Relation between classical and quantum systems

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MAX-PLANCK-GESELLSCHAFT

Introduction

- Higher dimensional classical non-Abelian gauge theory leads to a lower dimensional quantum field theory in the sense of chaotic quantitation $\hbar = aT$ [T.S. Biró et. al.]
- Bohm interpretation of quantum mechanics, Schrödinger equation as Hamilton-Jacobi but with nonlocal quantum potential
- Systematic effective quantum potentials on binary level for classical simulations (Kelbg, Deutsch)
- Dense classical system correlation restrict phase space for motion, analogy to Pauli-blocking for quantum systems at low temperature ?

Outline

1. Exact equivalence between N particle classical and N-1 particle quantum systems
2. Derive effective quantum potentials (Kelbg and higher order)
3. Conjecture: Dense classical systems can be described by Quantum Born calculations replacing quantum parameter by classical ones
4. Test: Simulation of one component plasma

Classical partition function

configuration integral with Meyer's graphs $f_{ij} = \exp(-\beta u(x_i - x_j)) - 1$

$$Q_N(\beta) = \int dx_1 ... dx_N \prod_{i<j}^{N} (1 + f_{ij})$$

Trick
$$\begin{aligned} \bar{Q}_N(\beta) &= Q_N(2\beta) \\ &= \int dx_1 ... dx_N dx'_1 ... dx'_N \delta(x_1 - x'_1) ... \delta(x_{N-1} - x'_{N-1}) \\ &\times \quad (1 + f_{12})(1 + f_{13})(1 + f_{14}) ... (1 + f_{1N}) \\ &\times \quad (1 + f_{1'2})(1 + f_{13})(1 + f_{24}) ... (1 + f_{2N}) \\ &\times \quad ..... \\ &\times (1 + f_{N'1'})(1 + f_{N2'})(1 + f_{N3'}) ... (1 + f_{NN-1'}) \end{aligned}$$

Introduce

$$\delta(x_1 - x'_1) ... \delta(x_{N-1} - x'_{N-1}) = \sum_{i_1 ... i_{N-1}} \Psi^*_{i_1 ... i_{N-1}}(x'_1 ... x'_{N-1}) \Psi_{i_1 ... i_{N-1}}(x_1 ... x_{N-1})$$

with eigenvalue problem

$$\int dx_1 \prod_{j=2}^{N} (1 + f_{1j}) \Psi_{i_1 ... i_{N-1}}(x_1 ... x_{N-1}) = V e^{-\epsilon_{i_1}(\beta)} \Psi_{i_2 ... i_{N-1} i_1}(x_2 ... x_N | 1)$$

Result
$$\bar{Q}_N(\beta) = V^N \sum_{i_1 ... i_{N-1}} e^{-N\epsilon_{i_1}(\beta)}.$$

classical N-body system equivalent to a $N-1$-body quantum system with $N-1$-body Schroedinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - \sum_{i}^{N-1} \frac{p_i^2}{2m_i} - \bar{U} \right) \xi(p_1 ... p_{N-1}, t) = 0$$

and quantum $N-1$-particle potential

$$\begin{aligned} < x_1 i_1 ... i_{N-1} | U | x'_1 i'_1 ... i_{N-1} > &= e^{\beta |u_{12}(x_1 - x_2) + ... + u_{1N}(x_1 - x_{N-1})|} \\ &\times \Omega \delta(x_1 - x'_1) ... \delta(x_{N-2} - x'_{N-1}) \delta_{i_1 i'_1} ... \delta_{i_{N-1} i'_{N-1}} \end{aligned}$$

Applications

1. Factorization $\Psi_{i_1 ... i_N}(x_1 ... x_N) = \phi_{i_1} ... \phi_{i_N}$ in plane waves leads to:

$$P = T \frac{\partial}{\partial V} \ln Q_N = T \left(\frac{N}{V} - \frac{N(N-2)}{V^2} \int dr \left(e^{-|u|r|/2} - 1 \right) \right)$$

2. Quantum potential represent quantum effects by classical potential

- multiply (1) with $\Psi^*_{i_1 ... i_{N-1} i_1}(x_2 ... x_N)$ and statistical operator (nondegenerate correlation function) $l^2 = \hbar^2/\mu T = \lambda^2/2\pi$, $x = r/l$

$$\rho_{i_1 i_2}(x_1 - x_2) = \int \frac{dp}{(2\pi\hbar)^3} e^{ipr/\hbar} \lambda^3 e^{-\beta \frac{p^2}{2\mu}} = e^{-x^2}$$

- integrate over $x_2 ... x_N$ to obtain:

$$\begin{aligned} \frac{U}{V} &= \sum_{\{i\}} \int \frac{dy_1 ... dy_{N-1}}{V^{N-1}} \rho_{i_1 i_2}(y_1) \rho_{i_2 i_3}(y_2) ... \rho_{i_{N-2} i_1}(y_{N-1}) \\ &\times (1 - f_{12}(y_1))(1 - f_{13}(y_1 + y_2)) ... (1 - f_{1N}(y_1 + ... + y_{N-1})) \\ &\equiv \sum_{i_1 i_2} \int \frac{dx}{V} \rho_{i_1 i_2}(x) V_{12}^{\text{eff}} \qquad \text{mean correlation energy} \end{aligned}$$

From this read off lowest order (binary) Kelbg 1964 [1]:

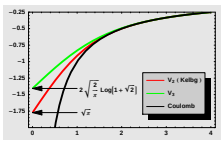
$$V_2^{\text{eff}}(r) \propto \sum_{ij} \int \frac{dx_1}{V} \rho_{12}(x_1) u_{12}(x_1) u_{23}(x_1 + r) = \frac{1}{x} \left(1 - e^{-x^2} + \sqrt{\pi}\, x\, \text{erfc}(x) \right)$$

Now next order (ternary):

$$\begin{aligned} V_3^{\text{eff}}(r) &\propto \sum_{ijl} \int \frac{dx_1 dx_2}{V^2} \rho_{12}(x_1) u_{12}(x_1) u_{13}(x_1 + x_2) \rho_{23}(x_2) u_{34}(x_1 + x_2 + r) \\ &= \frac{1}{x} \left(\text{erf}^2\left(\frac{x}{\sqrt{2}} \right) + \frac{2^{3/2} x}{\sqrt{\pi}} \int_x^\infty \frac{dz}{z} e^{-z^2/2} \text{erf}\left(\frac{z}{\sqrt{2}} \right) \right) \end{aligned}$$

Quantum potentials

Comparison binary (Kelbg) and ternary potential



Quantum potentials differ from Coulomb at smaller $\lambda = \sqrt{\frac{2\pi\hbar^2}{\mu T}} \sim d = (\frac{3}{4\pi n})^{1/3}$ distances than

CONJECTURE: good approximations for the dynamics of dense classical many-body systems by employing degenerate quantum-Born approximations and replace quantum parameter by classical ones

Non-Markovian kinetic equation

Time diagonal part of Kadanoff/Baym equation Levinson equation

$$\begin{aligned} \frac{\partial}{\partial t} f_a(t) &= \frac{2}{\hbar^2} \sum_b \int \frac{dp\, dq}{(2\pi\hbar)^6} V_D^2(q) \int_0^t d\bar{t} \exp\left\{ -\frac{t - \bar{t}}{\tau} \right\} \cos\left\{ \frac{1}{\hbar}(t - \bar{t}) \Delta_E \right\} \\ &\times \left\{ \bar{f}_a \bar{f}_b (1 - \bar{f}_a)(1 - \bar{f}_b) - \bar{f}_a \bar{f}_b (1 - \bar{f}_a)(1 - \bar{f}_b) \right\}_{\bar{t}}, \end{aligned}$$

where $\Delta_E = \frac{q^2}{2m_a} + \frac{p^2}{2m_b} - \frac{|\vec{k} - \vec{q}|^2}{2m_a} - \frac{|p + q|^2}{2m_b}$

- particle-number conservation $\frac{\partial}{\partial t} n = 0$
- momentum conservation $\frac{\partial}{\partial t} \langle p_i \rangle = 0$.
- Time variation of kinetic energy is [2]: $\frac{\partial}{\partial t} (\langle \frac{p_a^2}{2m} \rangle + \langle V_{12} \rangle) \equiv 0$

Solution at transient time regime

Analytical solution of Levinson's equation at short-times $t \ll \tau$

- neglect of time evolution of distributions, $\bar{f}_a(t) = f_a(0)$
- life-time factor, $\exp\left\{ -\frac{|t - \bar{t}|}{\tau} \right\} = 1$

deviation from initial value, $f_a(t) = f_a(0) + \delta f_a(t)$, reads

$$\begin{aligned} \delta f_a(t) &= 2 \sum_b \int \frac{dp\, dq}{(2\pi\hbar)^6} V_D^2(q) \frac{1 - \cos\left\{ \frac{1}{\hbar} t \Delta_E \right\}}{\Delta_E^2} \\ &\times \{ f'_a f'_b (1 - f_a)(1 - f_b) - f_a f_b (1 - f'_a)(1 - f'_b) \} \end{aligned}$$

two-particle and the single-particle concept of the transient behavior meet in kinetic equation

- right hand side: two particles correlate their motion to avoid the strong interaction regions
- Since process is very fast, the on-shell contribution to δf_a, has pure off-shell character
- off-shell character of mutual two-particle correlation is thus reflected in the single particle Wigner's distribution

One component plasma

Time dependent formation from kinetic theory [3-5]
static Debye with $z = \omega_p \sqrt{t^2 - it\frac{\hbar}{T}}$.

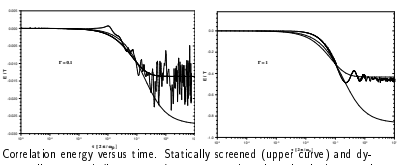
$$\frac{\partial}{\partial t} E_{\text{corr}}(t) = -\frac{e^2 n \kappa T}{2} \frac{1}{\hbar} \text{Im} \left[(1 + 2z^2) e^{z^2} (1 - \text{erf}(z)) - \frac{2z}{\sqrt{\pi}} \right]$$

dynamical screening with $z_1 = \omega_p \sqrt{2t^2 - it\frac{\hbar}{T}}$

$$\frac{\partial}{\partial t} \frac{E_{\text{corr}}^{\text{dynam}}(t)}{n} = -\frac{e^2 \kappa T}{\hbar} \text{Im} \left[e^{z_1^2} (1 - \text{erf}(z_1)) \right]$$

classical limit

$$\begin{aligned} E_{\text{corr}}^{\text{static}}(t) &= -\frac{1}{4} \kappa e^2 n \left[1 + \frac{2\omega_p t}{\sqrt{\pi}} - (1 + 2(\omega_p t)^2) e^{|\omega_p t|^2} (1 - \text{erf}(\omega_p t)) \right] \\ E_{\text{corr}}^{\text{dynam}}(t) &= -\frac{1}{2} e^2 n \kappa \left\{ 1 - \exp\left(\frac{\omega_p^2}{2} t^2 \right) \left[1 - \text{erf}(\frac{\omega_p t}{\sqrt{2}}) \right] \right\}. \end{aligned}$$



Correlation energy versus time. Statically screened (upper curve) and dynamically screened (lower curve) are compared with moleculardynamical simulations [6, 7].

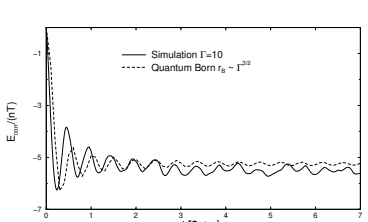
Dense classical OCP by quantum Born

Quantum Born at low temperatures [3, 4]:

$$\frac{E_{\text{corr}}^{\Gamma}(t) - E_{\text{corr}}^{0}(t)}{nT} = \frac{1}{(36\pi^4)^{1/6}} \frac{r_s^3}{\Gamma} \left(\frac{\sin y\tau}{y\tau} - 1 \right) \left(\frac{1}{b_t} \arctan(\frac{1}{b_t}) + \frac{1}{b_t^2 + b_t^3} \right)$$

Bruckner parameter $r_s = \frac{d}{a_B}$, $b_t = \frac{b_\kappa}{2y_\tau} = \sqrt{\Gamma}(48\pi^2)^{-1/6}$, time in plasma periods $\tau = \frac{2\pi t}{\omega_p}$ or $y_\tau = 4\epsilon_f t/\hbar = (2)^{4/3} \pi^{5/3} 3^{5/6} \tau / \sqrt{r_s}$

Simulation of dense classical plasma [G. Zwicknagel]



$$r_s^{\text{fit}} = \frac{1}{2} \sqrt{\frac{3}{\pi}} \Gamma^{3/2}$$

best fit ($\hbar \sim T$)

$$\lambda^2 = \frac{d}{\kappa} = \frac{d^2}{(3\Gamma)^{1/2}} \approx d^2$$

Summary

1. Classical N particle partition function can be represented by a quantum N-1 particle Eigenwert problem
2. Quantum potentials can be derived which describe classically quantum effects (Kelbg, 3-particle corrections)
3. Oppositely quantum Born results can be used to describe dense classical systems $\Gamma \sim 1..10$ by properly replacing quantum parameter $\lambda \to d$ or $r_s \to \Gamma^{3/2}/4$
4. Test: formation time of correlations by kinetic theory and moleculardynamical simulations
   - low temperature value is universal; ratio $\hbar$ to Fermi energy corresponds to the formation time of quasiparticles
   - high temperature limit shows roughly a time scale a particle needs to travel through the potential range (inverse plasma frequency)
   - dynamical result approaches Debye Hückel, while static leads to half the result
   - quantum Born results describe time evolution of dense classical system replacing $\lambda \to d$ or $r_s \to \Gamma^{3/2}/4$

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