reversal symmetry:

- Fractional QHE: fluid-solid transtion

- Normal Matter in superstrong magnetic fields

Excitations:

- Vortices in boson superfluids

— Fermions in curved space-time:

Applications:

- (Dirac) monopole-particle problem

- Fractional QHE on the sphere: energy gaps

## C) Constraining the Slater-determinant (state) space:

— General auxiliary-field formulation

— Lattice Fermions:

Applications:

- Hofstadter-type problems

"Trying to live with the **demon**"

## A) Improving a given phase function

— Cumulant expansion

Applications:

- Vortex problem revisited·

## B) Releasing the Constraints: → "exact"

— General quantum mechanical formulation

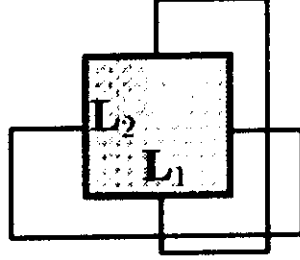— Ground and excited states of a given symmetry

Applications:

- Understanding the optical spectra of compact stellar remnants: Atoms and Molecules in astrophysical conditions

# The Fixed-Phase Method

GS properties of a 2D quantum system in a **B**-field

**—System:**



$N$-fermions of mass $m^*$

on a flat torus $\mathbf{L_1} \wedge \mathbf{L_2}$

$$\widehat{\mathbb{H}} = \sum_{i=1}^{N} \frac{\mathbf{\Pi}_i^2}{2m^*} + \sum_{i>j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \Lambda \quad (\widehat{\mathbb{H}} = \widehat{\mathbb{H}}^\dagger)$$

$$\mathbf{\Pi}_i = \mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i) \; ; \mathbf{B} = \nabla \wedge \mathbf{A} \; ; \text{and} \begin{cases} \mathbf{A}(\mathbf{r}) = (-By,\, 0) & \text{Landau} \\ \mathbf{A}(\mathbf{r}) = (-By/2,\, Bx/2) & \text{Symmetric} \end{cases}$$

$$\left[\widehat{\mathbb{H}}; \widehat{K}\right] \neq 0 \quad (\widehat{K} : \text{time} - \text{reversal}) \quad \Longrightarrow \quad \Psi \in \mathbb{C}$$

**—Hydrodynamic Eqs.:** Reformulation of the eigenvalue problem.

$$E\left[|\Psi|; \varphi\right] = \frac{\left\langle \Psi \left| \widehat{\mathbb{H}}\, \Psi \right\rangle\right.}{\langle \Psi | \Psi \rangle} \quad,$$

where $\Psi(\mathcal{R}) = |\Psi| \exp\left[i\varphi\right] \in \mathcal{L}^2(\mathbb{R}^{2N})$ and $\mathcal{R} \in \mathbb{R}^{2N}$

From $\delta E = 0 \Longrightarrow \begin{cases} \mathfrak{Re} \left\{ \exp\left[-i\varphi\right]\left(\widehat{\mathbb{H}} - E\right)\Psi \right\} = 0 \\ \\ \mathfrak{Im} \left\{ \exp\left[-i\varphi\right]\left(\widehat{\mathbb{H}} - E\right)\Psi \right\} = 0 \end{cases}$

or (in atomic units):

$$\begin{cases} \widehat{H} \, |\Psi(\mathcal{R})| \;=\; \left[ \Sigma_{i=1}^{N} \frac{\mathbf{p}_i^2}{2} + V(\mathcal{R}) \right] |\Psi(\mathcal{R})| \;=\; E\,|\Psi(\mathcal{R})| \\[2em] \Sigma_{i=1}^{N} \nabla_i \cdot \left[ |\Psi(\mathcal{R})|^2 \left( \nabla_i\,\varphi(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i) \right) \right] \;=\; 0 \end{cases} ,$$

where the *effective* potential $V(\mathcal{R})$ is given by

$$V(\mathcal{R}) \;=\; \sum_{i>j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{i=1}^{N} \left( \nabla_i\,\varphi(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i) \right)^2 + \Lambda$$

$$\boxed{\widehat{\mathbb{H}}\Psi = E\Psi \;\equiv\; \text{"Hydrodynamic MB Eqs."}}$$

- Interpretation:

    ⊙ Fermion ⟶ Boson Mapping for $|\Psi|$ (The phase $\varphi$ contains the statistics)

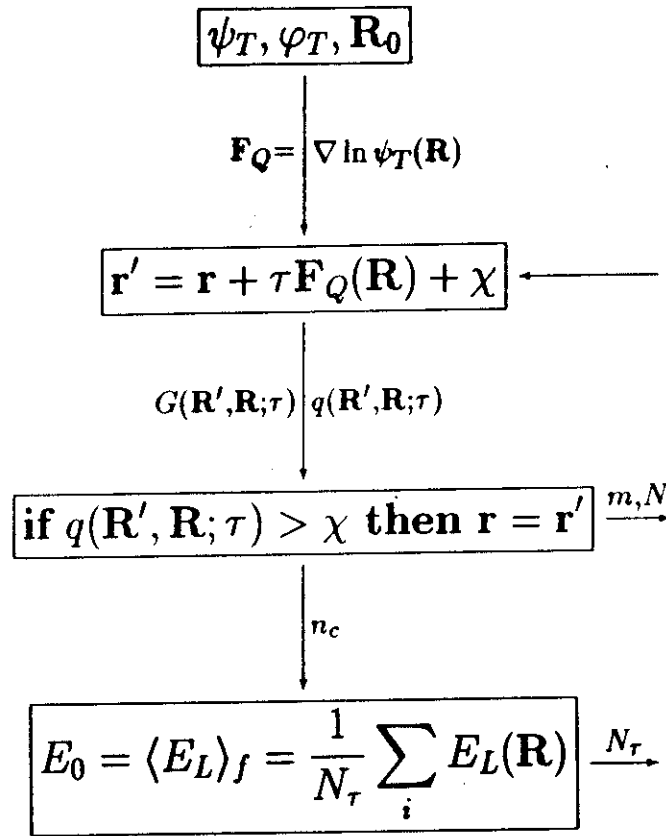    ⊙ "Singular" Gauge Transformation ⟶ fictitious vector potential ($\nabla_i\varphi$)

    —**The Fixed-Phase Method (FPM)**: Two steps:

    1) Make a choice for $\varphi$ ($\varphi_T$).

    2) Solve *exactly* the bosonic problem for $|\Psi|$.

FPM provides a Variational bound for the energy and, for a prescribed trial phase $\varphi_T$,the *lowest* energy consistent with this phase.

# FP Method Schematic

$$\boxed{\psi_T, \varphi_T, \mathbf{R}_0}$$

$\mathbf{F}_Q = \Big| \nabla \ln \psi_T(\mathbf{R})$

$$\boxed{\mathbf{r}' = \mathbf{r} + \tau \mathbf{F}_Q(\mathbf{R}) + \chi} \longleftarrow$$

$G(\mathbf{R}',\mathbf{R};\tau) \Big| q(\mathbf{R}',\mathbf{R};\tau)$

$$\boxed{\text{if } q(\mathbf{R}', \mathbf{R}; \tau) > \chi \text{ then } \mathbf{r} = \mathbf{r}'} \xrightarrow{m,N}$$

$\Big| n_c$

$$\boxed{E_0 = \langle E_L \rangle_f = \frac{1}{N_\tau} \sum_i E_L(\mathbf{R})} \xrightarrow{N_r}$$

## Metropolis acceptance probability

$$A = \min(1, q), \qquad q(\mathbf{R}', \mathbf{R}; \tau) = \frac{|\psi_T(\mathbf{R}')|^2}{|\psi_T(\mathbf{R})|^2} \frac{G(\mathbf{R}, \mathbf{R}'; \tau)}{G(\mathbf{R}', \mathbf{R}; \tau)}$$

## Branching

$$n_c = \mathbf{int} \left[ \exp\left(-\tau(E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T)/2\right) \right]$$

- Remark:

For Real Symmetric Hamiltonians the **FPM** reduces to the *Fixed-Node Method* [*] when we make the choice

$$\varphi = \pi \left[1 - \Theta(\Psi_T)\right] \mod (2\pi)$$

$$\Psi_T > 0 \qquad\qquad \Psi_T < 0$$

$$\pi \mod (2\pi)$$

$$\mathbb{R}^{2N}$$
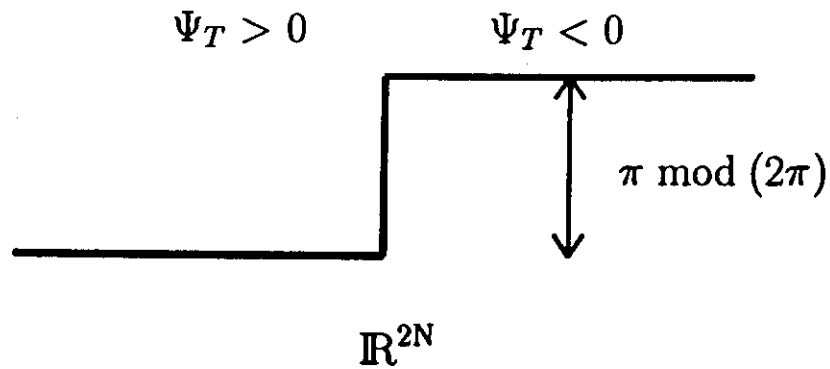
where $\Theta$ is the Heaviside step function.

In this way the Bosonic Eq. is solved in domains of the configuration space where hard wall boundary conditions are imposed. Notice that the "continuity" Eq. is exactly satisfied inside these domains if there is no **B**-field !!

[*] J. B. Anderson $\sim$ 1975

# Exploring the set of phases $\varphi$

## — General criteria:

- Conservation of the group of symmetries of $\widehat{\mathbb{H}}$ (unless some of them are spontaneously broken).

- Physical insight !!

## — Special set of admissible phases:

Consider trial functions of the form

$$\Psi_T(z_1, z_2, \cdots, z_N) = F(\{z_j\}) \exp\left[-\Omega(\{z_j, z_j^*\})\right] \quad ; z_j = x_j + \imath y_j \quad ,$$

where $F(\{z_j\}) \in$ analytic (holomorphic) function of $\{z_j\}$ (i.e., it belongs to the Bargmann space of analytic functions), and

$$\Omega(\{z_j, z_j^*\}) = \begin{cases} \Sigma_{j=1}^N \, y_j^2/2\ell^2 & \text{Landau Gauge} \\ \\ \Sigma_{j=1}^N \, |z_j|^2/4\ell^2 & \text{Symmetric Gauge} \end{cases}$$

These conditions on $\Psi_T$ imply:

$$\nabla_i \cdot \left[|\Psi_T(\mathcal{R})|^2 \left(\nabla_i \, \varphi_T(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)\right)\right] = 0 \quad ,$$
$$\nabla_i \cdot \left(\nabla_i \, \varphi_T(\mathcal{R}) + \mathbf{A}(\mathbf{r}_i)\right) = 0$$

and

$$E_{loc}(\mathcal{R}) = \frac{N}{2\ell^2} + \sum_{i>j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \Lambda \quad .$$

# Solving the Boson Problem on the Torus

We use Stochastic Methods which are based on the observation that the N-particle Schrödinger Eq. in Euclidean time (Wick rotation, $t = i\tau$) can be interpreted as a diffusion and branching process.

<u>For DMC</u>: The master Eq. for the *importance-sampled* distribution $P(\mathcal{R}, t) = |\Psi_T(\mathcal{R})| |\Psi(\mathcal{R}, t)|$ is given by:

$$\frac{\partial P(\mathcal{R}, t)}{\partial t} = \sum_{i=1}^{N} \nabla_i \cdot \left[ \frac{1}{2} \nabla_i P(\mathcal{R}, t) - \mathbf{F}_i(\mathcal{R}) P(\mathcal{R}, t) \right] - (E_{loc}(\mathcal{R}) - E_T) P(\mathcal{R}, t)$$

$$|\Psi_T(\mathcal{R})| \quad \longrightarrow \text{\textit{guide} the random-walk.}$$

$$\mathbf{F}_i(\mathcal{R}) = \nabla_i \ln |\Psi_T| \quad \longrightarrow \textit{drift velocity.}$$

$$E_{loc}(\mathcal{R}) = |\Psi_T|^{-1} \widehat{H} |\Psi_T| \quad \longrightarrow \text{local energy.}$$

- Stochastic dynamics:

$$P(\mathcal{R}', t + \Delta t) = \int d\mathcal{R} \, G(\mathcal{R} \to \mathcal{R}', \Delta t) P(\mathcal{R}, t) \quad ,$$

$G(\mathcal{R} \to \mathcal{R}', \Delta t)$ : Multiparticle Green's function.

- Asymptotic distribution:

$$P(\mathcal{R}, t \to \infty) \to |\Psi_T(\mathcal{R})| |\Psi_0(\mathcal{R})| = P_\infty(\mathcal{R})$$

$|\Psi_0|$ : Lowest FP-energy state with $\langle |\Psi_0| \, | \, |\Psi_T| \rangle \neq 0$.

- GS energy:

$$E_0 \; = \; \lim_{t \to \infty} \langle E_{loc}(\mathcal{R}) \rangle_{P(\mathcal{R},t)} \; = \; \frac{\int d\mathcal{R} \; P_\infty(\mathcal{R}) \; E_{loc}(\mathcal{R})}{\int d\mathcal{R} \; P_\infty(\mathcal{R})}$$

- Generalized Periodic Boundary Conditions:

— If $\mathbf{B} = \mathbf{0}$, $\left[ \widehat{\mathbb{H}}; \widehat{\mathbb{P}} \right] = 0 \implies$ Periodic

$$\Psi_T(\{\mathbf{r}_j + \mathbf{L}\}) \; = \; \exp\left[ \imath \, \theta \cdot \mathbf{L} \right] \Psi_T(\{\mathbf{r}_j\})$$

— If $\mathbf{B} \neq \mathbf{0}$, $\left[ \widehat{\mathbb{H}}; \widehat{\mathbb{P}} \right] \neq 0 \implies$ Quasi-Periodic

$$\Psi_T(\{\mathbf{r}_j + \mathbf{L}\}) = \exp\left[ \imath \, \theta \cdot \mathbf{L} \; - \; \imath \sum_{j=1}^{N} \Delta_j(\mathbf{L}) \right] \Psi_T(\{\mathbf{r}_j\}) \quad ,$$
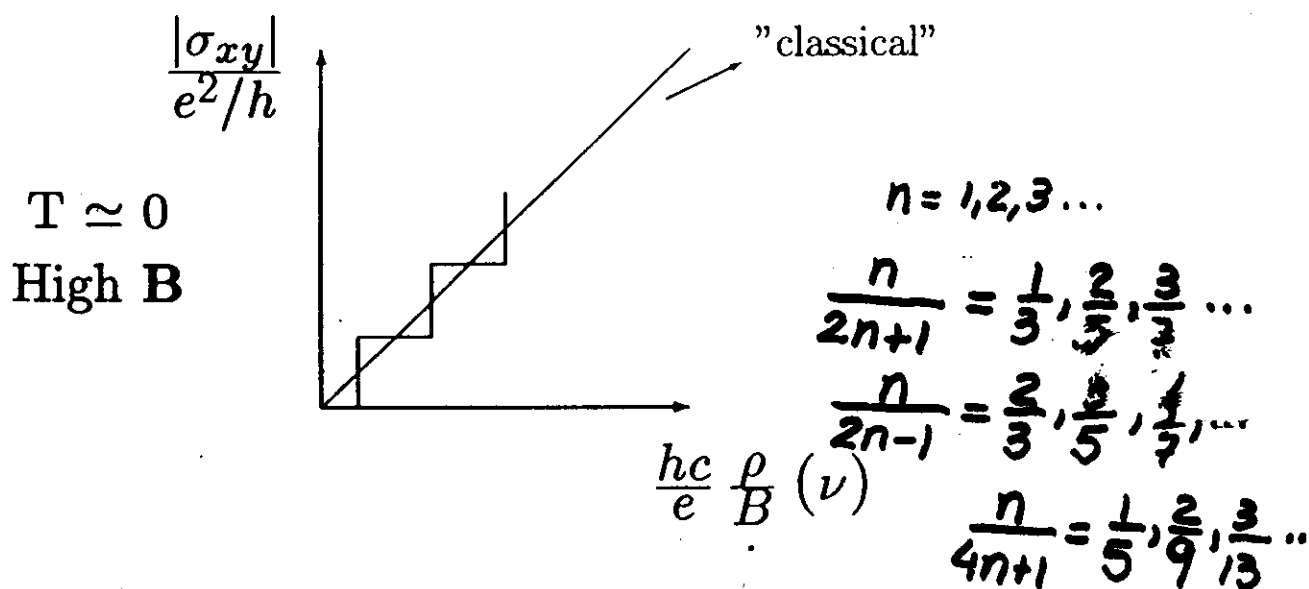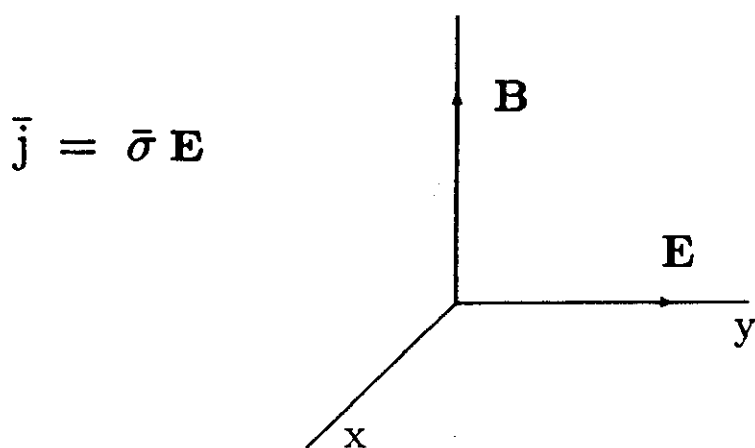
$$\Delta_j(\mathbf{L}) \; = \; \begin{cases} x_j \, L_y / \ell^2 & \text{Landau Gauge} \\[2mm] (x_j \, L_y - y_j \, L_x) / 2\ell^2 & \text{Symmetric Gauge} \end{cases}$$

$\ell = \sqrt{\frac{\hbar c}{eB}}$ "magnetic length"

Consistently $\mathbf{A}$ must change by a Gauge $\implies$ "Flux Quantization" ($\Phi = N_\phi \phi_o$)

However, all quantities needed to solve the Boson Eq. ( $|\Psi_T|$, $\mathbf{F}_i$ ) are genuine periodic functions on the torus $\longrightarrow$ Simplification of the sampling.

# Physics of 2D electrons in high B-fields

$$\bar{j} = \bar{\sigma}\,\mathbf{E}$$

$$\frac{|\sigma_{xy}|}{e^2/h}$$

"classical"

$T \simeq 0$

High $\mathbf{B}$

$$\frac{hc}{e}\,\frac{\rho}{B}\,(\nu)$$

$$n = 1, 2, 3 \ldots$$

$$\frac{n}{2n+1} = \frac{1}{3}, \frac{2}{5}, \frac{3}{7} \ldots$$

$$\frac{n}{2n-1} = \frac{2}{3}, \frac{3}{5}, \frac{4}{7}, \cdots$$

$$\frac{n}{4n+1} = \frac{1}{5}, \frac{2}{9}, \frac{3}{13} \cdots$$

$$\frac{n}{4n-1} = \frac{2}{7}, \frac{3}{11}, \frac{4}{15}$$

QHE $\begin{cases} \text{Integer :} & \text{Single-body Problem} \\[2mm] \text{Fractional :} & \text{Many-body Problem} \end{cases}$

FQHE: Important issue (GS):

Incompressible Liquid $\overset{(r_s, \nu)}{\longleftrightarrow}$ Wigner Crystal

$\ell$

$r_s$ $\qquad\qquad\qquad\qquad$ $r_s$

"Long-range order" $\qquad\qquad$ "Liquid"

# Incompressible Laughlin Liquid

— **Disk Topology**:

Laughlin's construction:

$\quad\quad\quad$ 1) No gapless excitations

$\quad\quad\quad$ 2) $\Psi \in \mathbb{C}$

$\quad\quad\quad$ 3) $\Psi \in$ antisymmetric

$$\Psi_m = \prod_{1 \leq i < j \leq N} (z_i - z_j)^m \exp\left[-\frac{1}{4\ell^2} \sum_{j=1}^{N} |z_j|^2\right] \quad , \quad \nu = \frac{1}{m} \quad m \in \text{ odd integer}$$
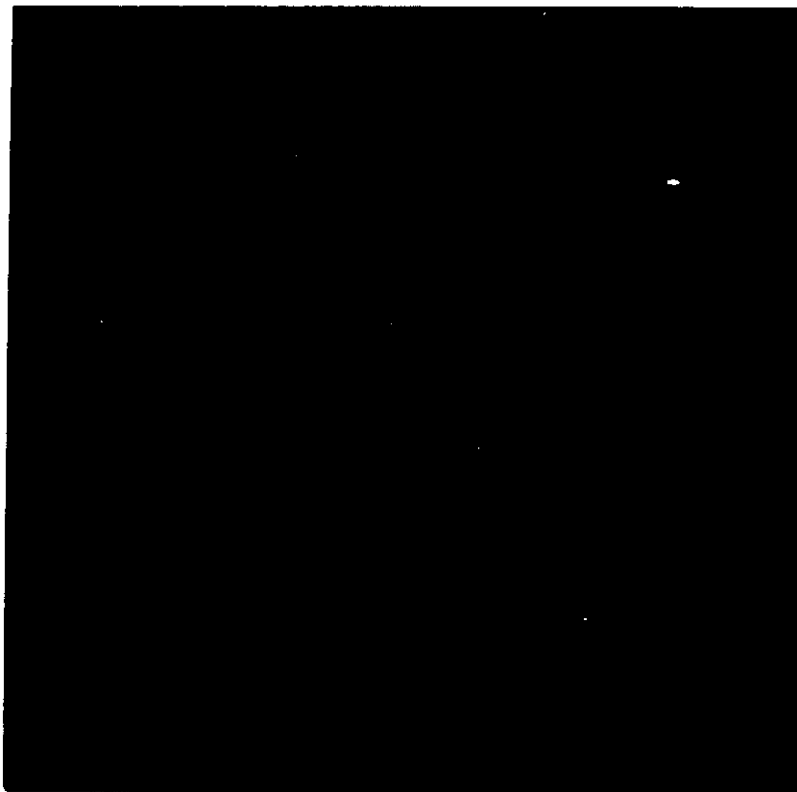
Then, Laughlin's phase corresponds to:

$$\varphi_m = m \, \Im m \sum_{i<j} \ln(z_i - z_j) \quad \text{"statistical phase"}$$

— **Torus Topology**:

Haldane's analysis $\longrightarrow$ Elliptic Theta functions

# Wigner Crystal State



$$\mathbf{R}_j = r_s \sqrt{\frac{2\pi}{\sqrt{3}}} \left( j_1 + \frac{j_2}{2} : \frac{\sqrt{3}}{2} j_2 \right) \qquad (j_1 : j_2) \quad \in \mathbb{Z}$$

$$\Phi_W = \widehat{\mathcal{A}} \prod_{i=1}^{N} \phi_i(\mathbf{r}_i) \qquad \text{(Slater Determinant)}$$

(Symmetric Gauge)

$$\phi_i(\mathbf{r}) = \frac{3}{\sqrt{2\pi\ell^2}} \sum_{\mathbf{L}} \exp\left[ -\frac{1}{4\ell^2} \left( \beta^2 (\mathbf{r} - \mathbf{R}_i - \mathbf{L})^2 - 2i\,(\mathbf{r} \wedge \mathbf{R}_i + \mathbf{r} \wedge \mathbf{L} + \mathbf{R}_i \wedge \mathbf{L})_z \right) \right]$$

$\beta$: variational parameter

# Magnetophonon correlations

- Free boundary conditions:

$$\widehat{\mathbb{H}}_{MP} = \sum_{i=1}^{N} \frac{[\mathbf{p}_i - \mathbf{A}(\mathbf{x}_i)]^2}{2} + \frac{1}{2} \sum_{i,j} x_\mu(i) D_{\mu,\nu}(i-j) x_\nu(j) \quad ,$$

$$\mathbf{x}_i = \mathbf{r}_i - \mathbf{R}_i$$

In the large **B**-field limit:

$$\Psi_{MP} = \Phi_W \, \exp\left[-\frac{1}{4\ell^2} \sum_{i,j} \xi_i \, B_{ij} \, \xi_j\right] \quad , \quad \xi_i = z_i^* - R_i^* \quad ,$$
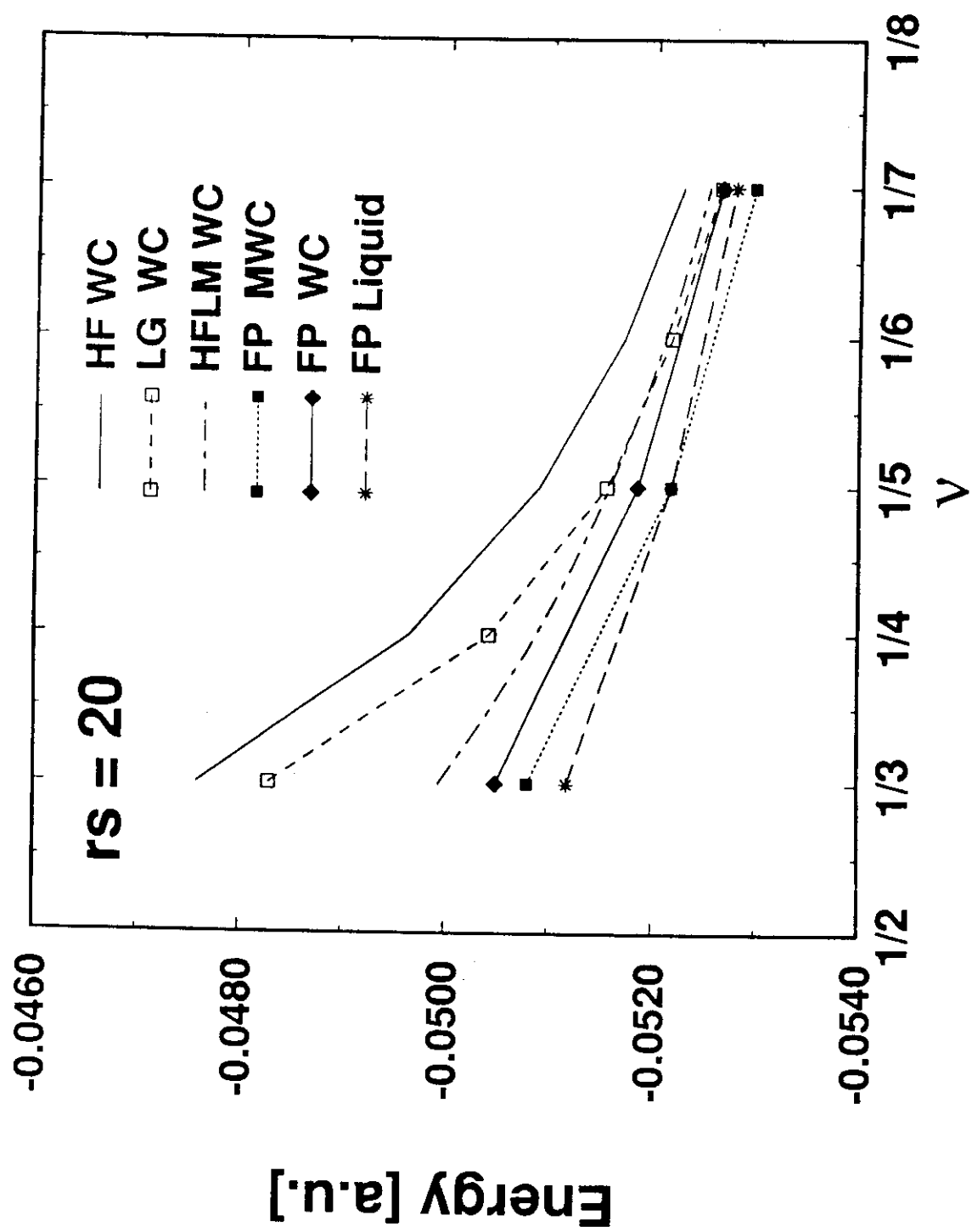
$$B_{ij} = \frac{-1}{\mathcal{N}} \sum_{\mathbf{k}} \frac{\omega_L - \omega_T}{\omega_L + \omega_T} \exp\left[i(\Theta_{\mathbf{k}} + \mathbf{k} \cdot \mathbf{R}_{ij})\right] \quad ,$$

$$\exp[i\Theta_{\mathbf{k}}] = \frac{\delta}{(\delta^2 + D_{12}^2)^{1/2}} + \frac{i \, D_{12}}{(\delta^2 + D_{12}^2)^{1/2}} \quad , \quad \delta = \frac{D_{11} - D_{22}}{2}$$

- Torus Topology:

Pragmatic solution:

$$\Psi_{MP} = \Phi_W^T \, \exp\left[-\frac{1}{4\ell^2} \sum_{i,j} \xi_i \, B_{ij} \, \xi_j\right]$$

rs = 20

Energy [a.u.]

HF WC
LG WC
HFLM WC
FP MWC
FP WC
FP Liquid

V

"If you like excitement, conflict, and contro-
versy, especially when nothing very serious
is at stake, then you will love the history of
quantization on curved spaces."

L.S. Shulman

# Quantum Projector Methods on Curved Manifolds

Let me illustrate the general idea with the following $1d$ equation:

$$\partial_x^2(D(x)v(x,t)) = \partial_t v(x,t)$$

The 'standard' approach to finding the Green's function for this problem is simply to solve the equation

$$\partial_x^2(D(x)G(x,t)) = \partial_t G(x,t)$$

subject to the boundary condition

$$G(x,0) = \delta(x)$$

We can do this by taking the Fourier transform in $x$:

$$-k^2 \int D(k - k')G(k',t)dk' = \partial_t G(k,t)$$

with the boundary condition

$$G(k,0) = 1$$

This is more complex than the usual diffusion equation because we get a convolution of D(k) and G(k.t). However, we can find an approximate solution for $G(k,t)$, valid for small time, by noting that the boundary condition implies that. for small times $t$.

$$G(k,t) - G(k',t) \sim \mathcal{O}(t)$$

and so we have

$$-k^2 \int D(k - k')G(k,t)dk' + \mathcal{O}(t) = \partial_t G(k,t)$$

or, simply,

$$-k^2 D(x = 0)G(k,t) + \mathcal{O}(t) = \partial_t G(k,t)$$

where $D(x = 0)$ is $D$ evaluated at the *prepoint*. For small times we can ignore the order $t$ term (more about this later) and solve for $G$ with the result

1

$$G(k,t) = e^{-k^2 D(0)t}$$

Taking the inverse Fourier transform we finally have

$$G(r,t) \simeq \frac{1}{\sqrt{4\pi D(0)t}} e^{-r^2/(4D(0)t)}$$

which is just the plain old Green's function with $D$ evaluated at the **prepoint** and with **no quantum corrections**. This is, in fact, the result that the Green's function for the Jacobian times $f$ has no quantum corrections. In the context of the expansions this result involved the seemingly miraculous cancellation of many terms. Here it is, I think, more natural.

(Of course $G(r,t)$ is really an approximate Green's function, valid to order $\mathcal{O}(t^2)$, which satisfies the equation

$$\partial_x^2 (D(x)G(x,t)) = \partial_t G(x,t) + \mathcal{O}(t)$$

One can easily show that this is all we need for the small time Green's function (I can tell you more on this if you like — it can be made every bit as rigorous as the expansions...).)

To make things clear let's look at a different equation

$$D(x)\partial_x^2 G(x,t) = \partial_t G(x,t)$$

where we know **there \*are\* quantum corrections**, and see how things go.

Again, taking the Fourier transform we get

$$-\int k'^2 D(k-k')G(k',t)dk' = \partial_t G(k,t)$$

Making the same approximation as above, replacing $G(k',t)$ with $G(k,t)$ in the integrand, making an error of order $t$, we have

$$-\int k'^2 D(k-k')dk' G(k,t) + \mathcal{O}(t) = \partial_t G(k,t)$$

but

$$\int (k+k')^2 D(k')dk' = k^2 D(0) + 2k\partial_x D(0) + \partial_x^2 D(0)$$

2

$$G(k.t) \simeq e^{-(k^2 D(0)+2k\partial_x D(0)+\partial_x^2 D(0))t}$$

when we take the inverse Fourier transform the terms with derivatives of $D$ give precisely the quantum corrections for this simple case.

We see a simple rule. If *all* the derivatives are brought all the way to the left of the diffusion 'constant'. then the Green's function is simply that for a constant diffusion constant. no **quantum corrections**. with the diffusion constant evaluated at the **prepoint**.

The general case is just as simple. Following the same argument as above, given a differential equation of the form

$$\partial_x^2(D(x)f(x.t)) - \partial_x(D(x)F(x)f(x.t)) - E_L(x)f(x.t) = \partial_t f(x.t)$$

where all the derivatives are all the way to the left, the Green's function is simply the conventional Green's function with $D$ and $F$ evaluated at the prepoint, with no quantum corrections.

The quantum corrections are then seen to be simply those extra terms we get when writing the equation

$$D(x)\partial_x^2 f(x,t) - D(x)\partial_x(F(x)f(x,t)) - E_L(x)f(x,t) = \partial_t f(x,t)$$

in the appropriate form. (You can check this for yourself — the extra terms are precisely the corrections obtained using the 'traditional' Feynman expansion approach.)

The same is true for the general metric $g^{\alpha\beta}$:

$$ds^2 = g_{\alpha\beta} \, dx^\alpha dx^\beta$$

and

$$g^{1/2} = \sqrt{\det g_{\alpha\beta}}$$

In order to find the Green's function for the wonderful 'Laplace-Beltrami' (L-B) operator

$$g^{-1/2}\partial_\alpha g^{1/2} g^{\alpha\beta}\partial_\beta f$$

3

we must first write it in the form

$$\partial_i \partial_j (g^{\alpha j} f) + \partial_\alpha (g^{\alpha j} F_j f) + E_L f$$

The extra terms should be, precisely, the quantum corrections for the L-B operator.

I should also say that (Bachelet-Ceperley...)'s correction to the force for the position dependent diffusion constant can be derived in one line using this approach:

$$\nabla a \nabla f = \nabla^2 (a f) - \nabla (a (\nabla a / a) f)$$

We simply read off $\nabla a / a$ as the correction to the force and we're done.

---

Let me summarize the key results.

(1) Given any second order differential equation (first order in $t$), no matter how many dimensions, with or without curvature, with or without a position dependent diffusion constant, with or without any complication you can dream up, the rule for obtaining the Green's function with everything evaluated at the prepoint is simple: **Bring all derivatives in all the terms all the way to the left.** One can then simply write down the Green's function assuming the $D$, $F$, $g^{\alpha \beta}$, whatever position dependent terms they may be, are constant and evaluated at the prepoint. Distilled to its essence, the proof of this statement is three lines long.

(2) *All* the quantum corrections we have been considering are simply the extra terms we get when commuting the derivatives to the left.

---

4

In a curved space with metric $g^{\alpha\beta}$ ($g$=det $g_{\alpha\beta}$) the generalized Fixed-Phase Hamiltonian is:

$$\hat{H}_{FP} = -Dg^{-1/2}\partial_\alpha(g^{\alpha\beta}g^{1/2}\partial_\beta) + \tilde{V}$$

where

$$D = \frac{\hbar^2}{2m}$$

and $\tilde{V}$ is the effective potential. Notice that in this section $D$ is a constant.

_____

Some words on Notation:

$$ds^2 = g_{\alpha\beta}\, dx^\alpha dx^\beta\ , \qquad g_{\alpha\beta} = g_{\beta\alpha}\ . \ \ \text{Suppose}\ \ x^\alpha = t^\alpha(x'^1, x'^2, \cdots)$$

$$
\begin{aligned}
A^\alpha &= \frac{\partial x^\alpha}{\partial x'^\beta} A'^\beta &&\text{contravariant} \\
A_\alpha &= \frac{\partial x'^\beta}{\partial x^\alpha} A'_\beta &&\text{covariant}
\end{aligned}
$$

$$A^\alpha = g^{\alpha\beta}A_\beta \qquad A_\alpha = g_{\alpha\beta}A^\beta$$

_____

The generalized diffusion equation in curved space for the importance-sampled function $f = \psi\psi_T$ ($\psi_T$ is a trial wave function) is:

$$\partial_t f = Dg^{-1/2}\partial_\alpha\left(g^{\alpha\beta}g^{1/2}(\partial_\beta f - fF_\beta)\right) - (E_L - E_T)f$$

where $\qquad F_\beta = 2\frac{\partial \ln\psi_T}{\partial x^\beta}, \quad E_L = \frac{\hat{H}_{FP}\psi_T}{\psi_T}$

5

To fix notation suppose $N = 1$ and $d = 2$ ($z = x^1 + ix^2$, $x^1 = x$, $x^2 = y$). Then, the iterated integral representation is

$$f(z, t + \tau) = \int dz' g^{1/2}(z') G(z, z'; \tau) f(z', t)$$

where

$$G(z, z'; \tau) = v_T(z) \left\langle z | e^{-\tau H_{FP}} | z' \right\rangle v_T^{-1}(z')$$

with its short-time approximation given by

$$G(z, z'; \tau) = \frac{1}{4\pi D\tau} \quad \exp\left[ \frac{\left(x'^\alpha - x^\alpha + D\tau \tilde{F}^\alpha(z')\right) g_{\alpha\beta}(z') \left(x'^\beta - x^\beta + D\tau \tilde{F}^\beta(z')\right)}{4D\tau} \right]$$

$$\times \exp\left[ \left( \frac{\tilde{E}_L(z) + \tilde{E}_L(z')}{2} \right) - E_T \right]$$

where

$$\begin{cases} \tilde{F}_\alpha = F_\alpha + \delta F_\alpha \\ \tilde{E}_L = E_L + \delta E_L \end{cases}.$$

The **"quantum corrections"** to the Green's function:

$$\delta F^\alpha = \partial_\beta g^{\beta\alpha} - g^{\alpha\beta} \Gamma^\gamma_{\beta\gamma}$$

$$\delta E_L = D F^\alpha \Gamma^\beta_{\alpha\beta} + D\partial_\alpha (g^{\alpha\beta} \Gamma^\gamma_{\beta\gamma})$$

where $\Gamma^\gamma_{\alpha\beta}$ is the Christoffel symbol of the second kind

$$\Gamma^\gamma_{\alpha\beta} = \frac{1}{2} g^{\gamma\mu} \left( \partial_\alpha g_{\beta\mu} + \partial_\beta g_{\alpha\mu} - \partial_\mu g_{\alpha\beta} \right)$$

Exercises:
1) Suppose the space interval is: $ds^2 = R^2(\sin^2\theta(d\varphi)^2 + (d\theta)^2)$. Calculate the metric tensor in the following coordinate system ($z = x + i\,y$):

$$\begin{cases} x = \mathrm{tg}\left(\frac{\theta}{2}\right) \cos\varphi \\ y = -\mathrm{tg}\left(\frac{\theta}{2}\right) \sin\varphi \end{cases}.$$

2) Get the quantum corrections in the general metric case
3) Write the short-time approximation to $G$ for a single particle in an external magnetic field. (Assume the metric is constant)

6

# FQHE on the Haldane Sphere

The key point of the method is that the function $P$ is $\psi$ times both the trial function *and* the Jacobian. It is then easy to show that the generalized diffusion equation is the one given, with all derivatives to the left. It follows from the arguments given above that the Green's function is just the conventional one with $D$ evaluated at the prepoint — and this is what we use in the simulation. It is important to mention that in $2d$ it is always possible to find a 'conformal gauge' where the metric tensor is diagonal (see Polyakov "Gauge fields and strings").

In the spherical geometry introduced by Haldane [?] electrons are confined to the surface of a sphere of radius $R$ with a magnetic monopole at its center. Let $N$ denote the number of electrons, which we take to be spin polarized, and $2S$ denote the number of flux quanta piercing the surface of the sphere due to the monopole. The magnetic field strength at the surface of the sphere is then $B = S\hbar c/eR^2$, and, for filling fraction $\nu = 1/q$, where $q$ is an odd integer, $2S = q(N-1)$. If the positions of the electrons are described using the stereographic coordinates $\mathbf{r}_i = (\cos\phi, \sin\phi)\tan\theta/2$ where $\theta$ and $\phi$ are the usual spherical angles then the Hamiltonian describing this system becomes

$$H = \frac{1}{2m}\sum_i D(\mathbf{r}_i)(-i\hbar\nabla_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i))^2 + \frac{e^2}{\epsilon l_0}V(\mathcal{R}) \tag{1}$$

where $D(\mathbf{r}_i) = (1 + r_i^2)^2/4R^2$ (using previous notation: $g^{\alpha\beta} = \delta^{\alpha\beta}g^{-1/2}$ and $g^{-1/2} = D(\mathbf{r})$). The interaction between the electrons is taken to be

$$V(\mathcal{R}) = \sum_{i<j}\frac{1}{\sqrt{d(\mathbf{r}_i,\mathbf{r}_j)^2 + \lambda^2}} \tag{2}$$

where $\mathcal{R} = (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ denotes the coordinates of the $N$ particles and where

$$d(\mathbf{r}_i, \mathbf{r}_j) = \frac{2R|\mathbf{r}_i - \mathbf{r}_j|}{\sqrt{(1 + r_i^2)(1 + r_j^2)}} \tag{3}$$

is the chord distance on the sphere and $\lambda$ is a parameter which accounts for the finite thickness of the 2DEG [?]. We work in the gauge for which

$$\mathbf{A}(\mathbf{r}_i) = \frac{B}{2(1 + r_i^2)}(y_i, -x_i, 0) \tag{4}$$

7

With this gauge choice the spherical analog of the Laughlin state for $\nu = 1/q$ is

$$\psi_{l=0} = \prod_i \left( \frac{1}{1 + |z_i|^2} \right)^S \prod_{i<j} (z_i - z_j)^q. \tag{5}$$

where $z_i = x_i + iy_i$ is the complex valued stereographic coordinate.

In the spherical geometry the excited state which corresponds to a charge $e/q$ quasiparticle and a charge $-e/q$ quasihole with infinite separation is constructed by putting the quasielectron and quasihole at opposite ends of the sphere. For this state we use the following trial wave function constructed using Jain's composite fermion approach [?]

$$\psi_{l=N} = \prod_i \left( \frac{1}{1 + |z_i|^2} \right)^S \prod_{i<j} (z_i - z_j)^{q-1} \begin{vmatrix} 1 & z_1 & \cdots & z_1^{N-2} & \sum_{i \neq 1} \frac{1}{z_1 - z_i} \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & z_N & \cdots & z_N^{N-2} & \sum_{i \neq N} \frac{1}{z_N - z_i} \end{vmatrix}. \tag{6}$$

The energy gap, defined to be the difference in energy $\psi_{l=N}$ and $\psi_{l=0}$, has been calculated using these states, with the result for $\nu = 1/3$ of $\Delta = 0.106(2)e^2/\epsilon l_0$.

In order to apply the diffusion Monte Carlo method to this problem we must first convert the Hamiltonian into an effective bosonic problem. To do this we follow Ortiz, Ceperley, and Martin [?] and fix the phase of the wave function using the phase of a many-body trial wave function $\psi_T$. We first write $\psi_T$ as follows

$$\psi_T(\mathcal{R}) = |\psi_T(\mathcal{R})| e^{i\phi_T(\mathcal{R})}. \tag{7}$$

The overall phase of this wave function can be used to perform a gauge transformation on the Hamiltonian as follows,

$$\hat{H} = e^{-i\phi_T(\mathcal{R})} H e^{i\phi_T(\mathcal{R})} = H_R + iH_I \tag{8}$$

where

$$H_R = -\frac{\hbar^2}{2m} \sum_i D(\mathbf{r}_i) \nabla_i^2 + U(\mathcal{R}) \tag{9}$$

and

$$H_I = -\frac{\hbar e}{2mc} \sum_i D(\mathbf{r}_i) \left( \nabla_i \cdot \tilde{\mathbf{A}}(\mathbf{r}_i) + \tilde{\mathbf{A}}(\mathbf{r}_i) \cdot \nabla_i \right) \tag{10}$$

8

where

$$\tilde{\mathbf{A}}_i = \mathbf{A}_i + \frac{\hbar c}{e}\nabla_i \varphi_T. \tag{11}$$

It is straightforward to show that the ground state of the 'real part' of the Hamiltonian. $H_R$ corresponds to the energy of the lowest energy state with the same phase as the trial function.

To use the diffusion Monte Carlo method to study the properties of the ground state of this Hamiltonian we first transform the time dependent Schrödinger equation into the generalized diffusion equation $H_R\psi(\mathcal{R},t) = -\frac{\partial}{\partial t}\psi(\mathcal{R},t)$. It is further convenient to consider the diffusion equation for the the importance-sampled distribution

$$P(\mathcal{R},t) = \psi(\mathcal{R},t)|\psi_T(\mathcal{R})|\prod_{i=1}^{N}\frac{1}{D(\mathbf{r}_i)}. \tag{12}$$

The resulting diffusion equation is

$$-\frac{\partial}{\partial t}P(\mathcal{R},t) = \sum_{i=1}^{N}\left[\nabla_i^2(D(\mathbf{r}_i)P(\mathcal{R},t)) + \nabla_i \cdot (D(\mathbf{r}_i)\mathbf{F}_i(\mathcal{R})P(\mathcal{R},t))\right] + E_L(\mathcal{R})P(\mathcal{R},t) \tag{13}$$

where

$$\mathbf{F}_i(\mathcal{R}) = \nabla_i \ln|\psi_T| \tag{14}$$

and

$$E_L(\mathcal{R}) = \frac{\hat{H}|\psi_T|}{|\psi_T|} \tag{15}$$

All of the trial wave functions we will be using here are entirely in the lowest Landau level. From this it follows that

$$E_L = \lambda V(\mathcal{R}) \tag{16}$$

This differential equation can be solved numerically by stochastically iterating the integral equation

$$P(\mathcal{R}',t+\tau) = \int G(\mathcal{R} \to \mathcal{R}',\tau)P(\mathcal{R},t)d\mathcal{R}. \tag{17}$$

9

The problem of finding the correct short time Greens function for this problem is made nontrivial by the fact that the electrons move in a curved space. We have, in fact, solved the general problem of finding the Greens function for the case of a general metric — the result we give now is a special case of this result.

$$G(\mathcal{R} \to \mathcal{R}', \tau) = \exp\left[-\tau\left(\frac{[E_L(\mathcal{R}) + E_L(\mathcal{R}')]}{2} - E_T\right)\right] \prod_{i=1}^{N} G_i^0(\mathcal{R} \to \mathcal{R}', \tau) \quad (18)$$

where

$$G_i^0(\mathcal{R} \to \mathcal{R}', \tau) = \frac{1}{4\pi D(\mathbf{r}_i)\tau} \exp\left[\frac{-(\mathbf{r}_i' - \mathbf{r}_i - D(\mathbf{r}_i)\tau \mathbf{F}_i(\mathcal{R}))^2}{4D(\mathbf{r}_i)\tau}\right] \quad (19)$$

Note that $D(\mathbf{r}_i)$ and $F_i(\mathcal{R})$ are evaluated at the 'prepoint' in the integral equation. This fact is crucial for performing the Monte Carlo simulation.

Having included the Jacobian in our definition of $P(\mathcal{R}, t)$ it follows that the expectation value of the energy is simply

$$\langle H \rangle = \frac{\int d\mathcal{R} P(\mathcal{R}, t \to \infty) E_L(\mathcal{R})}{\int d\mathcal{R} P(\mathcal{R}, t \to \infty)} \quad (20)$$

10

# Particle moving on the surface of a sphere
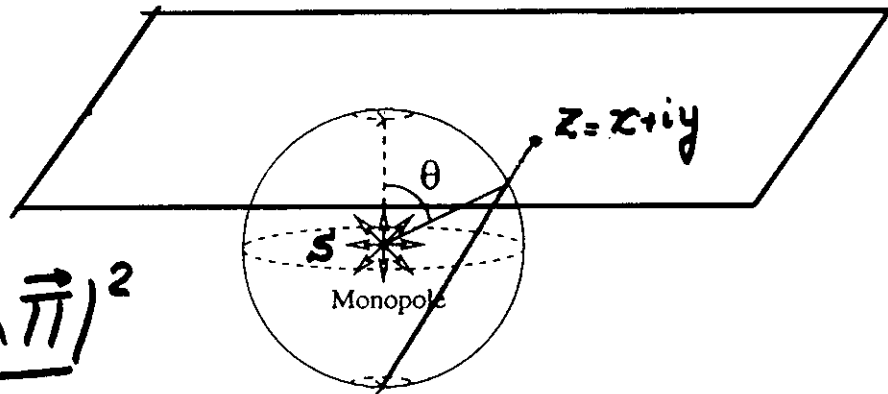


$$\hat{H} = \frac{|\breve{r} \wedge \vec{\Pi}|^2}{2m}$$

$$\hat{H} = \frac{\hbar^2}{2mR^2}\left\{-\partial_\theta^2 - \frac{1}{\sin^2\theta}\partial_\varphi^2 - \frac{\cos\theta}{\sin\theta}\partial_\theta + 2iS\frac{\cos\theta}{\sin^2\theta}\partial_\varphi + \right.$$

$$\left. + S^2\frac{\cos^2\theta}{\sin^2\theta}\right\}$$

$$B = \frac{\hbar c S}{e R^2} > 0 \quad ; \quad \omega_c = \frac{eB}{mc}$$

$$\hat{H}\Psi_0 = \frac{\hbar\omega_c}{2}\Psi_0$$

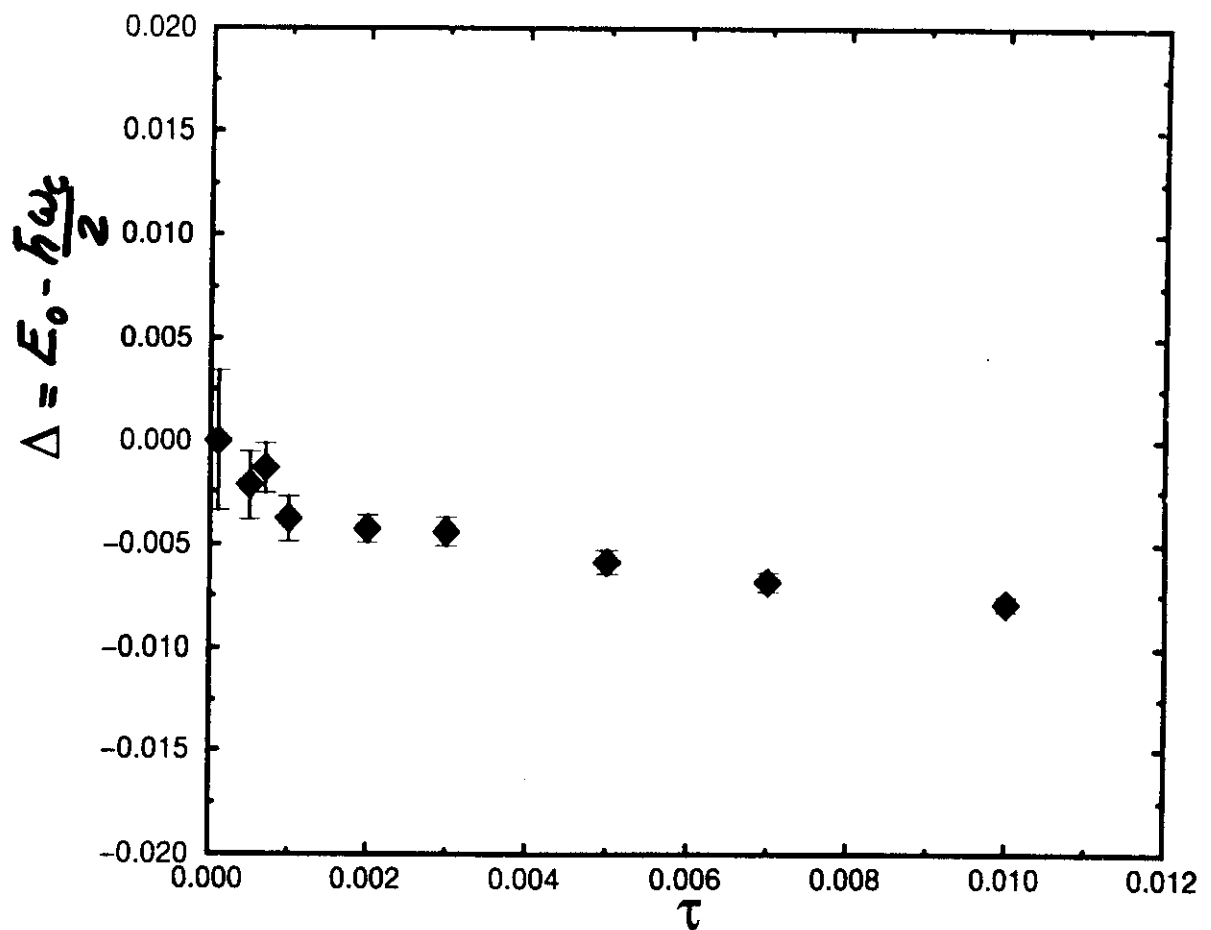$$\Psi_0(z) = \left(\frac{|z|}{1+|z|^2}\right)^S \left(\frac{\alpha^*}{z} + \beta^* z\right)^S \qquad /$$

$$|\alpha|^2 + |\beta|^2 = 1$$

$\downarrow$

ground state
(lowest Landau level)

# One Particle Problem

We test our method by solving one particle problem. If the exact phase is chosen as a trial phase, the exact solution is obtained in $\tau \to 0$ limit.
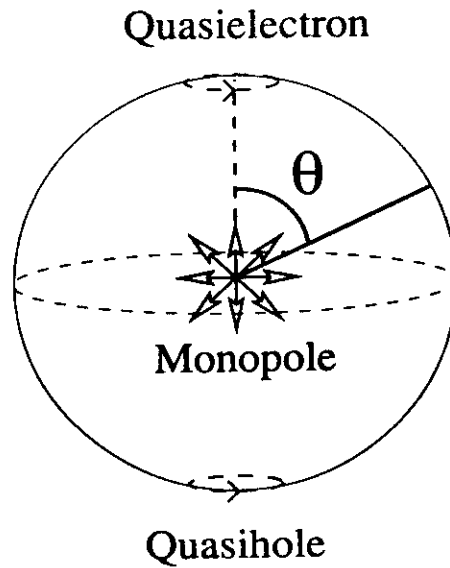


$\Delta \to -0.05$ when the corrections are not included.

# Introduction

1.  We present calculation of the quasiparticle-quasihole excitation gap in the FQHE.

2. Haldane Sphere:

Quasielectron



Quasihole

(F.D.M. Haldane, PRL **51**,605 (1983))

3.  We generalize the Fixed-Phase Diffusion Monte Carlo (FPDMC) for the case of curved space and study the Landau Level Mixing (LLM) effect $(\lambda = \frac{e^2/\epsilon l_0}{\hbar \omega_c})$. In additon finite thickness effect $(\beta)$ is included.
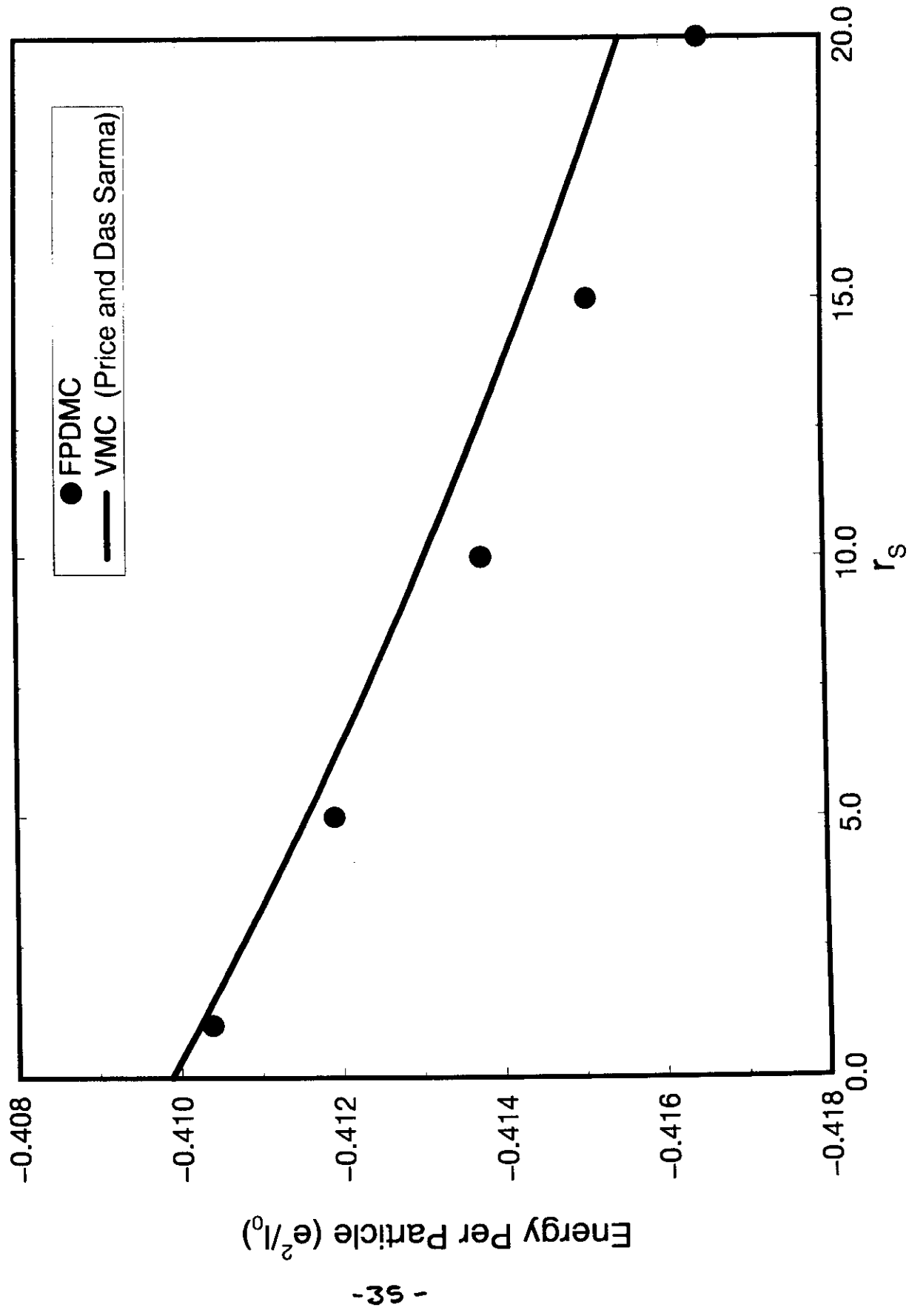
# Comparison to Experiments on Energy Gaps

(R.R.Du et.al., PRL **70**,2944(1993))

Experiment $\left[\Delta^E \simeq 0.05(e^2/\epsilon l_0)\right]$ Theory $\left[\Delta^E \simeq 0.056(e^2/\epsilon l_0)\right]$
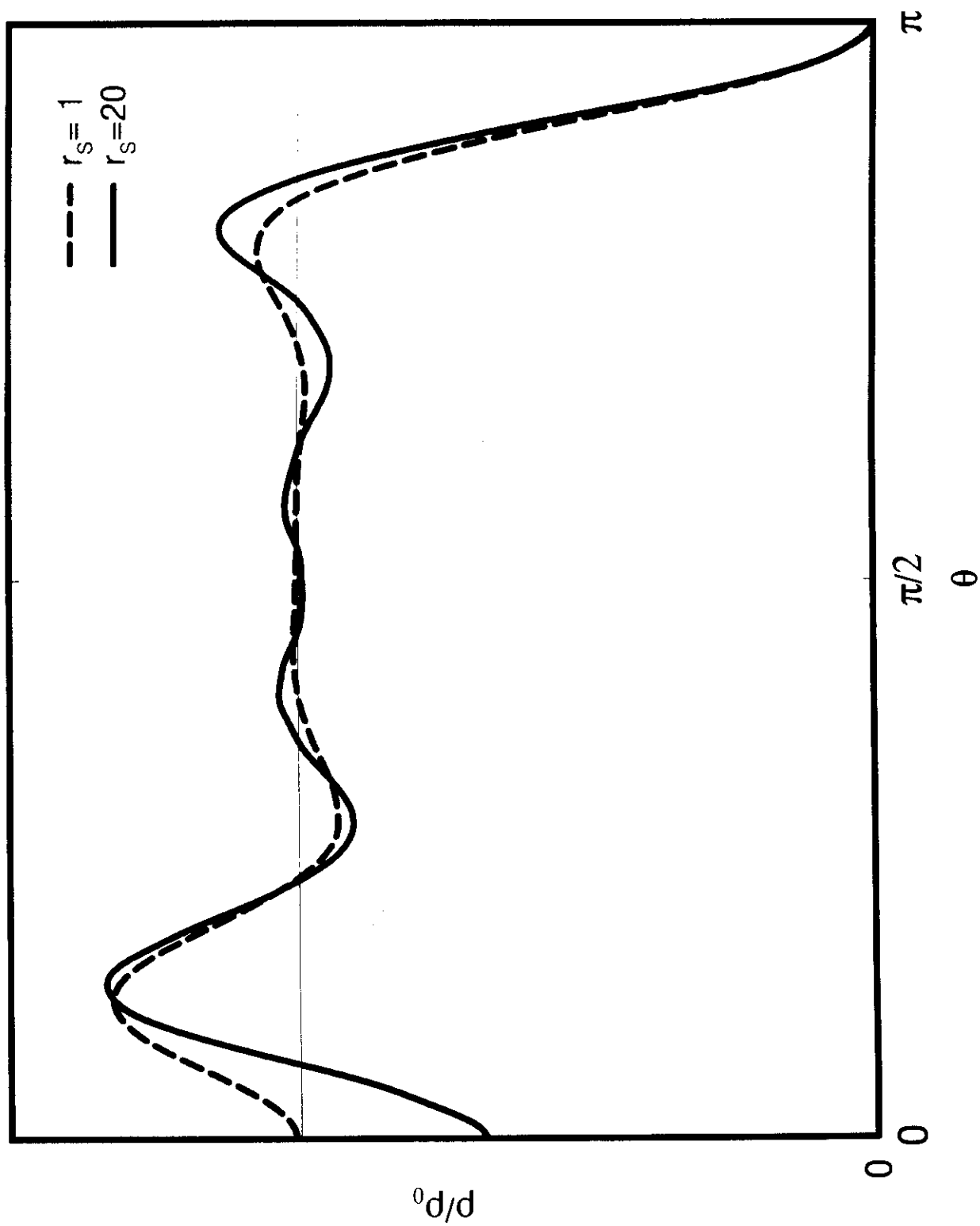
(H.C.Manoharan et.al., PRL **30**,3270(1994))

Experiment $\left[\Delta^H \simeq 0.023(e^2/\epsilon l_0)\right]$ Theory $\left[\Delta^H \simeq 0.049(e^2/\epsilon l_0)\right]$
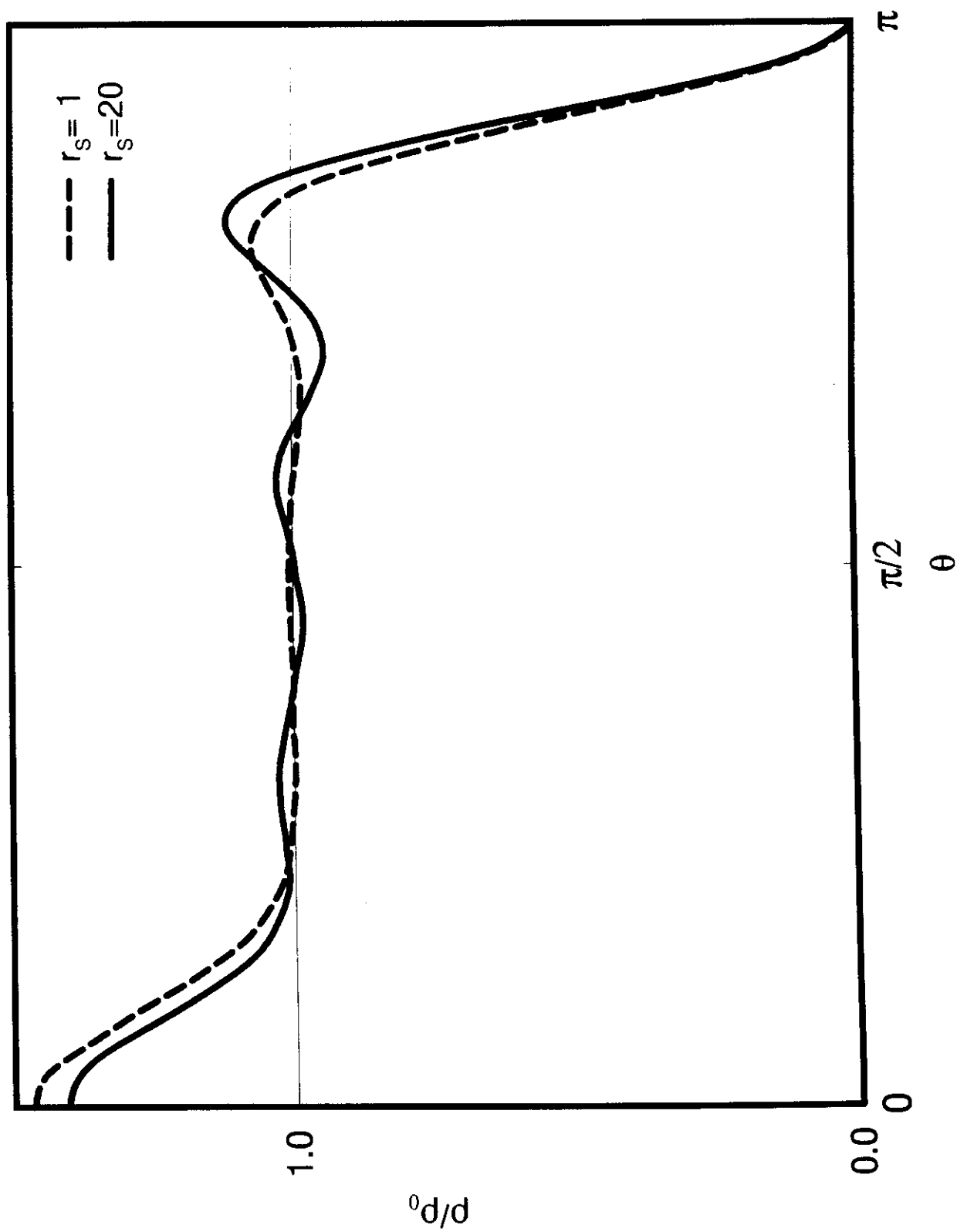
Ground State Energy vs. $r_S$ for $\nu = 1/3$

● FPDMC
—— VMC (Price and Das Sarma)

Energy Per Particle ($e^2/l_0$)

$r_S$

Spin Polarized Excited State Density Profile

ν=1/3 : 20 Electrons

$r_S= 1$
$r_S=20$

$\rho/\rho_0$

$0$     $\pi/2$     $\pi$

$\theta$

Spin Flip Excited State Density Profile

$\nu=1/3$ : 20 Electrons

$r_s=1$
$r_s=20$

$\rho/\rho_0$

$\theta$

Spin Polarized Energy Gap vs. $r_S$

$\nu = 1/3$ : 20 Electrons

Energy Gap ($e^2/l_0$)

$r_S$

$\lambda = 0$

$\lambda = 1.5$
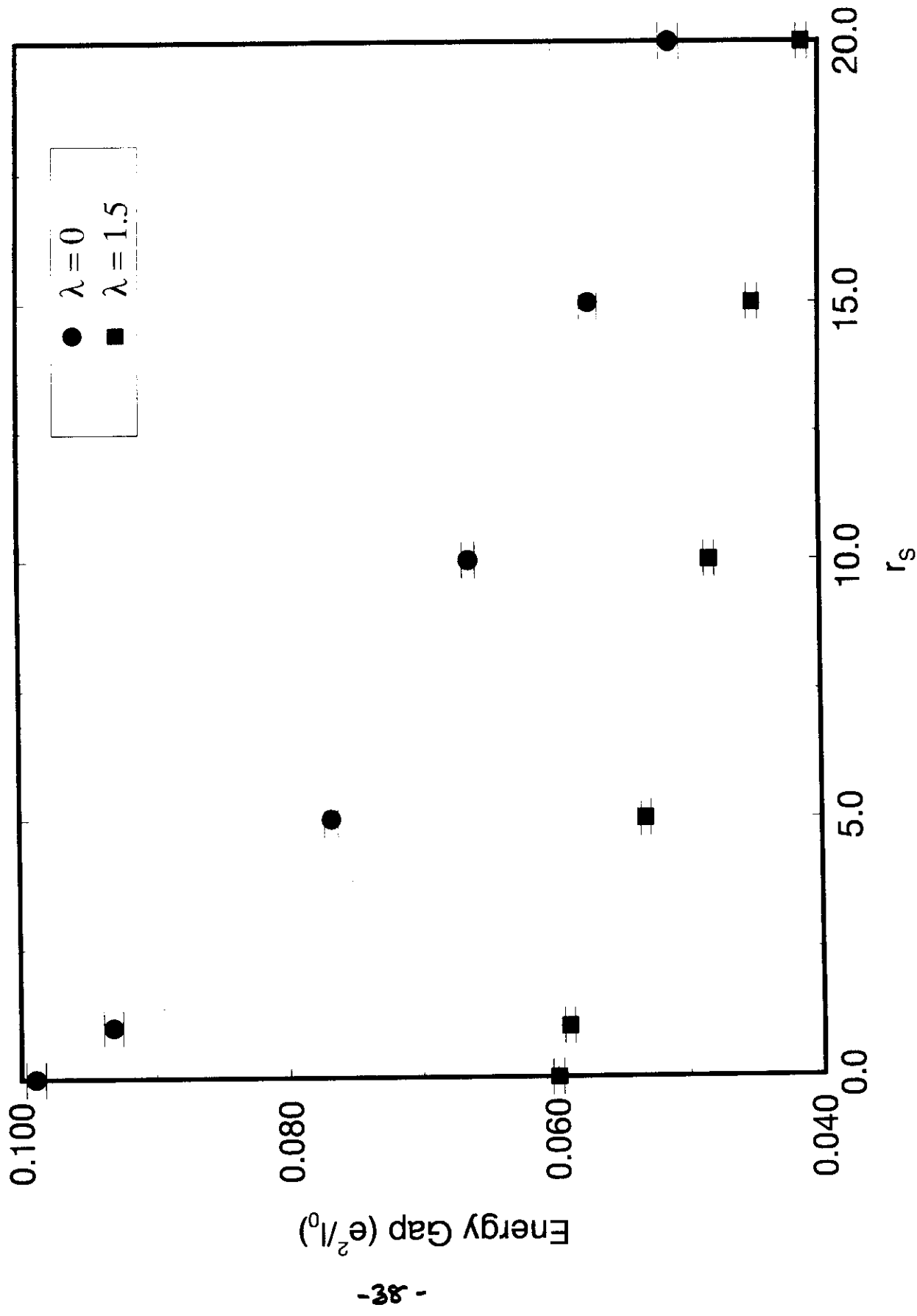
Spin Flip Energy Gap vs. $r_S$

$\nu = 1/3$ : 20 Electrons

Energy Gap ($e^2/l_0$)

$r_S$

$\lambda = 0$

$\lambda = 1.5$