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"Variational Monte Carlo: Shadow wave function for boson excited states"

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VARIATIONAL MONTE CARLO:

SHADOW WAVE FUNCTION FOR

BOSON EXCITED STATES

Low temperature $\Rightarrow$ low-lying states

Elementary Excitations in Liquid ^{4}He

The Phonon-Roton Spectrum

<u>Feynman trial function</u>

- $\Psi_0(R)$ the ground state representation
- To construct low-lying excited states
  - promote 1 particle to a state with momentum $\mathbb{K}$
  - simmetrize

$$\rho_{\mathbb{K}} = \sum_{j=1}^{N} e^{i\mathbb{K}\cdot\mathbb{r}_j}$$

- Excitation as a density fluctuation

$$\Psi_{\mathbb{K}}(R) = \rho_{\mathbb{K}}\,\Psi_0(R)$$

<u>The excitation spectrum</u>

$$\varepsilon_K = E_K - E_0$$

The Ground State Trial Function

The pair product structure

Liquid phase: $\Psi_J(R) = \prod_{i<j} e^{-\frac{1}{2}\left(\frac{b}{r_{ij}}\right)^5}$

Capture the dominant character of the particle-particle interaction

Three-Body Correlations: $\Psi_T(R) = \prod_{i<j<k} f_{ijk} \prod_{i<j} f(r_{ij})$

The shadow wave function

Liquid-solid phases

$$\Psi_{sh}(R) = \int dS\, \Xi(R,S)$$

$$\Xi(R,S) = \prod_{i<j} e^{-\frac{1}{2}\left(\frac{b}{r_{ij}}\right)^5} \prod_i e^{-c|\mathbf{r}_i - \mathbf{s}_i|^2} \prod_{i<j} e^{-\beta v(\gamma s_{ij})}$$

where v is the He-He potential

b, c, β and γ variational parameters

$\{\mathbf{s}_i\}$ coordinates of quantum holes or shadow particles

Introduces High-order correlations

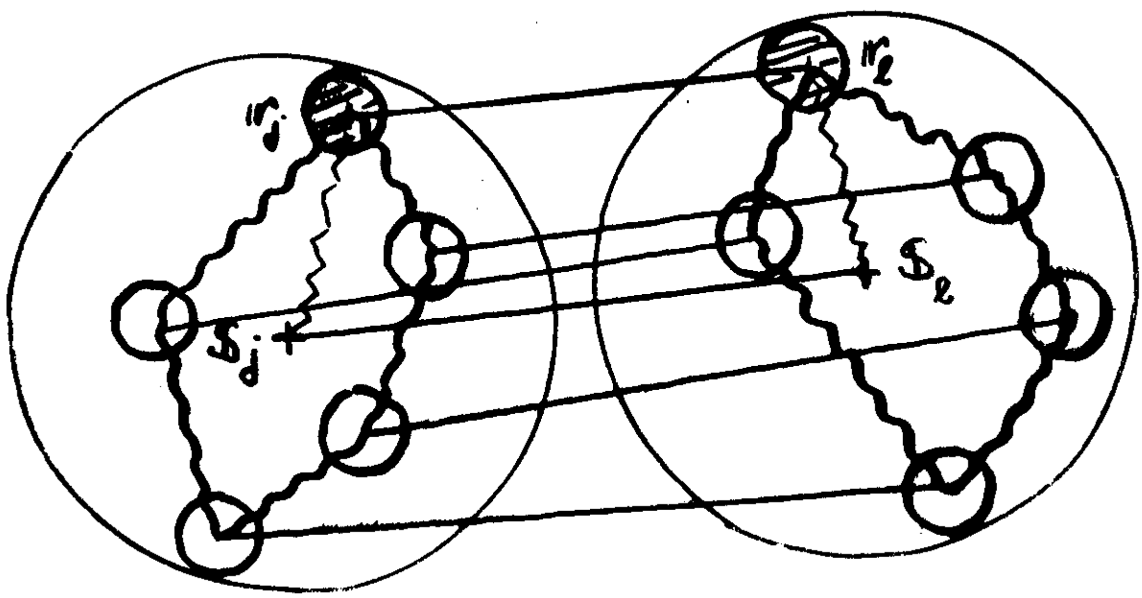
Takes into account the quantum delocalization

PHYSICAL MOTIVATION

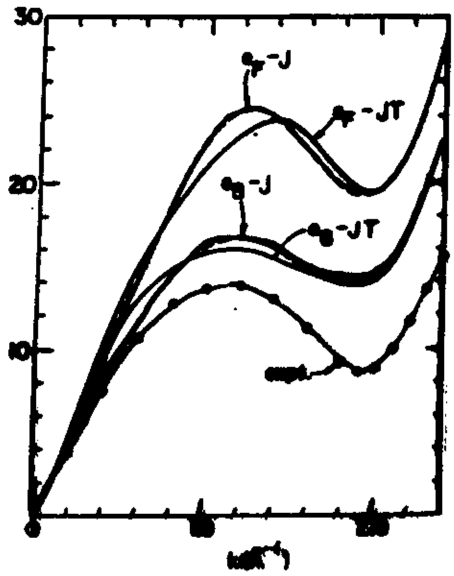
Discretized path-integral

of the density matrix

- **each particle $\Longleftrightarrow$ "polymer"**
- **path of a particle $\Longleftrightarrow$ "center of mass" + fluctuations**
- $e^{-C(\mathbf{r}_j-\mathbf{s}_j)^2}$ **$\Longleftrightarrow$ model for the fluctuations along the path with respect to the CM**
- $\mathbf{s}_l$ **$\Longleftrightarrow$ center of mass**
- **The CM behave as quasi-classical particles**



Excitation Spectrum



The Feynman-Cohen Ansatz

A wave-packet built out of Feynman states does not satisfy conservation of probability

Correction: dipolar backflow centered on each particle

- Backflow coordinates the motion of the souroundimg atoms
- It is very important at high values of K

The Trial Function

$$\Psi_{B\mathbb{K}}(R) = \sum_j \exp i\mathbb{K}\cdot\left[\mathbf{r}_j - \sum_{\ell\neq j} \eta(r_{j\ell})\,\mathbf{r}_{j\ell}\right]\Psi_0$$

$$\simeq \sum_j \exp i\mathbb{K}\cdot\mathbf{r}_j \left[1 - \sum_{\ell\neq j} \eta(r_{j\ell})\,\mathbb{K}\cdot\mathbf{r}_{j\ell}\right]\Psi_0$$

$\eta(r)$ a variational function

Feynman-Cohen choice: $\eta(r) = \frac{A}{r^3}$, A a parameter

Backflow $\Rightarrow$ mixing $\begin{cases} \rho_{\mathbb{K}} \\ \rho_{\mathbb{K}-\mathbf{q}}\,\rho_{\mathbf{q}} \end{cases}$

$$\rho_{B\mathbb{K}} = \rho_{\mathbb{K}} - \frac{1}{N}\sum_{\mathbf{q}} \mathbb{K}\cdot\mathbf{q}\,\eta(q)\left[\rho_{\mathbb{K}-\mathbf{q}}\,\rho_{\mathbf{q}} - \rho_{\mathbb{K}}\right]$$

$$\eta(q) = \rho\int d^3r\, e^{i\mathbf{q}\cdot\mathbf{r}}\,\eta(r)$$

The Feenberg approach determines η by perturbation theory

The FC trial function improves significantly the results

Mamousakis - Pandharipande

Integral equation method

Terms up to the 4^{th} order in $\{\rho_{k}\}$

Calculation	Roton Energy
M-P	10 K
F-C	14 K
F	20 K

The Shadow Particle Approach to The Phonom-Roton Spectrum

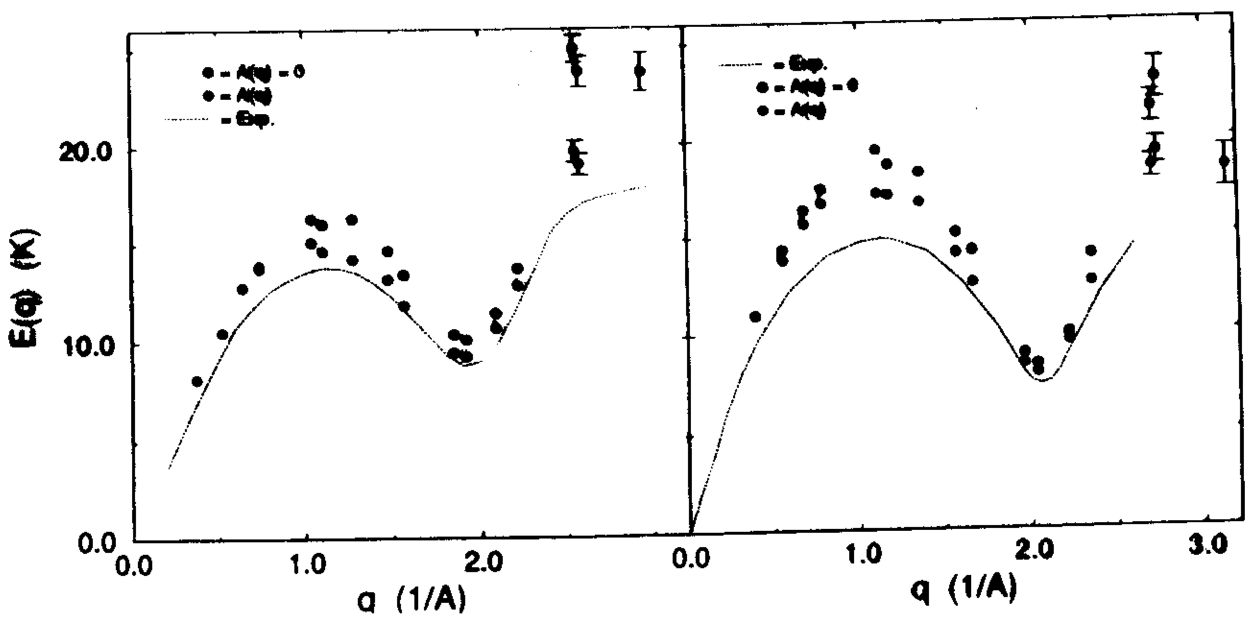
$$\Psi_{sh\,\mathbb{K}}(R) = \prod_{i<j} f(r_{ij}) \int ds\, \sigma_{\mathbb{K}} \prod_{i} e^{-C|\mathbf{r}_i - \mathbf{s}_i|^2} \prod_{i<j} e^{-\beta v(\alpha s_{ij})}$$

$$\sigma_{\mathbb{K}} = \sum_{j} e^{i\mathbb{K}\cdot \mathbf{s}_j}$$

zero-point motion } quantum holes or
hard core potential } SHADOW PARTICLES

Consequences

- Imposes particle modulations in a flexible way
- Backflow is introduced in a nonpolynomial structure in $\rho_{\mathbb{K}}$
- The amount of backflow is not controled

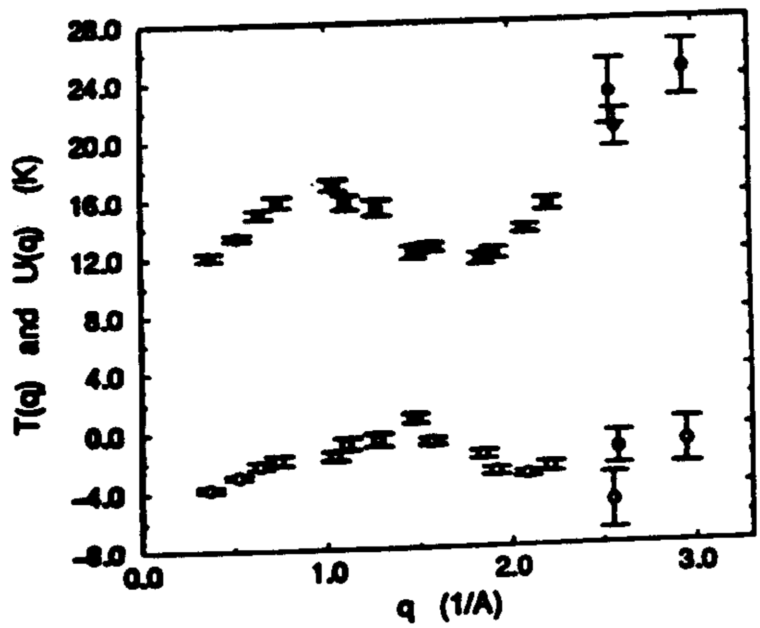


Comtributions of The Kimectic And Potential Emergies to The Excitation Spectrum

The roton region

$$\Delta \simeq 9\,K \simeq \underbrace{12\,K}_{\text{Kimectic}} - \underbrace{3\,K}_{\text{Potential}}$$

Rotom:
- a strongly amharmomic excitation
- imcreases the local order



The Shadow Particle Approach to The Phonon-Roton Spectrum With Explicit Backflow

$$\Psi_{BSh\,\mathbb{K}}(R) = \prod_{i<j} f(r_{ij}) \int ds\, \sigma_{B\mathbb{K}} \prod_i e^{-c|\mathbf{r}_i - \mathbf{s}_i|^2} \prod_{i<j} e^{-\beta v(\epsilon s_{ij})}$$

$$\sigma_{B\mathbb{K}} = \sum_j e^{i\mathbb{K}\cdot[\mathbf{s}_j - \sum_{\ell\neq j} \lambda_{\mathbb{K}}(s_{j\ell})\mathbf{s}_{j\ell}]}$$

$$\lambda_{\mathbb{K}}(s) = \begin{cases} A_{\mathbb{K}} \left(\frac{s}{s_0} - 2\right)^2 e^{-\left(\frac{s-s_0}{\omega}\right)^2} & \text{if } s \leq s_0 \\ 0 & \text{otherwise} \end{cases}$$

$A_{\mathbb{K}}$, s_0 and ω parameters

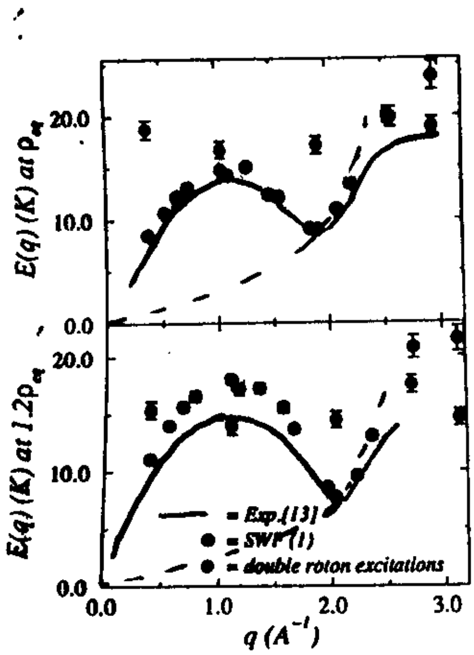
- The amount of backflow is a function of $\mathbb{K}$

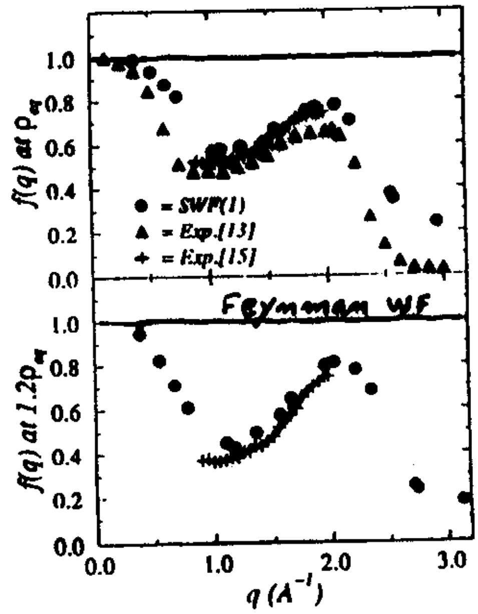
Density	WF	ε_{roton}	ε_{maxon}
ρ_0	Sh	10.0	16.2
	Sh-B	9.2	14.8
	Exp	8.6	13.9
$1.2\rho_0$	Sh	8.5	18.2
	Sh-B	7.9	17.1
	Exp	7.3	15.0

Optimized Shadow Wave Function

(Galli, Cecchetti & Reatto, PRL 77, 5401, 1996)

$$\Psi_{BShK}(R) = \prod_{i<j} f(r_{ij}) \int ds\, \sigma_{BK} \prod_i f(|r_i - s_i|) \prod_{i<j} e^{-\beta v(\delta s_{ij})}$$





$$f(q) = \frac{Z(q)}{S(q)}$$

Double roton excited state

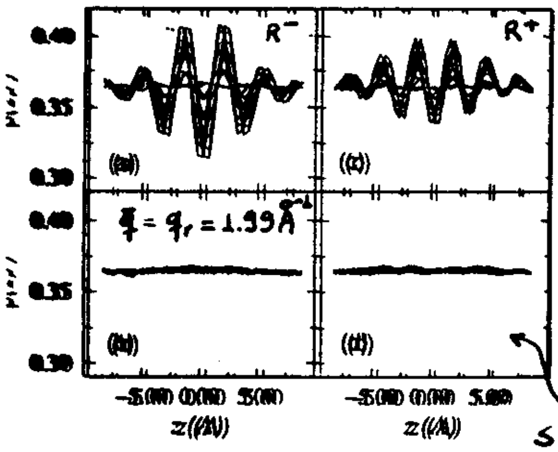
$$\sigma_{Bq} \longrightarrow \sigma_{Bq}\, \sigma_{B\,q-k}$$

Rotom Wave Packets

$$\sigma_{\mathbf{q}} \longrightarrow \sigma_{\mathbf{r}_0, \mathbf{q}_0, \Delta} = \sum_j f(|\tilde{\mathbf{s}}_j - \mathbf{r}_0|)\, e^{i\mathbf{q}_0 \cdot (\tilde{\mathbf{s}}_j - \mathbf{r}_0)}$$

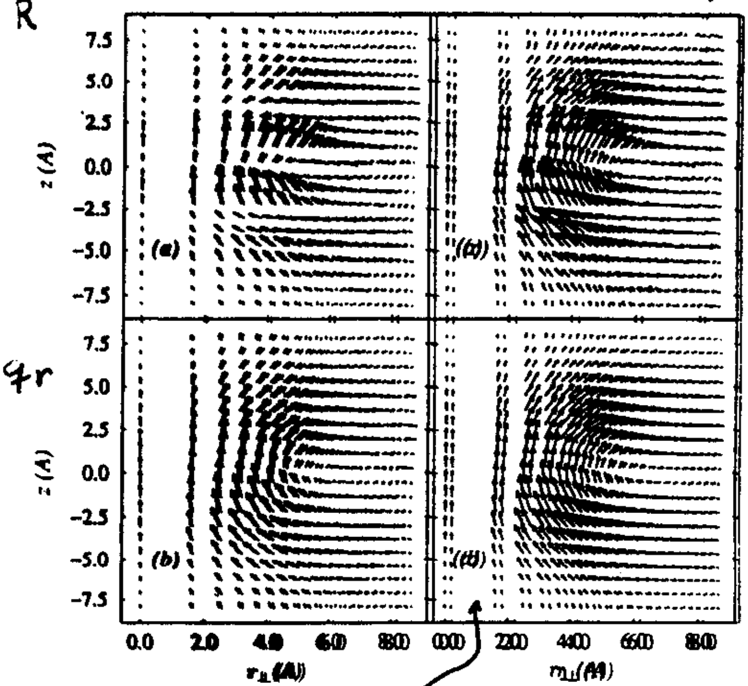
$$f(s) = e^{-\Delta^2 s^2} + e^{-\Delta^2 (s-L)^2} - 2e^{\Delta^2 (\frac{L}{2})^2}$$

$\langle \rho(z, r_\perp) \rangle$



single particle

$\langle \mathbf{j}(z, r_\perp) \rangle$



single particle

Gaussian wave packet $\begin{cases} \mathbf{q}_0 = q_0 \hat{k} & \text{wave vector} \\ \Delta = 0.25\,\text{Å} & \text{spread} \end{cases}$

At $q = q_r$

- backflow $\Rightarrow$ simple dipolar flow $\equiv$ vortex ring
- equivalent excitations $\begin{cases} \cdot \text{ distinguished particle} \\ \cdot \text{ collective} \end{cases}$

The nonpolynomial structure in $\rho_{\mathbf{k}}$

$$\Psi_{sh\,\mathbf{k}}(R) = \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \prod_{i<j} f(r_{ij})$$

$$\int ds\, e^{i\mathbf{k}\cdot(\mathbf{s}_j-\mathbf{r}_j)} \prod_i e^{-C|\mathbf{r}_i-\mathbf{s}_i|^2} \prod_{i<j} e^{-\beta v(s_{ij})}$$

Cumulant expansion

$$\langle e^{\varphi(\mathbf{r})} \rangle_r = e^{\langle \varphi(r) \rangle + \cdots}$$

$$\Psi_{sh\,\mathbf{k}}(R) = \sum_j e^{i\mathbf{k}\cdot[\mathbf{r}_j - \sum_{\ell\neq j} \varphi(r_{j\ell})\,\mathbf{r}_{j\ell}]}\, \Psi(R)$$

$$\varphi(r) = \frac{1}{2c}\,\beta\,\frac{v'}{r}$$

Backflow is not treated as a perturbatio

The Ground State Energy

The Hamiltonian

for a system of ^{4}He atoms

$$H = \sum_j T_j + V_j$$

$$T_j = -\frac{\hbar^2}{2m} \nabla_j^2 \quad \text{and} \quad V_j = \frac{1}{2} \sum_{\ell \neq j} v(|\mathbf{r}_j - \mathbf{r}_\ell|)$$

$$\Psi_T(R) = \int ds \, \Xi(R,S)$$

$$E_T = \frac{\int dR \, \Psi_T(R) \, H \, \Psi_T(R)}{\int dR \, \Psi_T^2(R)} \geqslant E_0$$

$$= \frac{\int dR\,ds\,ds' \, \Xi(R,S') \, H \, \Xi(R,S)}{\int dR\,ds\,ds' \, \Xi(R,S') \, \Xi(R,S)}$$

$$= \int dR\,ds\,ds' \, f(R,S,S') \, E_L(R,S)$$

$$f(R,S,S') = \frac{\Xi(R,S)\,\Xi(R,S')}{\int dR\,dS\,dS'\,\Xi(R,S)\,\Xi(R,S)}$$

$$\Xi(R,S,S') = \prod_{i<j} f(r_{ij}) \prod_i e^{-c|\mathbf{r}_i - \mathbf{s}_i|^2} \prod_{i<j} e^{-\beta v(s_{ij})}$$

$$E_L(R,S) = \frac{H \prod_{i<j} f(r_{ij}) \prod_i e^{-c|\mathbf{r}_i - \mathbf{s}_i|^2}}{\prod_{i<j} f(r_{ij}) \prod_i e^{-c|\mathbf{r}_i - \mathbf{s}_i|^2}}$$

$$\hat{E}_T = \frac{1}{M} \sum_{i=1}^{M} E_L(R_i, S_i)$$

$$Var(\hat{E}_T)_f$$

$$E_T = \langle E_L(R,S) \rangle$$

The Excited State Energy

$$E_K = \frac{\int dR\,ds\,ds'\,\sigma_{IK}'\,\sigma_{IK}\,\Xi(R,s')\,H\,\Xi(R,s)}{\int dR\,ds\,ds'\,\sigma_{IK}'\,\sigma_{IK}\,\Xi(R,s')\,\Xi(R,s)}$$

$$= \frac{\dfrac{\int dR\,ds\,ds'\,\sigma_{IK}'\,\sigma_{IK}\,\Xi(R,s')\,\Xi(R,s)\,\dfrac{H\,\Xi(R,s)}{\Xi(R,s)}}{\int dR\,ds\,ds'\,\Xi(R,s')\,\Xi(R,s')}}{\dfrac{\int dR\,ds\,ds'\,\sigma_{IK}'\,\sigma_{IK}\,\Xi(R,s')\,\Xi(R,s)}{\int dR\,ds\,ds'\,\Xi(R,s')\,\Xi(R,s')}}$$

$$= \frac{\int dR\,ds\,ds'\,f(R,s,s')\,\sigma_{IK}'\,\sigma_{IK}\,E_L(R,s)}{\int dR\,ds\,ds'\,f(R,s,s')\,\sigma_{IK}'\,\sigma_{IK}}$$

$$= \frac{\langle \sigma_{IK}'\,\sigma_{IK}\,E_L(R,s)\rangle}{\langle \sigma_{IK}'\,\sigma_{IK}\rangle}$$

The Excitation Spectrum

$$\mathcal{E}_K = E_K - E_T$$

Shadow Density Matrix

A model to compute properties at finite temperature

An extention of the
Penrose-Reatto-Chester density matrix

$$\langle R|\rho_T|R'\rangle = \sum_n \Psi_n^*(R)\,\Psi_n(R')\,e^{-\beta E_n}$$

At $T=0$ R and R' are uncoupled

$$\langle R|\rho_0|R'\rangle = \Psi_0(R)\,\Psi_0(R')$$

Independent excitations at Low T

Total energy: $E_{\{n_q\}} = E_0 + \sum_K n_K \epsilon_K$

- ϵ_K → excitation spectrum
- n_K → number of excitations
- E_0 → ground state energy

The shadow particle approach to a
multiple excited state

$$\Psi_{Sh\{n_K\}}(R) = \prod_{i<j} f(r_{ij}) \int dS \prod_{K} \sigma_{K}^{n_K} \prod_i e^{-C|r_i - s_i|^2} \prod_{i<j} e^{-\beta v(\gamma s_{ij})}$$

Shadow Density Matrix

$$\langle R | \rho_T | R' \rangle =$$

$$= \int ds\, ds'\, \Xi(R,S)\, \Xi(R',S') \prod_{i<j} e^{-\chi_1^T(s_{ij}) - \chi_1^T(s'_{ij})} \prod_{i,j} e^{-\chi_2^T(|s_i - s'_j|)}$$

$$\chi_i^T(s) = \frac{\rho^{-1}}{(2\pi)^3} \int d^3k\, \chi_i^T(k)\, e^{i \mathbf{k} \cdot \mathbf{s}}$$

$$\chi_1^T(k) = \frac{e^{-\beta\varepsilon_k}}{e^{\beta\varepsilon_k} - e^{-\beta\varepsilon_k}} \frac{N}{\langle \sigma'_k \sigma_k \rangle} \qquad \chi_2^T(k) = \frac{-1}{e^{\beta\varepsilon_k} - e^{-\beta\varepsilon_k}} \frac{N}{\langle \sigma'_k \sigma_k \rangle}$$

- Contributions to χ_i^T come from $\mathbf{k}$ regions where $\varepsilon_{\mathbf{k}}$ is small
  - The roton region: $\varepsilon_k = \varepsilon_r + \frac{\hbar^2}{2\mu}(k - k_r)^2$ (from experiment)
  - The phonon region: disregarded long range function

Results

All quantities are easelly computed

E(T) from Landau formula

$$E(T) = E_0 + \frac{1}{N} \sum \varepsilon_k \frac{1}{e^{\beta \varepsilon_k} - 1}$$

E(T) from simulations

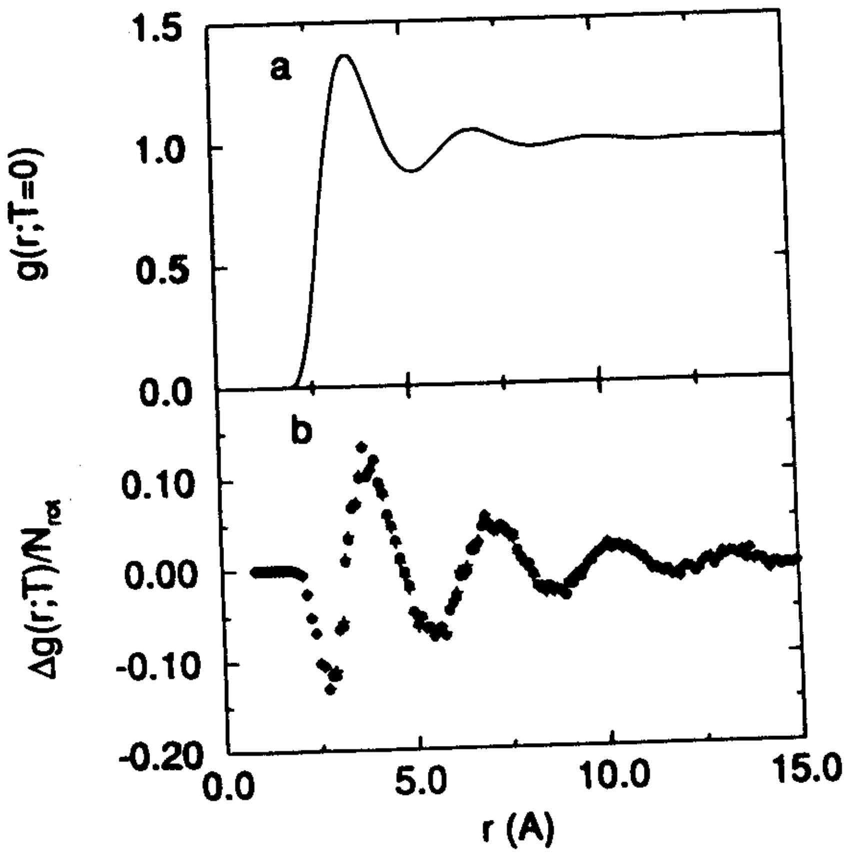
} agreement better than 1%

$$\Delta g(r;T) = g(r;T) - g(r;T=0)$$

$$\Delta g(r;T) \propto N_{rot}$$

A roton excitation lowers the potential energy

- • $\Delta g(r;T=1.4)/N_r$
- + $\Delta g(r;T=2.1)/N_r$

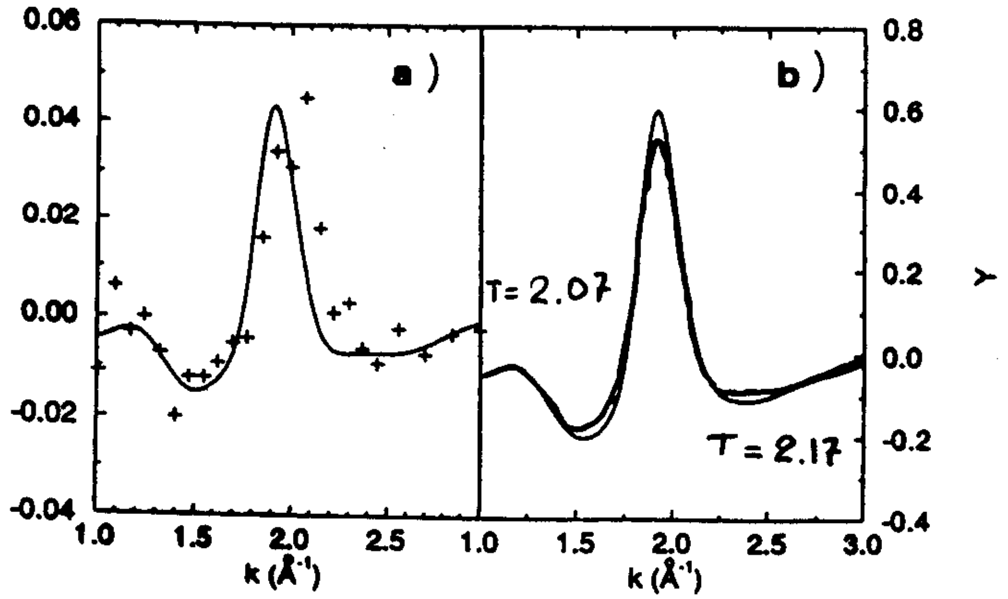


The Structure Factor

$$\Delta S(K;T) = S(K;T) - S(K;T=0)$$

$$Y(K;T) = \Delta S(K;T) / N_r$$

+ Exp. $S(K;2.07) - S(K;1.00)$



The Roton

At $q = q_R$

- Behavior of a vortex ring scaled down to atomic size
- Is essentially the same as a single particle excitation

As q moves away from q_R

- Interference effects between atoms modifies the properties of the collective excitation

Large effects of backflow in the full roton mimimum

Five to ten rotons are needed to deplete the condensate by one particle

Quantum Vortices

We want to clarify

- How the vorticity is distributed
- How the fluid density varies

FEYNMAN'S APPROACH
TO A VORTEX LINE

$$\Psi_F(R) = \prod_{j=1}^{N} f(\rho_j) e^{i\theta} \Psi_0(R)$$

$\Psi_0(R)$ is the ground-state wave function

$$R \equiv \{\mathbf{r}_j \mid j = 1, \ldots, N\}$$

$$\theta = \sum_{j=1}^{N} \theta_j$$

θ_j is the cylindrical angle of particle j

$$\lim_{\rho \to 0} f(\rho) = 0 \quad \text{and} \quad \lim_{\rho \to \infty} f(\rho) = 1$$

$$\rho_j = \sqrt{x_j^2 + y_j^2}$$

ρ_j is the radial distance to the vortex axis

THE SHADOW WAVE APPROXIMATION

$$\Psi_F(R) = \prod_{j=1}^{N} f(\rho_j) e^{i\theta} \Psi_T(R)$$

$$f(\rho) = 1 - e^{-\left(\frac{\rho}{a}\right)^2}$$

a **is a variational parameter**

$$\Psi_0(R) \simeq \Psi_T(R)$$

$\Psi_T(R)$ **is a trial shadow wave function**

Empty core - Localized vorticity

THE SHADOW WAVE FUNCTION
FOR THE GROUND-STATE

$$\Psi_T(R) = \psi(R) \int k(R,S)\psi_s(S)dS$$

$$S \equiv \{\mathbf{s}_j \mid j = 1, \ldots, N\}$$

$$dS = d\mathbf{s}_1 d\mathbf{s}_2 \cdots d\mathbf{s}_N$$

$$\psi(R) = \prod_{j<l} e^{-\frac{1}{2}u(r_{jl})} \quad \text{and} \quad \psi_s(S) = \prod_{j<l} e^{-u_s(s_{jl})}$$

$$u(r_{jl}) = \left(\frac{b}{|\mathbf{r}_j - \mathbf{r}_l|}\right)^5 \quad \text{and} \quad u_s(s_{jl}) = \left(\frac{b_s}{|\mathbf{s}_j - \mathbf{s}_l|}\right)^9$$

$$k(R,S) = \prod_j e^{-C(\mathbf{r}_j - \mathbf{s}_j)^2}$$

b, b_s and C are variational parameters

CYLINDRICAL CONTAINER

1-body terms for particles and

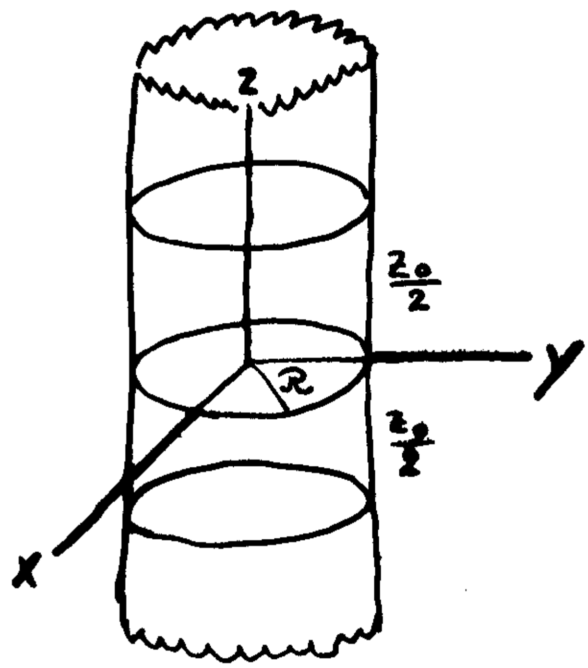
for shadow particles

$$\phi(R) = \prod_{j=1}^{N} \tanh d(\mathcal{R}^2 - \rho_j^2)$$

$$\varphi(R) = \prod_{j=1}^{N} \tanh d_s(\mathcal{R}^2 - \varrho_j^2)$$

d **and** d_s **are variational parameters**

$\mathcal{R}$ **is the cylinder's radius**



VORTEX LINE WAVE FUNCTION WITH DELOCALIZED VORTICITY

$$\Psi_d(R) = \psi(R) \int e^{i\vartheta} k(R,S) \psi_s(S) dS$$

$$\vartheta = \sum_{j=1}^{N} \vartheta_j$$

ϑ_j - cylindrical angle of shadow particle j

$\Psi_d(R)$ is an eigenstate of $\hat{L}$

$$\hat{L}\Psi_d(R) = N\hbar\Psi_d(R)$$

- **distributed vorticity**
- **non vanishing density at the vortex axis**
- **no extra variational parameters**

The Ground State Energy

The average number of particles

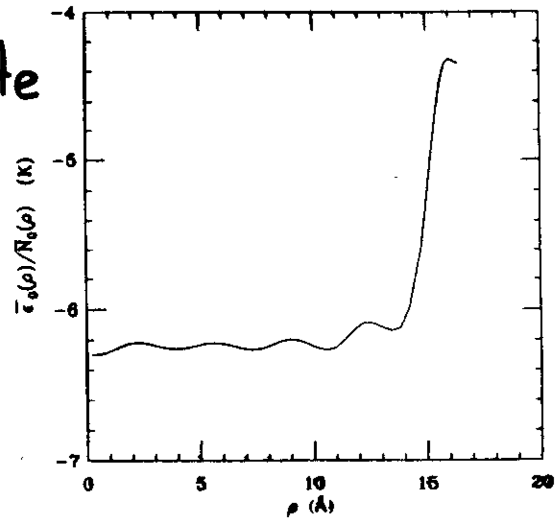
$$\bar{\mathcal{N}}_0(\rho) = z_0 \int_0^{\rho} n(\rho')\, d^2\rho'$$

The energy function

$$\bar{\mathcal{E}}_0(\rho) = \left\langle \sum_j \theta(\rho - \rho_j) \frac{(T_j + V_j)\,\Xi(R,S)}{\Xi(R,S)} \right\rangle$$

where $\theta(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$

$\dfrac{\bar{\mathcal{E}}_0(\mathcal{R})}{\bar{\mathcal{N}}_0(\mathcal{R})}$ is the estimate ground state energy per particle



SUMMARY

FEYNMAN WAVE FUNCTION

$$\Psi_F(R) = \prod_{j=1}^{N} f(\rho_j) e^{i\theta} \Psi_T(R)$$

$$f(\rho) = 1 - e^{-\left(\frac{\rho}{a}\right)^2}$$

a **is a variational parameter**

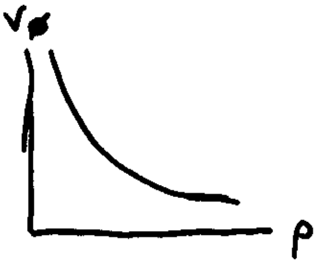
VORTEX LINE WAVE FUNCTION
WITH DELOCALIZED VORTICITY

$$\Psi_d(R) = \psi(R) \int e^{i\vartheta} k(R, S) \psi_s(S) dS$$

Vortex Lines in Superfluid ^4He

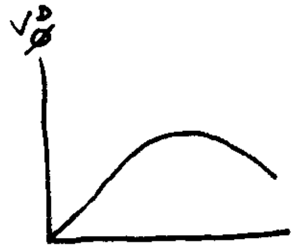
Feynman-Onsager

$$v_\phi = \frac{\hbar}{m}\,\frac{1}{\rho}$$

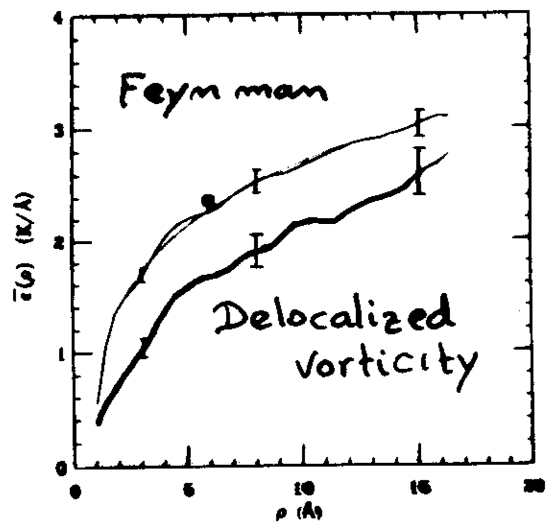


Delocalized vorticity

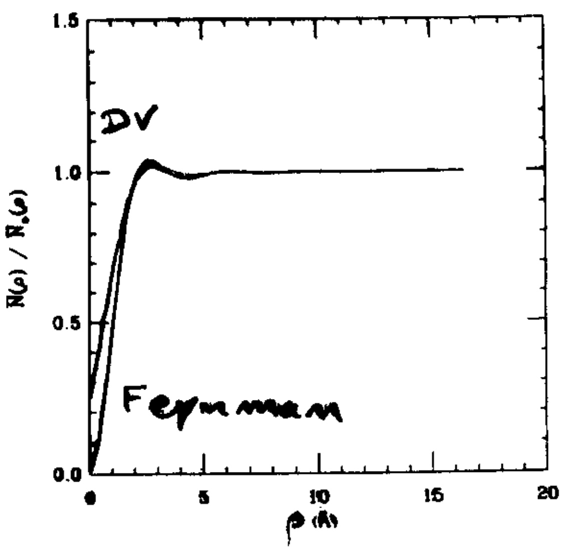
$$v_\phi^D = \frac{\hbar}{2m}\int d^3s\,\frac{n(\mathbf{r}|\mathbf{s})}{n(r)}\,\frac{1}{\ell}$$



The energy per unit length



The density profile



- To investigate properties of the roton spectrum and roton wave packets
- To construct a density matrix and compute properties at finite temperature
- To investigate vortex lines with distributed vorticity

Why use a Shadow Wave Function?

- To model the crystalization of a quantum many-body system
- To understand quantitative differences between theory and experiment
- To impose particle modulations in a very flexible way

For the low-lying states

- Introduces backflow in all orders of the density fluctuations in the roton spectrum
- Allows the investigation of vortices with distributed vorticity

In summary: The shadow particle approach is a very powerful tool to describe many different aspects of quantum liquids and solids

Conclusions

The Shadow Wave Function

- Introduces quantum delocalization of the particles explicitly in a variational description
- Describes the crystalline order as a spontaneously broken symmetry
- Allows the investigation of self-bound states of inhomogeneous systems
- A simple way of introducing high-order correlations