Thermodynamics, quasiparticle and collective excitations of dipolar Bose gases

Alexey Filinov

Christian-Albrechts-Universität Kiel, ITAP, Germany,
JIHT RAS, Izhorskaya Str., 13, 125412 Moscow, Russia

20.09.2011

Michael Bonitz, Nikolay Prokof'ev

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

FINESS 2011, Heidelberg 17-21 Sept.

Outline

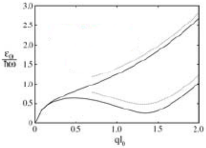
1. Dipole systems
2. Thermodynamics: eos, superfluidity, momentum distribution
3. Response functions
4. Stochastic optimization method
5. Single and two-particle Green's function
6. Collective and one-particle excitations: $S(q,\omega)$, $A(q,\omega)$
7. Summary
8. Appendix

Outline

Interesting physics of dipolar bosons

$$U_d(\mathbf{r}) = \frac{\mu_0}{4\pi}\mu^2 \frac{1 - 3\cos^2(\theta)}{r^3}$$

- **Anisotropy of the interaction**:
  – New dispersion relations of elementary excitations: roton minimum due to the vertical coupling
  – New equilibrium shapes
  – Stability depends on the trap geometry

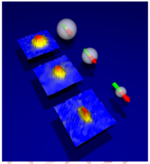


- **Theory:** Supersolid/Insulating phases in optical lattices

- **Pancake geometry**: Superfluid-normal phase transition – Berezinskii-Kosterlitz-Thouless scenario

- **Tuning of interactions**: Long-range dipolar forces compete short-range s-wave scattering

Lahaye, Griesmaier, Pfau et al., Nature 448, 672 (2007)



Physical realizations and some numbers

Key parameters:
– Effective radius of dipole-dipole interaction

$$\boxed{a_d = \frac{me^2 d^2}{\hbar^2}}$$

– Strength of dipole interaction

$$\boxed{D = a_d/a} \quad a = 1/\sqrt{n}$$

- Cold bosonic atoms with a permanent magnetic moment in tight pancake traps (^{52}Cr)
  – magnetic dipoles are aligned by a magnetic field

$$\mu_{Cr} = 6\mu_B, \quad a_d \approx 24\AA$$

- Molecules with an electric dipole moment
  – permanent moment (long molecules $^{15}ND_3, H^{12}C^{14}N$)

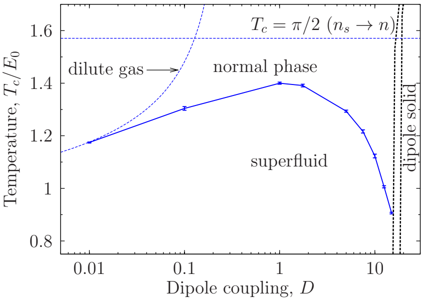
$$E \sim 10kV/cm, \quad ed = 0.1\ldots1 \text{ Debye } (1\mu_B \approx 10^{-2}\text{Debye}), \quad a_d = 10\ldots10^4\AA$$

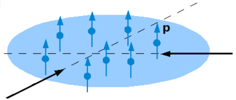
  – moment induced by DC electric field: $E \sim 10^3 kV/cm, \quad ed \sim 0.1\text{Debye}, \quad a_d \sim 10\AA$
- Composite bosons formed by two fermions: bound electron-hole pairs (excitons)

Moderate coupling: $\boxed{D = 1}$ $(a = a_d)$ **Typical densities**: $\boxed{n = a_d^{-2} = 10^{14}\ldots10^8 \text{ cm}^{-2}}$

Present analysis: $\boxed{D = 0.1\ldots15}$

Phase diagram in 2D





Phase transitions:

- Crystallization at $T = 0$ [1]
  $D = 17 \pm 1$
- Classical gas-solid transition [2]
  $\Gamma_D = 62 \pm 3$
- Normal-superfluid transition [3]

Hamiltonian: $\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j} \frac{p^2}{|\mathbf{r}_i - \mathbf{r}_j|^3}$

Classical regime

$\langle E_{\rm pot}\rangle \sim p^2/a^3, \quad \langle E_{\rm kin}\rangle = 1/\beta$

Coupling: $\Gamma_D = \beta p^2/a^3$

Quantum regime

$\langle E_{\rm pot}\rangle \sim p^2/a^3, \quad \langle E_{\rm kin}\rangle \sim \hbar^2/ma^2$

Coupling: $D = mp^2/\hbar^2 a \ \propto n^{1/2}$

[1] Astrakharchik *et al.*, Phys. Rev. Lett. **98**, 060405 (2007); Büchler *et al.*, Phys. Rev. Lett. **98**, 060404 (2007)
[2] Kalia and Vashishta, J. Phys. C: Solid State Phys. **14**, 643 (1981)
[3] Filinov, Prokof'ev and Bonitz, Phys. Rev. Lett. **105**, 070401 (2010)

Methods: quantum Monte Carlo (PIMC)

- Symmetric/antisymmetric density matrix (bosons/fermions)

$$\langle R|\hat{\rho}^{S/A}|R'\rangle = \rho^{S/A}(R,R';\beta) = \frac{1}{N!}\sum_{P=1}^{N!}(\pm 1)^{\delta P}\rho(R,\hat{P}R';\beta)$$

$R = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ is the N-particle radius vector.

- Feynman's path integrals

$$\hat{\rho}(\beta) = e^{-\beta\hat{H}} = \left[e^{-\frac{\beta}{M}\hat{H}}\right]^M = [\hat{\rho}(\tau)]^M, \ \tau = \beta/M,$$

$$\rho(R,\hat{P}R';\beta) = \int \mathrm{d}R_1 \ldots \mathrm{d}R_{M-1}\,\rho(R,R_1;\tau)\ldots\rho(R_{M-1},\hat{P}R';\tau)$$

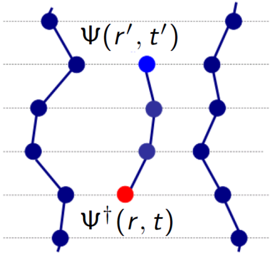
- Grand canonical ensemble [1]

$$Z = \sum_{N=0}^{\infty} e^{\beta\mu N}\ \mathrm{Tr}\left[e^{-\beta\hat{H}}\right]$$

Matsubara Green's function

$$G_1(r',t';r,t) = \langle\hat{\Psi}(r',t')\hat{\Psi}^{+}(r,t)\rangle =$$

$$\frac{1}{ZV}\ \mathrm{Tr}\left[e^{\beta\mu\hat{H}}e^{-(\beta-\tau)\hat{H}}\ \hat{a}(r')\,e^{-\tau\hat{H}}\ \hat{a}^{+}(r)\right]$$



[1] Boninsegni, Prokof'ev, and Svistunov, Phys. Rev. E 74, 036701 (2006)

Outline

Equation of state

$$\epsilon(n) = E(n)/N = \epsilon_{\text{pot}}(n) + \epsilon_{\text{kin}}(n) \approx a_1\, n^{3/2} + a_2\, n^{5/4}$$

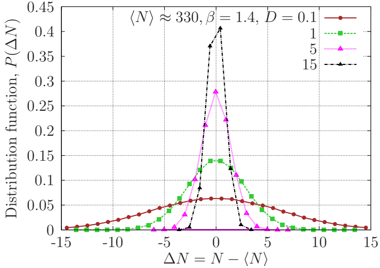
- Finite-size scaling

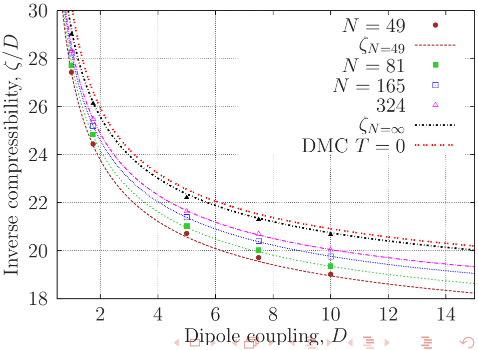
$$\epsilon_N(n) = \epsilon(n) - f_\epsilon(N), \quad f_\epsilon(N) = \frac{1}{2}\int_{L/2}^{\infty} \mathrm{d}r\, 2\pi r\, \frac{p^2}{r^3}\, g(r) + \tilde{f}_\epsilon(N)$$

- Chemical potential: $\mu(n) = \partial E(n)/\partial N$

  Compressibility: $\kappa V T = \langle (N - \langle N \rangle)^2 \rangle_\mu, \quad \zeta(n) = 1/\kappa(n)$

  Zero sound: $m c_T^2(n) = n\,\zeta(n)$





Normal fluid to superfluid transition

- Superfluid density n_s: winding number from PIMC simulations

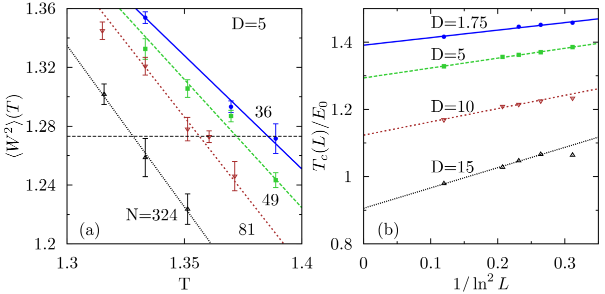
$$n_s(L,T) = \frac{mk_B T \langle \mathbf{W}^2(T) \rangle}{2\hbar^2}$$

- $T_c(L)$ from universal jump of superfluid fraction [1]

$$n_s(L,T_c) = \frac{2mk_B}{\pi\hbar^2} T_c, \quad \langle W^2 \rangle = 4/\pi$$

- $T_c(\infty)$, macroscopic system: finite-size scaling [2]

$$T_c(L) = T_c(\infty) + b/\ln^2(L)$$



[1] Nelson and Kosterlitz, Phys. Rev. Lett. 39, 1201 (1977)

[2] Filinov, Prokof'ev and Bonitz, Phys. Rev. Lett. **105**, 070401 (2010)

Normal fluid to superfluid transition

- Superfluid density n_s: winding number from PIMC simulations

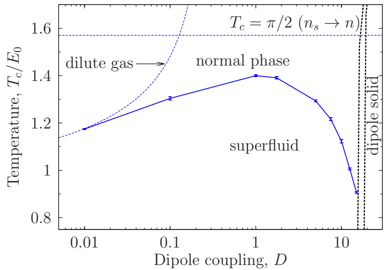
$$n_s(L,T) = \frac{mk_B T \langle \mathbf{W}^2(T) \rangle}{2\hbar^2}$$

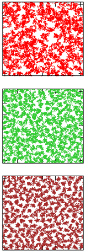
- $T_c(L)$ from universal jump of superfluid fraction [1]

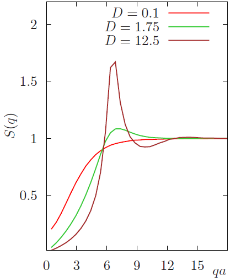
$$n_s(L,T_c) = \frac{2mk_B}{\pi\hbar^2} T_c, \quad \langle W^2 \rangle = 4/\pi$$

- $T_c(\infty)$, macroscopic system: finite-size scaling [2]

$$T_c(L) = T_c(\infty) + b/\ln^2(L)$$





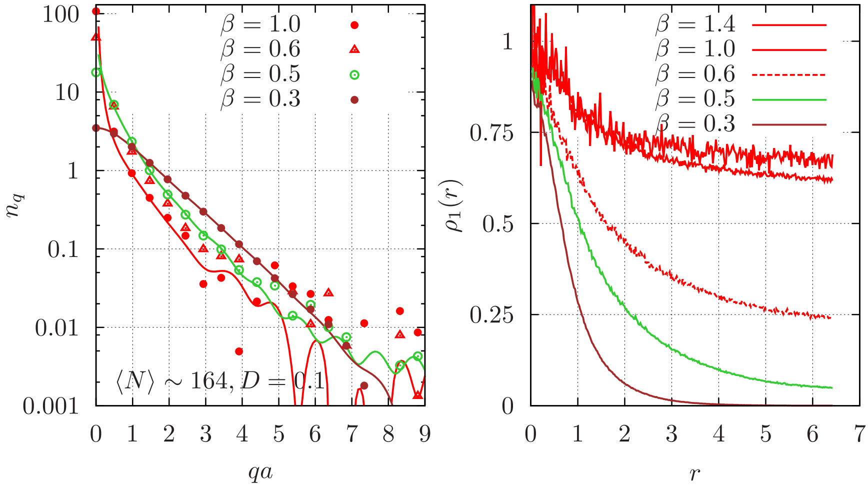


[1] Nelson and Kosterlitz, Phys. Rev. Lett. 39, 1201 (1977)

[2] Filinov, Prokof'ev and Bonitz, Phys. Rev. Lett. **105**, 070401 (2010)

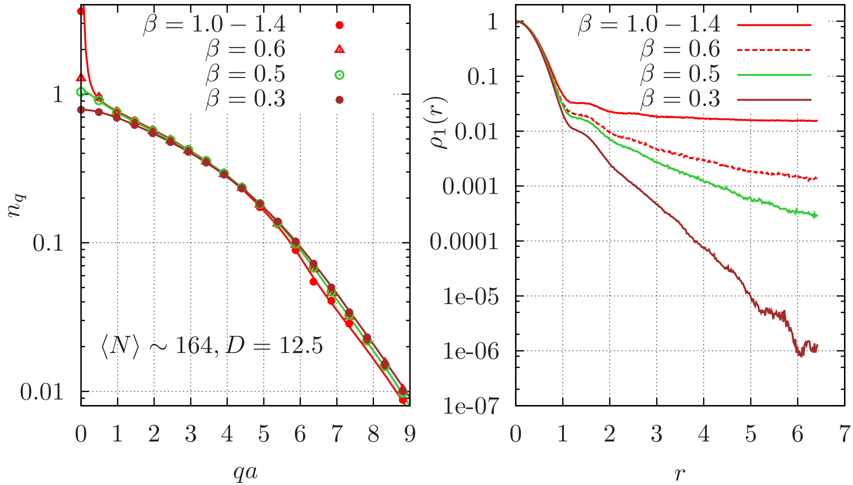
Momentum distribution: T-dependence

$$n_q = \langle \hat{a}_q^+ \hat{a}_q \rangle = \int \int_V \mathbf{dr}\, \mathbf{dr}'\, e^{i\mathbf{q}(\mathbf{r}'-\mathbf{r})} \langle \hat{\Psi}(\mathbf{r}', t) \hat{\Psi}^+(\mathbf{r}, t) \rangle$$



Momentum distribution: T-dependence

$$n_q = \langle \hat{a}_q^+ \hat{a}_q \rangle = \int \int_V \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}'\, e^{i\mathbf{q}(\mathbf{r}'-\mathbf{r})} \langle \hat{\Psi}(\mathbf{r}', t) \hat{\Psi}^+(\mathbf{r}, t) \rangle$$



Momentum distribution $T \ll T_c$: long-wave length limit

Collisionless $[T = 0,\ \rho_s = \rho]$ low-frequency regime (Gavoret and Nozie're s, 1964)

$$A(q,\omega) = 2\pi(Z(q) + 1/2\pi)\delta(\omega - cq) - 2\pi Z(q)\delta(\omega + cq)$$

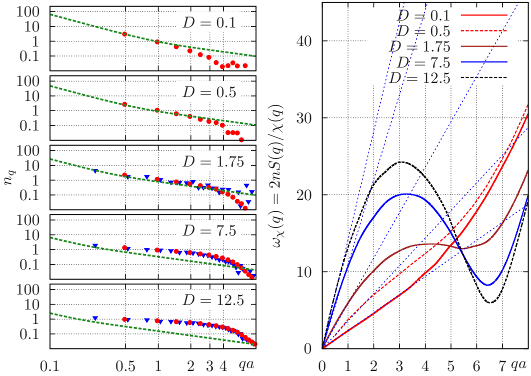
Sum rules for the spectral density

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(q,\omega) = 1, \qquad \lim_{q\to 0} -G_{11}(q,\omega=0) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{A(q,\omega)}{\omega} = \frac{m^2 n_0}{\rho_s q^2}$$

By substitution we obtain

$$\boxed{n_q = Z(q)\,[2N(cq)+1]}, \quad Z(q) = \frac{m^2 n_0 c}{2\rho_s q}, \quad N(\omega) = \frac{1}{e^{\beta\omega} - 1}$$

Momentum distribution $T < T_c$: long-wavelength limit



D	μ $(V = 165)$	c	$n_0 = N_{p=0}/\langle N\rangle$	
0.1	4.7	2.35	0.65	(107.1/163.69)
0.5	12.55	3.60	0.47	(77.0/163.18)
1.75	31.10	5.90	0.26	(43.15/162.97)
7.5	102.20	11.0	0.061	(9.81/162.05)
12.5	163.53	14.14	0.022	(3.61/164.46)

Outline

Excitations in Bose liquids: response functions

- Neutron scattering: $\frac{d^2\sigma}{d\Omega dE} = \frac{b^2}{\hbar}\frac{k_1}{k_0} S(\mathbf{q},\omega)$, $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_1$, $\hbar\omega = \frac{\hbar^2 k_0^2}{2m} - \frac{\hbar^2 k_1^2}{2m}$
- The dynamic structure factor

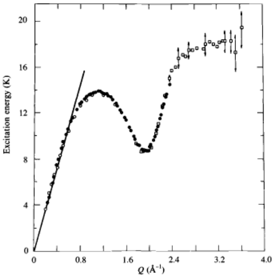
$$S(\mathbf{q},\omega) = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\langle \hat{\rho}_q(t)\hat{\rho}_q^+(0)\rangle$$

– density operator: $\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r}-\mathbf{r}_j)$, $\hat{\rho}_q = \sum_i e^{-i\mathbf{q}\mathbf{r}_i} = \hat{\rho}_{-q}^+ = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}-\mathbf{q}}^+ \hat{a}_{\mathbf{k}}$

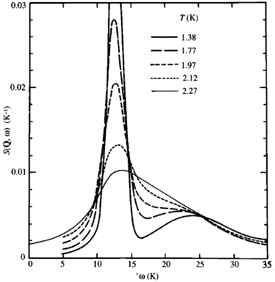
- Static structure factor (instantaneous correlations between atoms)

$$S(\mathbf{q}) = S(\mathbf{q}, t=0) = \frac{1}{N}\sum_{i,j}\langle e^{-i\mathbf{q}\mathbf{r}_i} e^{i\mathbf{q}\mathbf{r}_j}\rangle = \int_{-\infty}^{\infty} d\omega\, S(\mathbf{q},\omega)$$

Quasiparticle dispersion curve: phonon-maxon-roton



Scattering data $S(q,\omega)$ at $q = 0.8$ Å^{-1}. Woods, Svensson, Griffin



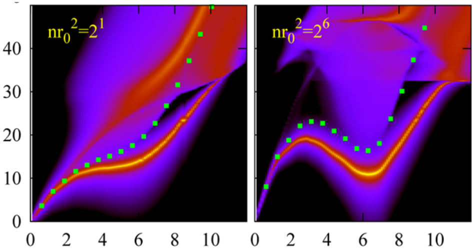
Dynamic structure factor: 2D dipolar bosons, $T = 0$

Dynamic structure factor in *correlated basis functions* (CBF) theory [1]

- Decay of single excitations (Feynman) into two due to the self-energy $\sum(q,\omega)$

$$S(q,\omega) = -\frac{1}{\pi} Im \frac{S(q)}{\epsilon(q) - \epsilon_F(q) - \sum(q,\omega) + i\nu}, \quad \epsilon_F(q) = \frac{\hbar^2 q^2}{2mS(q, T=0)}$$

- Spectrum of excitations (peak position): $\epsilon(q) - \epsilon_F(q) - Re\sum(q,\omega) = 0$



F. Mazzanti et.al., Phys.Rev.Lett. **102**, 110405(2009)

- $Im\sum(q,\omega) \neq 0$: damping/decay of excitations and peak broadening
- $Im\sum(q,\omega) \sim Re\sum(q,\omega)$: not a well defined dispersion, multiexcitation continuum
- Present analysis: $S(q,\omega)$ at $T \neq 0$ and near the superfluid phase transition $T \approx T_c$

[1] E. Feenberg, *Theory of Quantum Liquids* (Academic Press, NY 1967); C.C. Chang and C.E. Campbell, Phys.Rev.B **13**, 3779(1976)

Density operator in the presence of condensate

Decomposition of field operators (Beliaev, 1958)

$$\hat{\Psi}(\mathbf{r}) = \hat{\Psi}_0(\mathbf{r}) + \tilde{\Psi}(\mathbf{r}) = \frac{\hat{a}_0}{\sqrt{V}} + \frac{1}{\sqrt{V}} \sum_{\mathbf{q}\neq 0} e^{i\mathbf{qr}}\, \hat{a}_q$$

Number density operator for any system with condensate $\langle \hat{\Psi}_0(\mathbf{r}) \rangle = \sqrt{n_0} e^{i\phi}$

$$\hat{\rho}(\mathbf{Q}) = \sum_{\mathbf{q}} \hat{a}^+_{\mathbf{q}} \hat{a}_{\mathbf{q}+\mathbf{Q}} = \hat{a}^+_0 \hat{a}_Q + \hat{a}^+_{-Q} \hat{a}_0 + \sum_{\mathbf{q}\neq 0} \hat{a}^+_{\mathbf{q}} \hat{a}_{\mathbf{q}+\mathbf{Q}}$$

Coupling of the single-particle operators to the density operator

$$\hat{\rho}(\mathbf{Q}) = \sqrt{N_0} \hat{A}_{\mathbf{Q}} + \tilde{\rho}_{\mathbf{Q}}, \quad \hat{A}_{\mathbf{Q}} = \hat{a}_{\mathbf{Q}} + \hat{a}^+_{-\mathbf{Q}}$$

Dynamic structure factor $T \neq 0$

Dynamic structure factor

$$S(\mathbf{Q},\omega) = \mathcal{F}\{\langle \hat{\rho}_{\mathbf{Q}}(t)\hat{\rho}_{-\mathbf{Q}}(0)\rangle\}, \quad \mathcal{F} = \frac{1}{2\pi N}\int_{-\infty}^{\infty} dt\, e^{i\omega t}$$

$$S(\mathbf{Q},\omega) = S_1(\mathbf{Q},\omega) + S_{int}(\mathbf{Q},\omega) + \tilde{S}(\mathbf{Q},\omega)$$

Density fluctuations (Hugenholtz and Pines, 1959)

Normal fluid: $\tilde{S}(\mathbf{Q},\omega) = \mathcal{F}\{\langle \tilde{\rho}_{\mathbf{Q}}(t)\tilde{\rho}_{-\mathbf{Q}}(0)\rangle\}$,

Bose condensate: $S_1(\mathbf{Q},\omega) = \mathcal{F}\{N_0 \langle \hat{A}_Q(t)\hat{A}_{-Q}(0)\rangle\}$,

Interaction: $S_{int}(\mathbf{Q},\omega) = \mathcal{F}\{\sqrt{N_0}[\langle \tilde{\rho}_Q(t)\hat{A}_{-Q}\rangle + \langle \hat{A}_Q(t)\tilde{\rho}_{-Q}\rangle]\}$

Single particle Green's function

- Correlation function of single-particle operators

$$\langle \hat{A}_Q(t)\hat{A}_{-Q}(0)\rangle = \langle \hat{a}_{\mathbf{Q}}(t)\hat{a}^{+}_{\mathbf{Q}}\rangle + \langle \hat{a}^{+}_{-\mathbf{Q}}(t)\hat{a}_{-\mathbf{Q}}\rangle + \langle \hat{a}_{\mathbf{Q}}(t)\hat{a}_{-\mathbf{Q}}\rangle + \langle \hat{a}^{+}_{-\mathbf{Q}}(t)\hat{a}^{+}_{\mathbf{Q}}\rangle$$
$$\equiv -iG_{11}(Q,t) - iG_{22}(Q,t) - iG_{12}(Q,t) - iG_{21}(Q,t)$$

- Spectral density: spectrum of a single-particle excitations

$$A_{11}(Q,\omega) = \mathcal{F}\{\langle \hat{a}_{\mathbf{Q}}(t)\hat{a}^{+}_{\mathbf{Q}}\rangle\}$$

- In Bose condensate poles of $A_{\alpha\beta}(\mathbf{Q},\omega)$ and $S(\mathbf{Q},\omega)$ share common poles

$$S(\mathbf{Q},\omega) = N_0(A_{11}(\mathbf{Q},\omega) + A_{22}(\mathbf{Q},\omega) + \dots) + S_{int}(\mathbf{Q},\omega) + \tilde{S}(\mathbf{Q},\omega)$$

Single particle Green's function

- Switching to imaginary time: $\tau = it, \quad 0 < \tau \leq \beta = 1/k_B T$
  - Matsubara Green's function: can be evaluated via Path Integral Monte Carlo

$$G(Q,\tau) = \frac{1}{Z}\,\mathrm{Tr}\left[e^{\beta\mu\hat{H}} e^{-(\beta-\tau)\hat{H}}\,\hat{\mathbf{a}}_{\mathbf{Q}}\, e^{-\tau\hat{H}}\,\hat{\mathbf{a}}^{+}_{\mathbf{Q}}\right]$$

  - Expansion in Matsubara frequencies

$$G_{\alpha\beta}(Q,\tau) = k_B T \sum_{\omega_n} e^{-i\omega_n\tau}\, G_{\alpha\beta}(Q, i\omega_n)$$

  - Ill-posed problem: analytical continuation

$$G_{\alpha\beta}(Q, i\omega_n) \to A_{\alpha\beta}(Q, \omega + i\nu)$$

Outline

Stochastic optimization method [1] (STO)

1. Restore the spectral functions from the imaginary-time Green's function.
   QMC data: $\{G(\tau_i) \pm \delta G_i\}_{i=1\dots N}$, $0 \leq \tau_i \leq \beta$)

$$G_2(Q,\tau) = \frac{1}{\langle N \rangle} \langle \hat{\rho}_Q(\tau)\hat{\rho}_{-Q}(0)\rangle = \int_{-\infty}^{\infty} e^{-\tau\omega} S(Q,\omega)\, d\omega,$$

$$\boxed{\int_{-\infty}^{\infty} S(Q,\omega) d\omega = S(Q)}$$

$$G_1(Q,\tau) = \langle \hat{a}_Q(\tau)\hat{a}_Q^{+}(0)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-\tau\omega}}{1-e^{-\beta\omega}} A(Q,\omega),$$

$$\boxed{\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(Q,\omega) = 1}$$

[1] A.S. Mishchenko et al., Phys.Rev.B **62**, 6317(2000)

Stochastic optimization method [1] (STO)

1. Solution is not unique. Find the solutions $\tilde{G}_n$ with the deviation $D_n \leq D_{min}$

$$D_n[\tilde{G}_n] = \int_0^{\beta} |1 - \tilde{G}_n(Q,\tau)/G(Q,\tau)|\, d\tau, \quad D_{min} \approx \sum_{\tau_i} \Delta\tau |\delta G(Q,\tau_i)| G^{-1}(Q,\tau_i)$$

   – $\tilde{G}_n$ are generated from the trial spectral densities $\tilde{S}_n(Q,\omega)$:

$$\tilde{G}_n(Q,\tau) = \int_{-\infty}^{\infty} e^{-\tau\omega} \tilde{S}_n(Q,\omega)\, d\omega$$

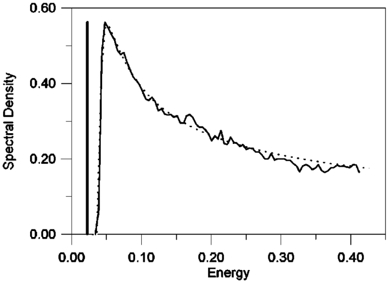
2. Final result: linear superposition of independent stochastic solutions

$$S_{est}(Q,\omega) = \frac{1}{M}\sum_{n=1}^{M} \tilde{S}_n(Q,\omega), \quad S(Q,\omega) \approx S_{est}(Q,\omega)$$

[1] A.S. Mishchenko et al., Phys.Rev.B **62**, 6317(2000)

Parametrization for stochastic optimization

Idea: try to avoid possible systematic errors, i.e. $\tilde{S}(\omega)$ on a preassigned discrete set of frequencies $\{\omega_m\}_{m=1\ldots K}$



Model spectral density. A sharp feature (delta peak) is difficult to match by a grid.

Parametrization by in a basis

$$\tilde{S}(\omega) = \sum_{m=1}^{K} P_m(\omega)$$

of rectangles $\{P\} = \{h, w, c\}$

$$P_m(\omega) = \begin{cases} h_m, & \omega \in \left[c_m - \frac{w_m}{2}, c_m + \frac{w_m}{2}\right] \\ 0, & \text{otherwise} \end{cases}$$

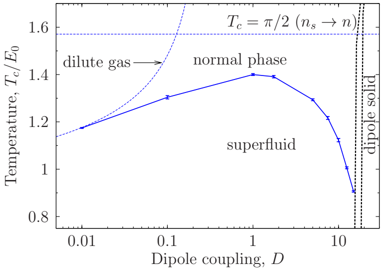
$$\int d\omega\, \tilde{S}(\omega) = \sum_{m=1}^{K} h_m w_m$$

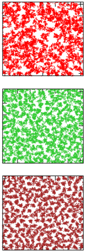
$$\tilde{G} = \begin{cases} S(q), & \tau = 0 \\ 2\tau^{-1} \sum_m h_m e^{-c_m \tau} \sinh(w_m \tau/2), & \tau \neq 0 \end{cases}$$

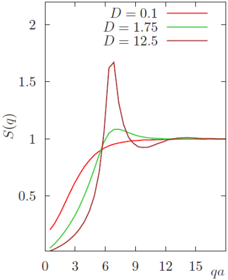
The initial configuration $C_0 = \{P_m, m = 1, \ldots K\}$ is optimized in the space of parameters $\{h_m, w_m, c_m\}$ until $D[\tilde{G}(C_i)] \leq D_{min}$

Outline

Coupling strength





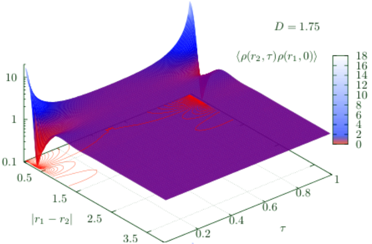


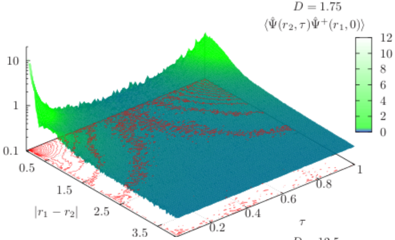
Single and two-particle Green's function

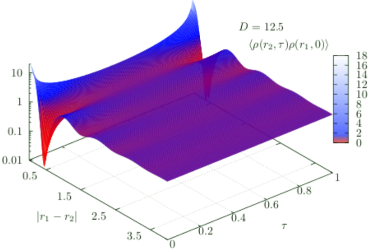
Dipole coupling: $D = 1.75$ and $D = 12.5$. Superfluid phase: $T = 1$ ($T < T_c$, $T_c \approx 1.2$).

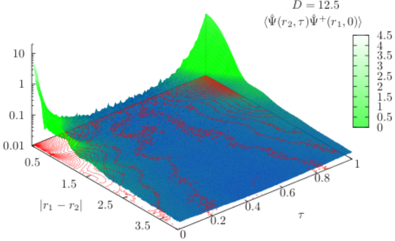
$G_2 = \langle \rho(r_2, \tau) \rho(r_1, 0) \rangle$

$G_1 = \langle \Psi(r_2, \tau) \Psi^+(r_1, 0) \rangle$



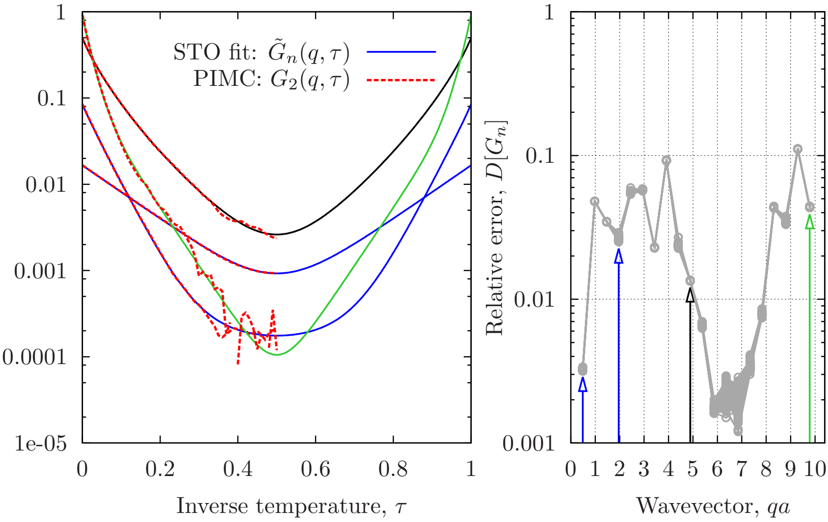






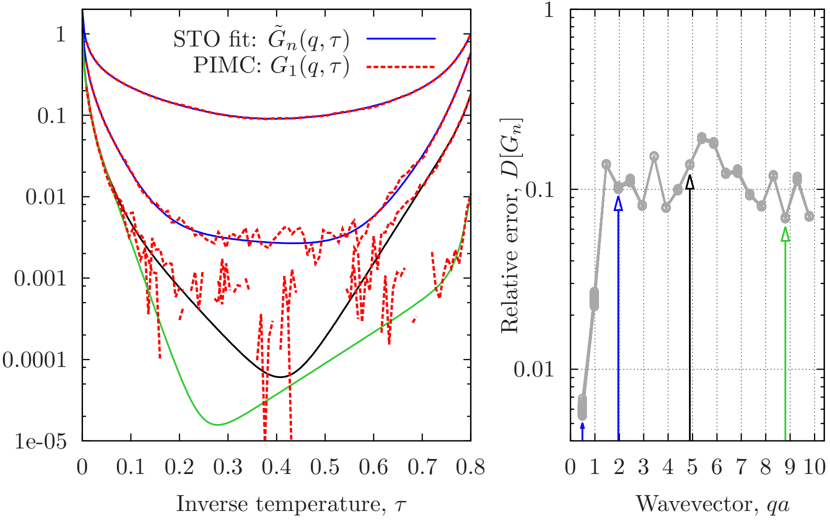
STO: Density correlation function $G_2(q, \tau)$

$D = 12.5, \quad \beta = 1/k_B T = 1.0, \quad 0 \leq \tau \leq \beta$



STO: Matsubara Green's function $G_1(q, \tau)$

$D = 12.5, \quad \beta = 1/k_B T = 0.8, \quad 0 \leq \tau \leq \beta$



Outline

Sum rules: upper bound for dispersion relation

Empirical decomposition (*damping is negligible*)

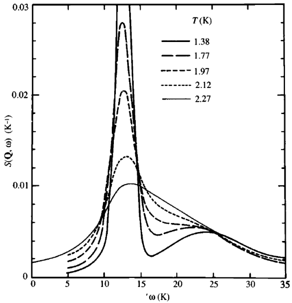
$$S(q,\omega) = S_1(q,\omega) + S_2(q,\omega)$$

– single-peaked quasiparticle part:

$$S_1(q,\omega)+S_1(q,-\omega) = Z(q)\delta(\omega-\omega_q)(1+e^{-\beta\omega})$$

– broad multiparticle background:

$$S_2(q,\omega) = \begin{cases} \neq 0, & \omega \geq \omega_q \\ 0, & \omega < \omega_q \end{cases}$$



^{4}He. Scattering data at $q = 0.8$ Å^{-1}.

Woods, Svensson, Griffin (1987).

- Sum rules: $\langle \omega^{-1} \rangle = \int_{-\infty}^{\infty} d\omega\, \frac{1}{\omega} S(q,\omega) = \frac{1}{2n}|\chi(q)|$, $\int_{-\infty}^{\infty} d\omega\, S(q,\omega) = S(q)$

$$\frac{1}{2n}|\chi(q)| = \omega_q^{-1} Z(q)(1+e^{-\beta\omega_q}) + \int d\omega\, \omega^{-1} S_2(q,\omega)$$

Sum rules: upper bound for dispersion relation

Empirical decomposition (*damping is negligible*)

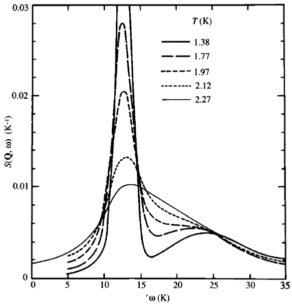
$$S(q,\omega) = S_1(q,\omega) + S_2(q,\omega)$$

– single-peaked quasiparticle part:

$$S_1(q,\omega)+S_1(q,-\omega) = Z(q)\delta(\omega-\omega_q)(1+e^{-\beta\omega})$$

– broad multiparticle background:

$$S_2(q,\omega) = \begin{cases} \neq 0, & \omega \geq \omega_q \\ 0, & \omega < \omega_q \end{cases}$$



^{4}He. Scattering data at $q = 0.8$ Å^{-1}.

Woods, Svensson, Griffin (1987).

- Sum rules: $\langle\omega^{-1}\rangle = \int_{-\infty}^{\infty} d\omega\, \frac{1}{\omega} S(q,\omega) = \frac{1}{2n}|\chi(q)|$, $\int_{-\infty}^{\infty} d\omega\, S(q,\omega) = S(q)$

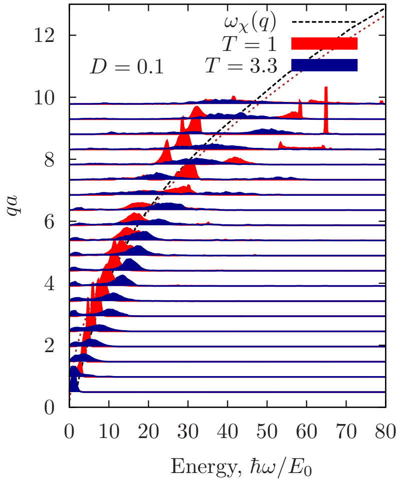
$$\frac{1}{2n}|\chi(q)| \leq \omega_q^{-1} Z(q)(1+e^{-\beta\omega_q}) + \omega_q^{-1}\left[S(q) - \int d\omega\, S_1(q,\omega)\right]$$

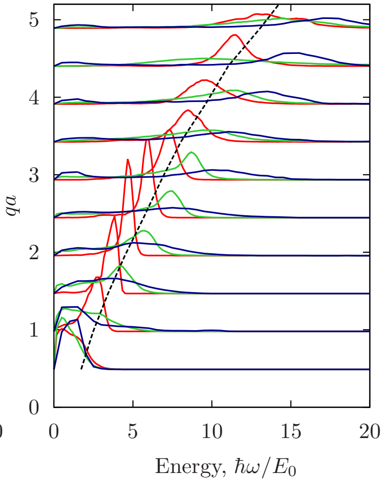
$$\boxed{\omega(q) \leq \omega_\chi(q) = 2nS(q)/|\chi(q)|}$$

Path integral data: $S(q)$, $\chi(q) = -\int_0^\beta d\tau\, G_2(q,\tau)$

Collective excitations $S(q, \omega)$: T-dependence

Weak coupling: $D = 0.1$ $(\mu = 4.7,\ V = 165,\ \langle N \rangle \sim 164)$
Superfluid fraction: $\rho_s(T = 1) = 0.95$, $\rho_s(T = 2) = 0.04$, $\rho_s(T = 3.3) = 0$





Collective excitations $S(q,\omega)$: T-dependence

Summary for weak coupling: $D = 0.1$

Superfluid phase:

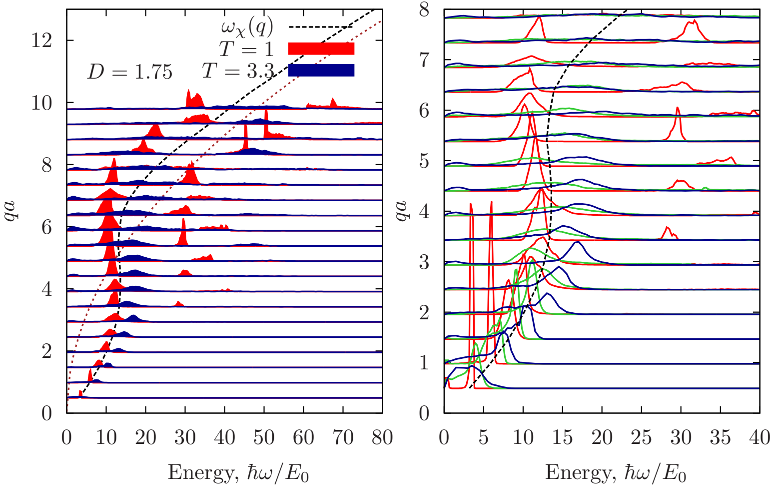
- Continuous single excitation branch
- $q < 6$: perfect agreement with the sum rule result. A single excitation branch!
- $q > 6$: appearance of the high energy branch, i.e. pair (multi)-excitations. The sum rule result, $\omega_\chi(q)$, is the upper bound for the lower branch.

Normal phase:

- $q < 7$: linear dispersion (compressional sound wave) and low energy multiexcitation continuum.
- Increase of the sound speed with temperature.
- $q > 7$: broadening of the spectrum and shift to the free-particle dispersion, $q^2/2m$.

Collective excitations $S(q,\omega)$: T-dependence

Moderate coupling: $D = 1.75$ $(\mu = 32.8,\ V = 165,\ \langle N\rangle \sim 166)$
Superfluid fraction: $\rho_s(T=1) = 1.0$, $\rho_s(T=2) = 0.17$, $\rho_s(T=3.3) = 0$



Collective excitations $S(q, \omega)$: T-dependence

Summary for moderate coupling: $D = 1.75$

Superfluid phase:

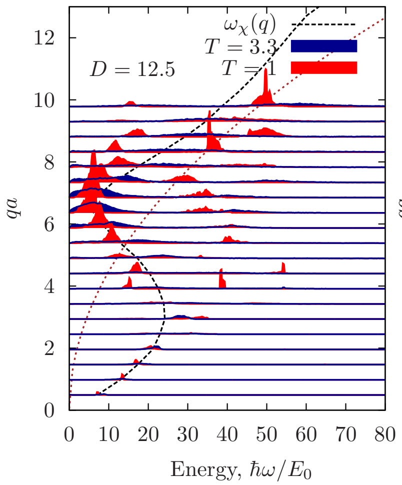
- Sharp peaks at the low energy excitation branch.
- $q < 3$: agreement with the sum rule result in the phonon and phonon-maxon regions.
- $q > 3$: high energy branch.
- Offset of a small roton minimum around $q \sim 6.3$.
- Partially superfluid phase, $\rho_s(T = 2) = 0.17$
  – Significant broadening of the peaks
  – Sharp peaks of the high energy branch disappear

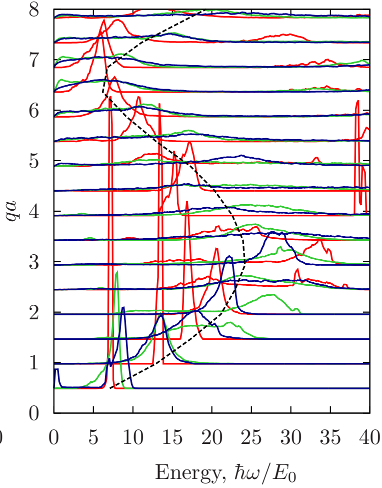
Normal phase:

- $q < 3$: linear dispersion (compressional sound wave). It is different from the low-T phonon-maxon dispersion.
- Low energy multiexcitation continuum.
- $3 < q < 8$: dispersion is independent on the q-vector.
- $q > 8$: multiexcitation continuum and shift to the free-particle dispersion, $q^2/2m$.

Collective excitations $S(q,\omega)$: T-dependence

Strong coupling: $D = 12.5$ $(\mu = 163.5,\ V = 165,\ \langle N \rangle \sim 165)$
Superfluid fraction: $\rho_s(1) = 0.85$, $\rho_s(2) = 0$, $\rho_s(3.3) = 0$



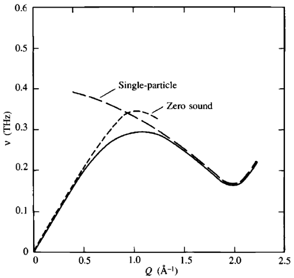


Collective excitations $S(q,\omega)$: T-dependence

Summary for strong coupling: $D = 12.5$

Superfluid phase:

- Low energy excitation branches: phonons and rotons.
- $2.5 \leq q \leq 4.5$: the maxon region is a cross-over. Hybridization due to crossing of two different excitation branches (phonons and rotons)?
  – If there are two branches do they appear in the single particle spectrum $A(Q,\omega)$?
- High energy branch: vanishes in the normal phase, similar to $D = 0.1, 1.75$.
- Large wavevectors, $q > 8$: free-particle excitations plus the two-roton branch.



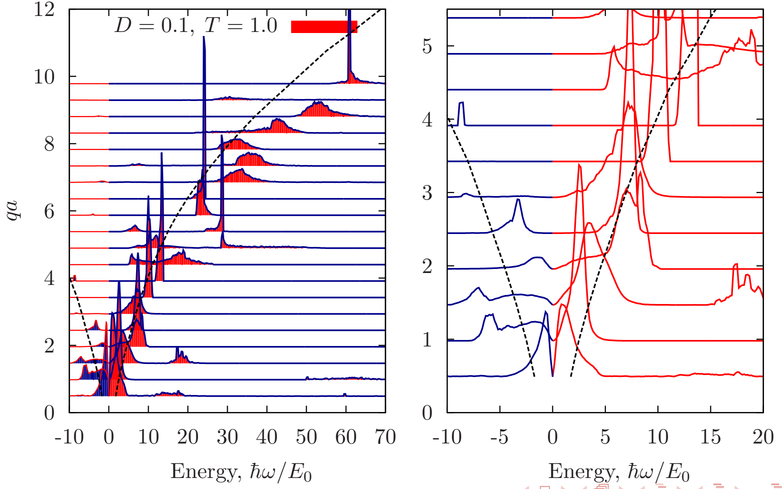
Glide, Griffin (1990)

Normal phase:

- $q < 3$: linear dispersion (compressional sound wave).
- Broad multiexcitation dispersion in the roton minimum.
- $q > 8$: multiexcitation continuum and shift to the free-particle dispersion, $q^2/2m$.

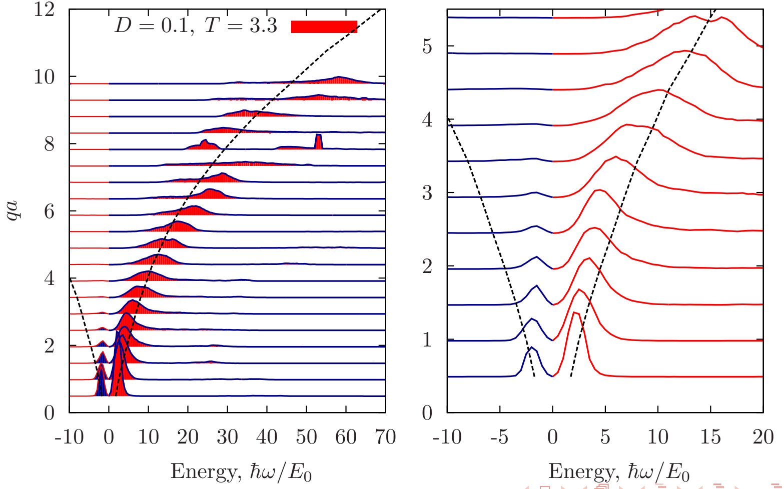
Spectral density $A(q,\omega)$: T-dependence

Weak coupling: $D = 0.1$ $(\mu = 4.7,\ V = 165,\ \langle N \rangle \sim 164)$
Superfluid fraction: $\rho_s(T = 1) = 0.95$



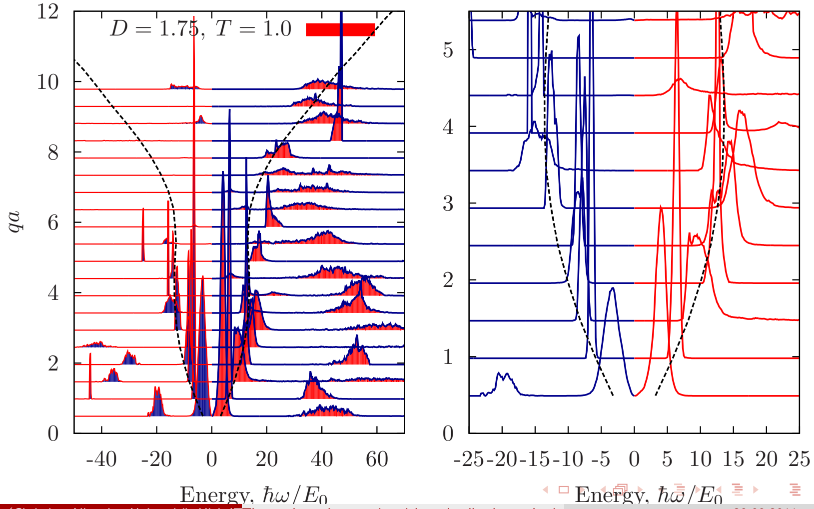
Spectral density $A(q, \omega)$: T-dependence

Weak coupling: $D = 0.1$ $(\mu = 4.7,\ V = 165,\ \langle N \rangle \sim 164)$
Superfluid fraction: $\rho_s(T = 3.3) = 0$



Spectral density $A(q,\omega)$: T-dependence

Moderate coupling: $D = 1.75$, $\mu = 32.8$, $V = 165$, $\langle N \rangle \sim 166$.
Superfluid fraction: $\rho_s(1) = 1.0$



Spectral density $A(q,\omega)$: T-dependence

Pitaevskii (1987): $A(p,\omega) \leq 0$ for $\omega < 0$

$$n_p = 2\int_0^\infty \frac{d\omega}{2\pi} N(\omega)\frac{1}{2}\left[A(p,\omega) + A(p,-\omega)\right] - \int_{-\infty}^0 \frac{d\omega}{2\pi} A(p,\omega)$$

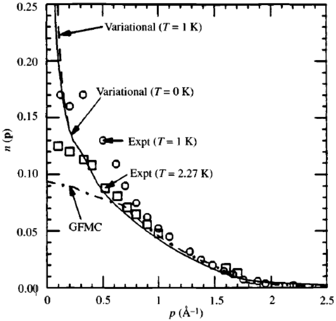
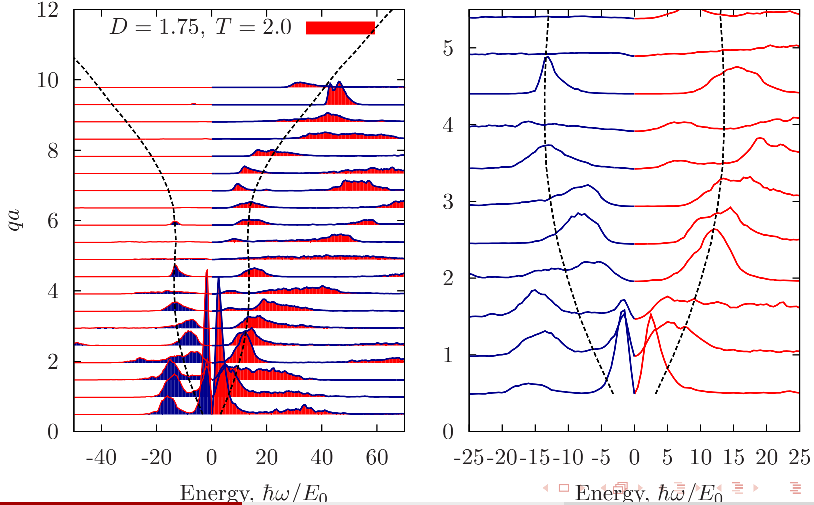


Fig. 4.2. The atomic momentum distribution $n(\mathbf{p})$ as given by three methods: variational; Green's function Monte Carlo GFMC (Whitlock and Panoff, 1987); and high-momentum $S(\mathbf{Q},\omega)$ data as analysed by Sears *et al.*, (1982) [Source: Manousakis, 1989].

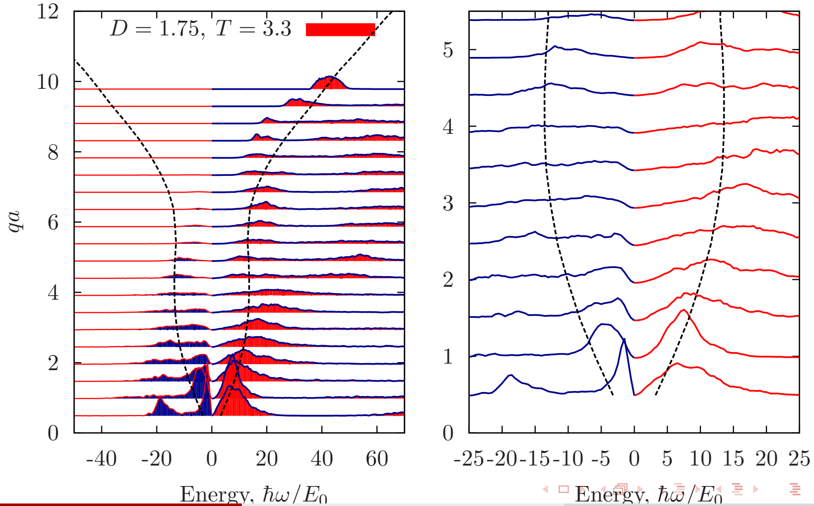
Spectral density $A(q,\omega)$: T-dependence

Moderate coupling: $D = 1.75$, $\mu = 32.8$, $V = 165$, $\langle N \rangle \sim 166$.
Superfluid fraction: $\rho_s(T = 2) = 0.17$



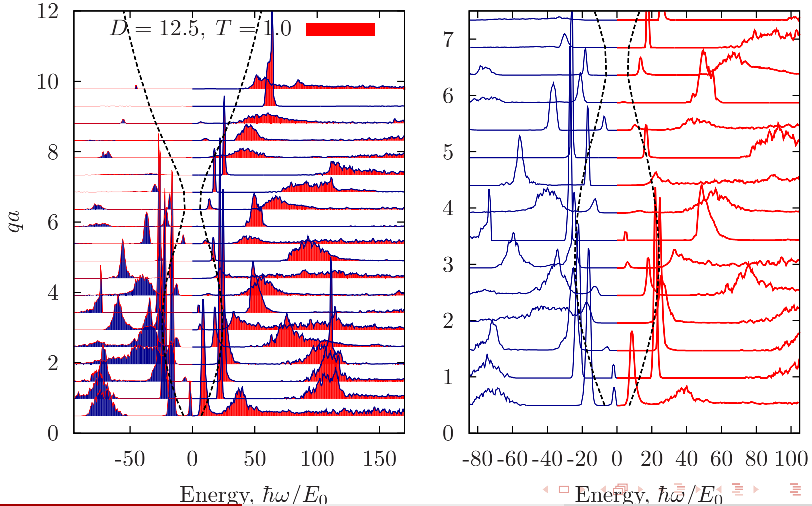
Spectral density $A(q,\omega)$: T-dependence

Moderate coupling: $D = 1.75$, $\mu = 32.8$, $V = 165$, $\langle N \rangle \sim 166$.
Superfluid fraction: $\rho_s(3.3) = 0$.



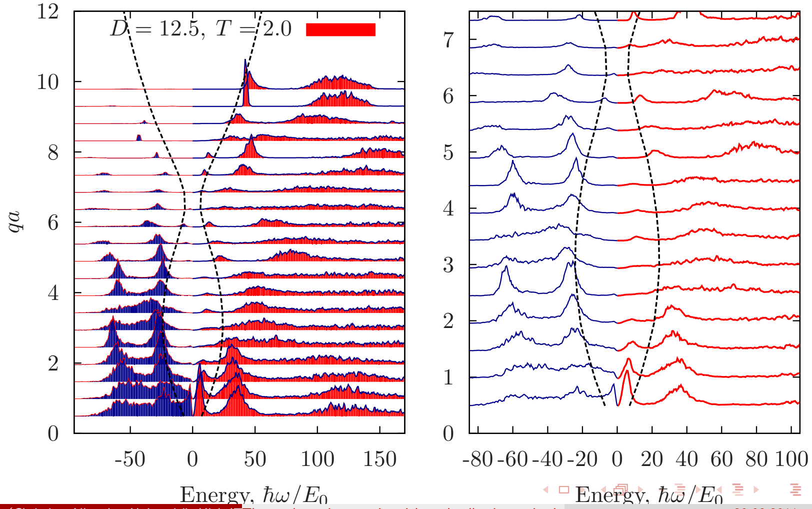
Spectral density $A(q, \omega)$: T-dependence

Strong coupling $D = 12.5$, $\mu = 163.5$, $V = 165$, $\langle N \rangle \sim 165$.
Superfluid fraction: $\rho_s(T = 1) = 0.85$



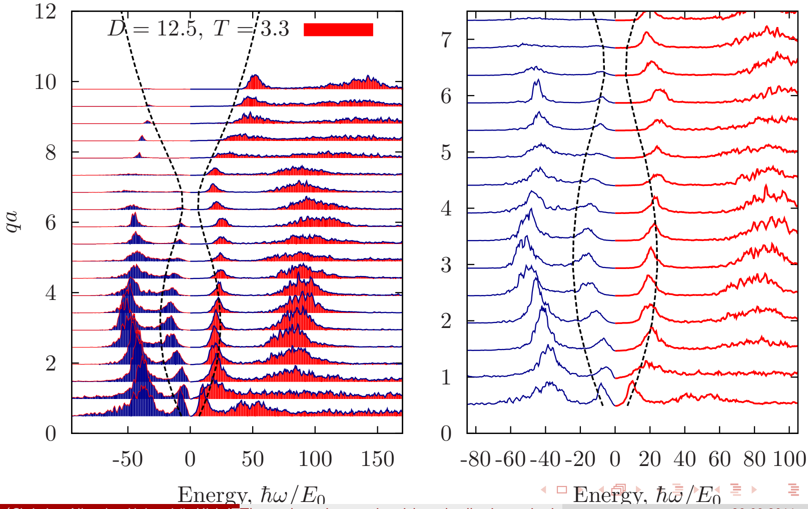
Spectral density $A(q,\omega)$: T-dependence

Strong coupling $D = 12.5$, $\mu = 163.5$, $V = 165$, $\langle N \rangle \sim 165$.
Superfluid fraction: $\rho_s(T=2) = 0$

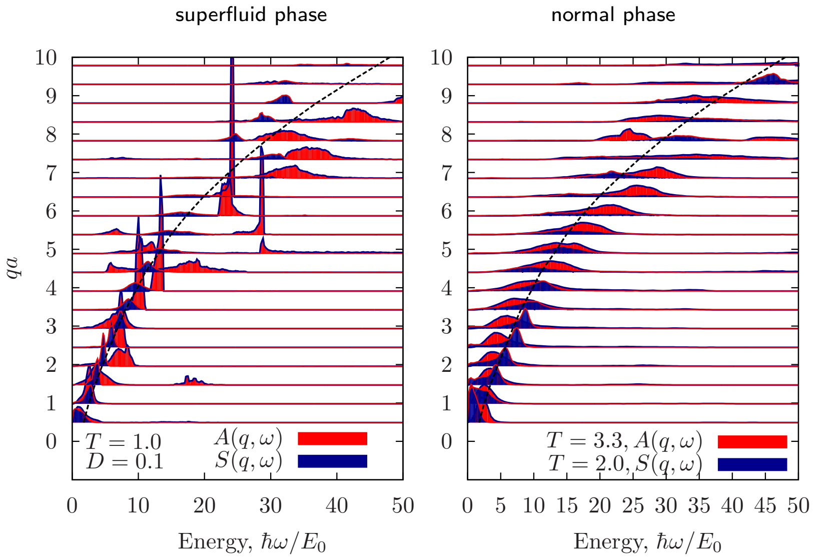


Spectral density $A(q,\omega)$: T-dependence

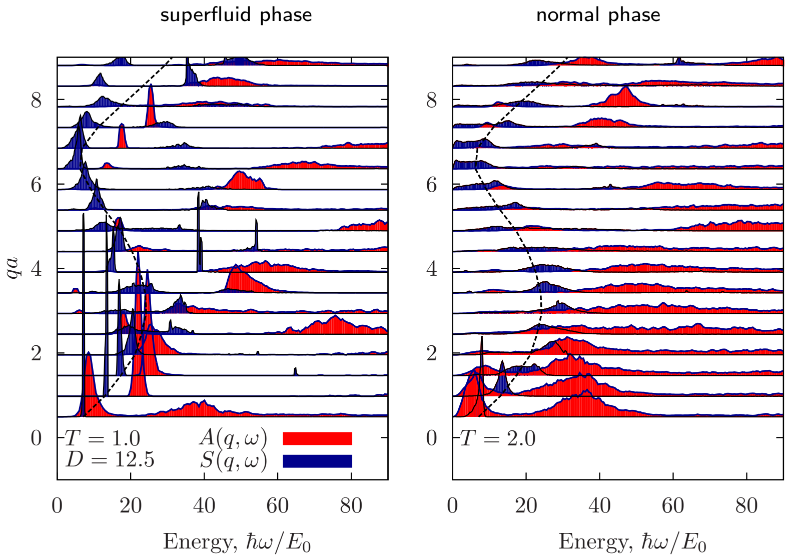
Strong coupling $D = 12.5$, $\mu = 163.5$, $V = 165$, $\langle N \rangle \sim 165$.
Superfluid fraction: $\rho_s(T = 3.3) = 0$



Particle-hole $S(q,\omega)$ vs. single-particle $A(q,\omega)$ spectrum



Particle-hole $S(q,\omega)$ vs. single-particle $A(q,\omega)$ spectrum



Outline

Summary

- We show that PIMC can be an effective method for computation of two- and single-particle Green's function, and, in general, other correlation functions of QM operators in imaginary time. $\Rightarrow$ Good check for the diagrammatic perturbation methods.
- STO method allows quite accurately reproduce the excitation spectrum (spectral densities) in linear response.

  – PIMC: allows to work out the single-particle excitations in a Bose liquid from first principles.
- We show that in the superfluid phase $S(q,\omega)$ share common poles with the single-particle excitation spectrum $A(q,\omega)$ as was theoretically predicted and analyzed by Hugenholtz, Pines, Bogoliubov, Gavoret, Nozieres,. . ., Glyde, Griffin,. . ..
- $A(q,\omega)$ shows some broadening but still a well defined dispersion even for $T \sim 2T_c$.

  – Rotons-maxons are observed as intrinsic single-particle excitations also in the normal phase.
- $S(q,\omega)$: in the normal phase we observe an acoustic plus a free-particle dispersion for weak-moderate coupling $D = 0.1, 1.75$.
- In a strongly coupled liquid, $D = 12.5$ (close to crystallization transition $D = 17 \pm 1$), we observe in addition a roton minimum as the intrinsic density excitation.

Summary

Thank you for your attention

Outline

Single particle Green's function II

Dyson equation involving 2×2 matrix self-energy $\Sigma_{\alpha\beta}$

$$G_{\alpha\beta} = G^0_{\alpha\beta} + G^0_{\alpha\nu}\Sigma_{\nu\mu}G_{\mu\beta}, \quad G^0_{\alpha\beta}(Q, i\omega_n) = \frac{\delta_{\alpha\beta}}{i\omega_n - (\epsilon_Q - \mu)}$$

Solutions in the Bogoliubov approximation

$$\Sigma^B_{11}(Q, i\omega_n) = \Sigma^B_{22}(Q, i\omega_n) = n_0 V(\mathbf{Q} = 0) + n_0 V(\mathbf{Q}),$$
$$\Sigma^B_{12}(Q, i\omega_n) = \Sigma^B_{21}(Q, i\omega_n) = n_0 V(\mathbf{Q})$$

$$G^B_{11}(Q, i\omega_n) = G^B_{22}(Q, -i\omega_n) = \frac{u_Q^2}{i\omega_n - \omega_Q} - \frac{\upsilon_Q^2}{i\omega_n + \omega_Q},$$
$$G^B_{12}(Q, i\omega_n) = G^B_{21}(Q, i\omega_n) = -u_Q\upsilon_Q\left(\frac{1}{i\omega_n - \omega_Q} - \frac{1}{i\omega_n + \omega_Q}\right),$$
$$\omega_Q^2 = \epsilon_Q^2 + 2n_0 V(Q)\epsilon_Q, \quad u_Q^2, \upsilon_Q^2 = \frac{\epsilon_Q + n_0 V(Q)}{2\omega_Q} \pm \frac{1}{2}$$

Single particle Green's function II

Gerenal solution for gas and liquid (Fetter and Walecka, 1971)

$$G_{11}(Q, i\omega_n) = \frac{i\omega_n + \epsilon_Q - \mu + \Sigma_{22}(Q, i\omega_n)}{D(Q, i\omega_n)},$$

$$G_{22}(Q, i\omega_n) = \frac{-i\omega_n + \epsilon_Q - \mu + \Sigma_{11}(Q, i\omega_n)}{D(Q, i\omega_n)},$$

$$G_{12}(Q, i\omega_n) = G_{21}(Q, i\omega_n) = \frac{-\Sigma_{12}(Q, i\omega_n)}{D(Q, i\omega_n)}$$

The poles (the energies of the single-particle excitations) are given by the zeros of

$$D(Q, i\omega_n) = [i\omega_n - (\epsilon_Q - \mu + \Sigma_{11})][i\omega_n + (\epsilon_Q - \mu + \Sigma_{22})] + \Sigma_{12}^2$$

Symmetry relations

$$G_{11}(Q, i\omega_n) = G_{22}(Q, -i\omega_n) \quad \Rightarrow \Sigma_{11}(Q, i\omega_n) = \Sigma_{22}(Q, -i\omega_n),$$
$$G_{12}(Q, i\omega_n) = G_{21}(Q, i\omega_n) \quad \Rightarrow \Sigma_{12}(Q, i\omega_n) = \Sigma_{21}(Q, i\omega_n)$$

Momentum distribution $T \ll T_c$: long-wave length limit

Collisionless $[T = 0,\ \rho_s = \rho]$ low-frequency regime (Gavoret and Nozie'res, 1964)

$$A(q,\omega) = 2\pi(Z(q) + 1/2\pi)\delta(\omega - cq) - 2\pi Z(q)\delta(\omega + cq)$$

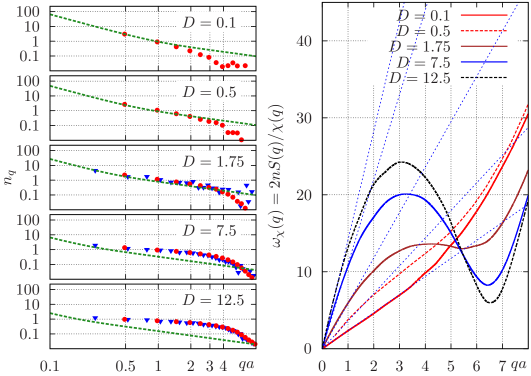
Sum rules for the spectral density

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(q,\omega) = 1, \quad \lim_{q\to 0} -G_{11}(q,\omega=0) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{A(q,\omega)}{\omega} = \frac{m^2 n_0}{\rho_s q^2}$$

By substitution we obtain

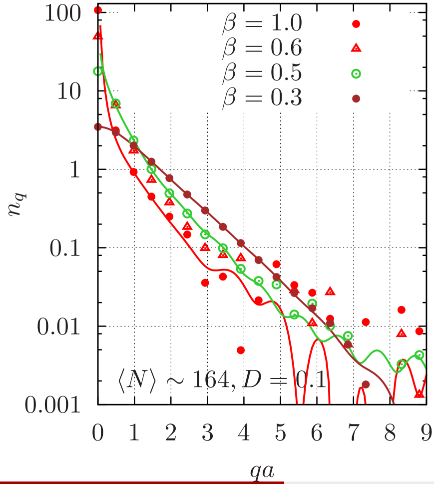
$$\boxed{n_q = Z(q)\,[2N(cq) + 1]}, \quad Z(q) = \frac{m^2 n_0 c}{2\rho_s q}, \quad N(\omega) = \frac{1}{e^{\beta\omega} - 1}$$

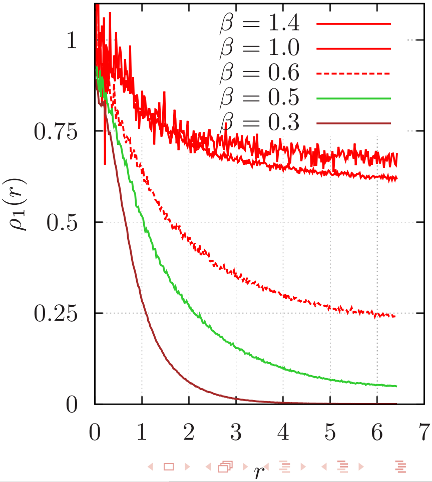
Momentum distribution $T < T_c$: long-wavelength limit



D	μ ($V = 165$)	c	$n_0 = N_{p=0}/\langle N \rangle$	
0.1	4.7	2.35	0.65	(107.1/163.69)
0.5	12.55	3.60	0.47	(77.0/163.18)
1.75	31.10	5.90	0.26	(43.15/162.97)
7.5	102.20	11.0	0.061	(9.81/162.05)
12.5	163.53	14.14	0.022	(3.61/164.46)

Momentum distribution: T-dependence





Momentum distribution: T-dependence