Mixture of Tonks-Girardeau gas and Fermi gas in one-dimensional optical lattices

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We study the Bose-Fermi mixture with infinitely boson-boson repulsion and finite boson-Fermion repulsion. By using a generalized Jordan-Wigner transformation, we show that the system can be mapped to a repulsive Hubbard model and thus can be solved exactly for the case with equal boson and fermion masses. By using the Bethe-ansatz solutions, we investigate the ground state properties of the mixture system. Our results indicate that the system with commensurate filling $n = 1$ is a charge insulator but still a superfluid with non-vanishing superfluid density. We also briefly discuss the case with unequal masses for bosons and fermions.

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Mixtures of quantum degenerate atoms recently became a subject of intense studies of both experiment and theory. One of particularly interesting systems is mixture of ultracold bosonic and fermionic atoms [1–3], which have become accessible through the development of sympathetic cooling [1, 2]. The experimental progress in manipulating cold atoms in effective one-dimensional (1D) waveguides and the ability of tuning the effective 1D interactions by Feshbach resonance leads experiment accessible to the strong correlation regime of 1D quantum gas [4, 5]. Meanwhile, by loading the atomic system into the optical lattice [6, 7], one can simulate not only the solid state systems in a highly tunable way but also new systems which may not be realized in condensed matter, such as mixtures of Bose-Fermi atoms. These advances open a new channel to investigate numerous phenomena of low-dimensional correlated lattice models which play important roles in condensed matter physics.

To gain a deep insight of properties of the low-dimensional quantum mixtures, some refined methods capable of dealing with strong correlations are especially important. For example, the method of Bose-Fermi mapping has been extensively exploited to study the Tonks-Girardeau (TG) gas [8, 9]. This method has been also generalized to study the multi-component quantum gas in the infinitely repulsive limit [10, 11]. The extended Bose-Fermi mapping method is only limited to a special case with no tunable parameter of interaction, where all the intra- and inter-component interactions go to infinite. In addition, the Bose-Fermi mixture with equal boson-boson and boson-fermion interactions can be exactly solved by Bethe-ansatz [12–14]. Unfortunately, its corresponding lattice model is no longer integrable. So far, the ground state phase diagram of the 1D Bose-Fermi Hubbard model in optical lattice has been studied by mean-field theory [15, 16], Bosonization method [17, 18], exact diagonalization method [19] and quantum Monte Carlo method [20–22]. Despite the intensive studies of the lattice model [15–20, 22–24], no analytically exact result has been given except the TG limit [10], in which however the model suffers the problem of a huge degeneracy of ground states (GSs). In this work, we shall study the boson-fermion mixtures with the aim to give some exact conclusions apart from the TG limit and focus on the case with an infinite boson-boson repulsion but a tunable boson-fermion interaction, which is found to be exactly solvable when the hopping amplitude t_b for boson equals to t_f for fermion.

We consider a mixture system of bosonic and spin-polarized fermionic atoms confined in a deep 1D optical lattice. For sufficiently strong periodic potential and low temperatures, the atoms will be confined to the lowest Bloch band and the low energy Hamiltonian is described by the Hamiltonian

$$\begin{aligned} H &= -\sum_{i,\sigma=b,f}\left(t_\sigma a_{i\sigma}^\dagger a_{i+1\sigma} + H.c.\right) \\ &\quad + \frac{1}{2}\sum_i U_b n_{i,b}\left(n_{i,b}-1\right) + U_{bf}\sum_i n_{i,b}n_{i,f}, \quad (1) \end{aligned}$$

where $a_{i\sigma}$ are bosonic or fermionic annihilation operators localized on site i, and $n_{i\sigma} = a_{i_\sigma}^\dagger a_{i_\sigma}$. In principle, the interaction parameters U_{bf} and U_b can be tuned experimentally by the Feshbach resonance. In this work, we shall focus on the case with infinitely strong boson-boson repulsion, i.e., $U_b = \infty$, and a tunable inter-species repulsion $U_{bf} = U$. In this case, the boson is a hard-core one or a TG gas, for which the states occupied by more than one boson are prohibited. Similarly, the states occupied by more than one fermion are not permitted due to the Pauli principle. However, a boson and a fermion can occupy the same site which contributes an on-site energy U. In the hard-core limit, the Bose-Fermi mixture model can be simplified to

$$H_{BF} = -\sum_{i,\sigma=b,f}\left(t_\sigma a_{i\sigma}^\dagger a_{i+1\sigma} + H.c.\right) + U\sum_i n_{i,b}n_{i,f}, \quad (2)$$

with additional on-site constraints $a_{ib}^\dagger a_{ib}^\dagger = a_{ib}a_{ib} = 0$ and $\left\{a_{ib}, a_{ib}^\dagger\right\} = 1$ assigned to avoid double or higher occupancy.

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Mixture with equal masses.— Firstly, we focus on the case that the bosonic and fermionc atoms have the same masses, which is approximately satisfied for the Bose-Fermi mixture of heavy isotopic atoms, for example, the ^{174}Yb-^{173}Yb mixture [3]. The Bose-Fermi mixture with equal masses provides a solvable limit, which may serve as a touchstone for various numerical simulations. For the model system with the fermion and the boson having the same mass, we have $t_b = t_f$. It is convenient to use the following extended Jordan-Wigner (JW) transformations

$$a_{ib} = \prod_{j<i} e^{i\pi c^{\dagger}_{j\uparrow} c_{j\uparrow}} c_{i\uparrow}, \quad a_{if} = \prod_{j=1}^{N} e^{i\pi c^{\dagger}_{j\uparrow} c_{j\uparrow}} c_{i\downarrow}, \quad (3)$$

which maps the Hamiltonian of hard-core Bose and Fermi mixture model into a Hubbard model

$$H_F = -\sum_{i,\sigma} \left(t_\sigma c^{\dagger}_{i\sigma} c_{i+1\sigma} + H.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (4)$$

The second mapping in eq. (3) is introduced to enforce the Fermion operators $c_{i,\uparrow}$ and $c_{i,\downarrow}$ fulfil the anti-commutation relation $\{c_{i,\uparrow}, c_{i,\downarrow}\} = 0$. The Hamitonians of H_{BF} and H_F have the same spectrum of energy. Therefore, we can get the eigen-energy of H_{BF} with $t_b = t_f = t$ from the well-known Lieb-Wu solution of the Hubbard model [25], i.e., the eigenenergy is given by $E = -2t\sum_j^N \cos k_j$ with k_j determined by the Bethe-ansatz equations

$$2\pi I_j \ = \ k_j L - \sum_{\beta=1}^{M} \theta_1(\Lambda_\beta - \sin k_j), \quad (5)$$

$$2\pi J_\alpha \ = \ \sum_{j=1}^{N} \theta_1(\Lambda_\alpha - \sin k_j) - \sum_{\beta=1}^{M} \theta_2(\Lambda_\alpha - \Lambda_\beta), \quad (6)$$

where $\theta_n(k) = 2\tan^{-1}(4k/nU)$, $j = 1, \cdots, N$, $\beta = 1, \cdots, M$, $N = N_b + N_f$, $M = N_f$, N_b (N_f) is the number of bosons (fermions), and L is the size of the system. Here the set $\{I_j, J_a\}$ play the role of quantum number. We also solve the ground state energy of H_{BF} by using the numerical exact diagonalization method and compare with the result obtained by solving the Bethe-ansatz equations. It is found that the numerical result agrees with the Bethe-ansatz solution exactly.

The unitary mapping builds a bridge between the hard-core Bose-Fermi mixture and the extensively studied Hubbard model. Since these two models sharing the same energy spectrum, we can conclude that they have the same thermodynamic properties. The GS properties of hard-core Bose-Fermi model also share some similarities with the Hubbard model, i.e., there exists no Mott transition from superfluid to Mott insulator for any finite U. For the incommensurate filling case, the system is in a superfluid phase, whereas the system with the commensurate filling $n = 1$ is in a Mott phase for any finite U, which is characterized by the presence of a charge gap and simultaneously a gapless mode of mixture composition fluctuations.

The superfluid density of the bosonic component can also be characterized by the bosonic phase stiffness, which reflects the response of a superfluid component to the imposed phase gradient and is defined as [26]

$$D_b = \frac{L}{2} \frac{\partial^2 E_0(\phi_b)}{\partial \phi_b^2} \bigg|_{\phi_b = 0}$$

which is proportional to the Drude weight. Similarly, the fermionic stiffness can be represented as

$$D_f = \frac{L}{2} \frac{\partial^2 E_0(\phi_f)}{\partial \phi_f^2} \bigg|_{\phi_f = 0}.$$

Here, E_0 is the ground-state energy, ϕ_b and ϕ_f are the component-dependent flux in units of $\hbar c/e$ for the boson and fermion respectively, which can be incorporated in the wavefunction by making the usual gauge transformation $a_{i,\sigma} \to e^{i\phi_\sigma r_i/L} a_{i,\sigma}$. A finite bosonic or fermionic stiffness is characteristic of a superfluid or conductor, whereas the stiffness vanishes for a insulator. In the presence of component-dependent flux, the eigenenergy of the system is also given by $E = -2t\sum_j \cos k_j$ with k_j determined by the revised Bethe-ansatz equations [26]

$$2\pi I_j \ = \ k_j L - \phi_b - \sum_{\beta=1}^{M} \theta_1(\Lambda_\beta - \sin k_j), \quad (7)$$

$$2\pi J_\alpha \ = \ \sum_{j=1}^{N} \theta_1(\Lambda_\alpha - \sin k_j) - \sum_{\beta=1}^{M} \theta_2(\Lambda_\alpha - \Lambda_\beta) + \phi_f - \phi_b. \quad (8)$$

By solving the revised BAEs, we can directly calculate the stiffness of system. In order to calculate the charge stiffness D_c, we set the magnetic flux of hard-core bosons ϕ_b and that of spinless fermions ϕ_f to be the same, i.e., $\phi_b = \phi_f = \phi$, whereas the spin stiffness D_s is calculated by taking $\phi_b = -\phi_f = \phi$. Explicitly, we have

$$D_c = \frac{L}{2} \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \bigg|_{\phi = \phi_b = \phi_f = 0}$$

and

$$D_s = \frac{L}{2} \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \bigg|_{\phi = \phi_b = -\phi_f = 0}.$$

For the case with commensurate filling, we display the charge, spin and boson stiffness in (a), (b) and (c) of Fig. 1, respectively. It is obvious that the charge stiffness goes to zero quickly when the interaction U exceeds a critical value. To extrapolate the critical U_c in the thermodynamic limit, we make finite size analysis of the transition point where the charge stiffness tends to vanish, which is characterized by the minimum of the derivative of the charge stiffness as shown in the Fig. 1(d).

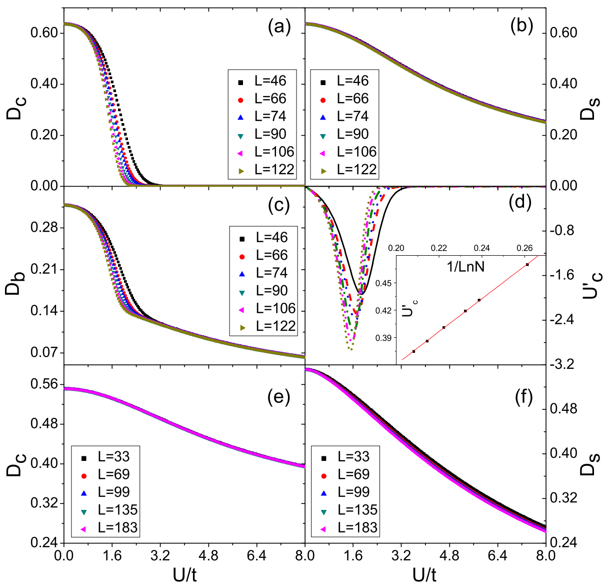

FIG. 1: (color online) The stiffness of system. The panels (a), (b), (c) and (d) correspond to the filling factor $n = 1$, whereas the panels (e) and (f) correspond to $n = 2/3$. Finite size analysis of the minimum of the derivative of the charge stiffness is shown in inset of (d). Here we have taken $N_b = N_f$.

The scaling behaviors of transition points can be fitted as $U_{cm} = 0.00104 + 1.79789/\ln N$. When the system-size tends to infinity, the critical on-site interactions reads $U_c = 0.00104 \pm 0.00354$, which covers the zero within the scope of fitting error. This means that the system is in a Mott phase with zero charge stiffness for any finite repulsion between the hard-core boson and fermion in the thermodynamic limit. However, as shown in Fig. 1(b) and 1(c), the spin and boson stiffness do not vanish even the system is in a Mott phase where the fluctuation of particle number (charge) on each site is greatly suppressed. Furthermore, our results show that the density of superfluid fulfills an interesting relation with the charge and spin stiffness, $D_b = (D_c + D_s)/4$ (see appendix). The non-vanishing D_b indicates that the boson is still in a superfluid phase even in the phase of charge insulator. This is induced by the fluctuation of bosons. Despite the charge fluctuation is suppressed, the boson can tunnel to the neighboring sites by a virtual second order process. For the incommensurate case with $n < 1$, both the charge and spin stiffness do not vanish as shown in Fig. 1(e) and 1(f), and no a Mott phase exists.

Particular attention should be paid to the special cases with a partial commensurate filling, for example, cases with $n_f = 1$, $n_b < 1$. Then the system favors that every site has one fermion which supplies a background and the bosons can hop on it freely. The energy of this state is

$$E = N_b U - \frac{tL}{\pi} \int_{-k_b}^{k_b} \cos(k + \phi_b/L) dk,$$

where $k_b = \pi n_b$. It is straightforward to get $D_b = t \sin(\pi n_b)/\pi$ and $D_f = 0$, which indicates that the bosons form a superfluid whereas the fermions form an insulator. Similarly, for the case with $n_b = 1$ and $n_f < 1$, the bosons are in an insulator state which provides a homogeneous background for the fermions which form a conductor with $D_f = t \sin(\pi n_f)/\pi$.

Despite H_{BF} and H_F sharing the same energy level structure, they have different ground state wavefunction due to the intrinsically different exchange symmetry of the wave functions for Bose and Fermi systems. Supposed the wavefunction of the Fermi Hubbard model is given by $\Psi_F(x_1, \cdots, x_n; x_{n+1}, \cdots, x_N)$, the wavefunction of H_{HB} can be constructed as

$$\begin{aligned} &\Psi_{BF}(x_1, \cdots, x_n; y_{n+1}, \cdots, y_N) \\ = &\prod_{i<j} sgn(x_i - x_j) \Psi_F(x_1, \cdots, x_n; y_{n+1}, \cdots, y_N), \end{aligned}$$

where $sgn(x_i - x_j) = (x_i - x_j)/|x_i - x_j|$ is the sign function. Consequently, the observable associated with the wave functions rather than the energy level structures should display different behaviors, which can be displayed in the off-diagonal density matrix and the momentum distributions of the hard-core boson. Explicitly, the density matrices of boson and fermion are defined as $\rho_{ij}^B = \left\langle a_{i,b}^\dagger a_{j,b} \right\rangle$ and $\rho_{ij}^F = \left\langle a_{i,f}^\dagger a_{j,f} \right\rangle$ respectively, which exhibit quite different behaviors for boson and fermion. The momentum distribution can be obtained by the Fourier transformation of the corresponding density matrix. For example, we have

$$n^{B,F}(k) = \frac{1}{2\pi L} \sum_{i,j} \rho_{ij}^{B,F} e^{-ik(i-j)}. \qquad (9)$$

In Fig. (2), we display the momentum distribution of the Bose and Fermi systems respectively for the case with commensurate filling $n_b = n_f = 1/2$. It is shown that the momentum distribution of the hard-core bosons has a sharp peak, which reflects the bosonic nature of the particles. With the increase in inter-component interactions, the momentum distribution spreads wider and wider but the pronounced peak around the zero momentum is kept. While the momentum distribution of the fermion exhibits the free Fermi distribution for $U = 0$, it becomes more wider and develops a wide tail with the increase in U.

Mixture with unequal masses.— Finally, we give a brief discussion on the case with $t_b \neq t_f$ which corresponds to the system where the bosonic and fermionc atoms have different masses, such as mixture of ^{7}Li and ^{40}K. In general, the single particle hopping amplitude is inversely proportional to the mass of atoms, *i.e.*, $t_f/t_b = m_b/m_f$.

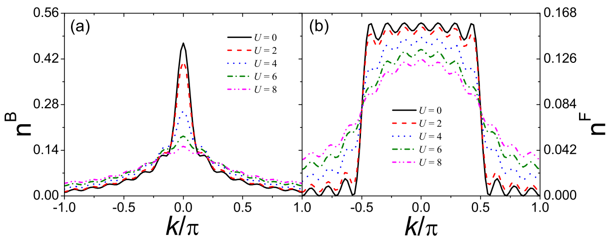

FIG. 2: (color online)Momentum distributions $n^B(k)$ for hard-core bosons (a) and $n^F(k)$ for spinless fermions (b). Here $L = 14$, $N_\mathrm{b} = 7$ and $N_\mathrm{f} = 7$.

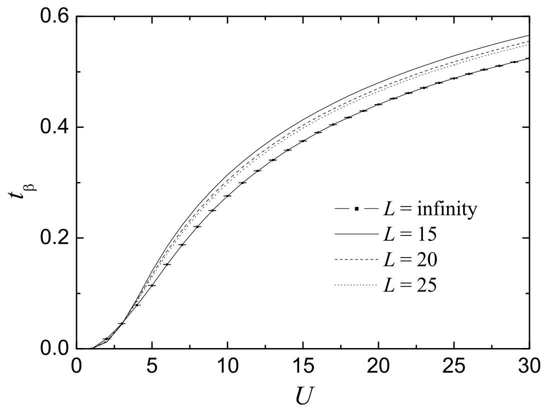

FIG. 3: Phase diagram for the asymmetric Bose-Fermi mixture with $n = 4/5$.

Taking the mixture ^{7}Li and ^{40}K as an example, we have $t_\beta = t_f/t_b \approx 0.175$. For the general case with $t_\beta \neq 1$, the mixture of hard-core bosons and fermions is no longer exactly solvable, although a mapping to the asymmetric Hubbard model [27] still holds true via the generalized JW transformation.

In the heavy Fermi mass limit $t_\beta \to 0$, the fermions lose the mobility and the asymmetric mixture model is related to the Falicov-Kimball model [28] via the generalized JW transformation. Away from integer-filling with $n < 1$, the heavy fermion and the light bosons are favorable to stay in different regimes to lower the kinetic energy of bosons. Therefore the system is expected to have a transition from density wave to phase separation. Next we shall use the density matrix renormalization group method to obtain a quantitative phase diagram for the mixture of TG gas and Fermi gas with $N_b = N_f$ and a filling $n = 4/5$.

Taking into account that the dominating configuration of fermionic atoms is quite different in the density-wave phase or phase with phase separation, we introduce the following structure factor of density wave (DW) of fermionic atoms

$$S_{\mathrm{FDW}}(q) = \frac{1}{L}\sum_{jl}\left[e^{iq(j-l)}(\langle n_{j,f}n_{l,f}\rangle - \langle n_f\rangle^2)\right], \quad (10)$$

where $q = 2n\pi/L$ and $n = 0, 1, \cdots, L$. We calculate the structure factor as a function of t_β for different modes for systems with different sizes L and strengthes of interactions U. The results show an obvious competition between the modes of $S_{\mathrm{FDW}}(q = 2\pi/L)$ and $S_{\mathrm{FDW}}(q = N\pi/L)$. In the heavy fermionic atom limit with small t_β, $S_{\mathrm{FDW}}(q = 2\pi/L)$ dominates, which indicates phase separation in this region [29] where configurations of fermionic atoms like $|f, f, f, f, \circ, \circ, \circ, \circ, \circ, \circ\rangle$ are found to be dominant. On the other hand, as $t_\beta \to 1$, $S_{\mathrm{FDW}}(q = N\pi/L)$ exceeds $S_{\mathrm{FDW}}(q = 2\pi/L)$, which implies that fermionic atoms distribute uniformly on the optical lattice. Then together with bosonic atoms, the ground state becomes the so called DW state similar to the state of symmetric model, which is the limiting case with $t_\beta = 1$ studied in the above section. Consequently, we can determine the transition point on the $U - t_\beta$ plane for a finite system from the intersection of the structure factor of two modes. In Fig. 3, we plot the phase diagram on the $U - t_\beta$ plane for systems with a filling factor $n = 4/5$ for different system-sizes $L = 15, 20, 25$. The infinite size limit is obtained by extrapolation from the finite-size analysis. Below the phase boundary line, the phase-separation phase dominates, while the DW phase is dominated above the boundary line.

In summary, we study the mixture of TG gas and fermions in a 1D optical lattice. We show that this system can be mapped to the Fermi Hubbard model by a generalized Jordan-Wigner transformation and thus is exactly solvable when the bosons and fermions have the same masses. Based on the Bethe-ansatz solution, we calculate the charge stiffness and the superfluid density for the systems with either commensurate or incommensurate filling. Our results show that the system with commensurate filling factor $n = 1$ is a charge insulator but remains to be a superfluid characterized by a non-vanishing superfluid density. We also give a brief discussion to the case with unequal boson and fermion masses. In the heavy Fermi mass limit, our result indicates that a phase-separation phase arise. The phase transition from the density wave phase to the phase-separation phase is discussed.

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Appendix A

In this appendix, we provide a derivation of the relation $D_b = \frac{1}{4}(D_c + D_s)$. In the presence of flux, the

Hamiltonian (2) becomes

$$\begin{aligned} H_{BF} &= -t\sum_i \left(a_{ib}^\dagger a_{i+1b} e^{i\phi_b/L} + H.c.\right) \\ &\quad -t\sum_i \left(a_{if}^\dagger a_{i+1f} e^{i\phi_f/L} + H.c.\right) + U\sum_i n_{i,b} n_{i,f}. \end{aligned}$$

Expanding the Hamiltonian in terms of ϕ_b/L and ϕ_f/L, we have

$$\begin{aligned} H_{BF} &= \left(T_b - \frac{\phi_b j_b}{L} - \frac{T_b}{2}\frac{\phi_b^2}{L^2}\right) + \left(T_f - \frac{\phi_f j_f}{L} - \frac{T_f}{2}\frac{\phi_f^2}{L^2}\right) \\ &\quad + U\sum_i n_{i,b} n_{i,f} + O(\phi_b^4, \phi_f^4), \end{aligned}$$

where $T_\sigma = -t\sum_i \left(a_{i\sigma}^\dagger a_{i+1\sigma} + H.c.\right)$ and $j_\sigma = it\sum_i \left(a_{i\sigma}^\dagger a_{i+1\sigma} - H.c.\right)$ with $\sigma = b, f$. So according to the perturbation theory,

$$D_c = \frac{1}{L}\left[\frac{1}{2}\langle -T_c\rangle - \sum_{n\neq 0}\frac{\langle 0|j_c|n\rangle^2}{E_n - E_0}\right],$$

$$D_s = \frac{1}{L}\left[\frac{1}{2}\langle -T_s\rangle - \sum_{n\neq 0}\frac{\langle 0|j_s|n\rangle^2}{E_n - E_0}\right],$$

$$D_b = \frac{1}{L}\left[\frac{1}{2}\langle -T_b\rangle - \sum_{n\neq 0}\frac{\langle 0|j_b|n\rangle^2}{E_n - E_0}\right],$$

$$D_f = \frac{1}{L}\left[\frac{1}{2}\langle -T_f\rangle - \sum_{n\neq 0}\frac{\langle 0|j_f|n\rangle^2}{E_n - E_0}\right],$$

where the current operators: $j_c = j_b + j_f$, $j_s = j_b - j_f$, and $T_c = T_s = T_f + T_b = 2T_b$. Then

$$\begin{aligned} D_c &+ D_s \\ &= \frac{1}{L}\left[\frac{1}{2}\langle -4T_b\rangle - 2\sum_{n\neq 0}\frac{\langle 0|j_c|n\rangle^2}{E_n - E_0} - 2\sum_{n\neq 0}\frac{\langle 0|j_s|n\rangle^2}{E_n - E_0}\right] \\ &= \frac{1}{L}\left[\frac{1}{2}\langle -4T_b\rangle - 4\sum_{n\neq 0}\frac{\langle 0|j_b|n\rangle^2}{E_n - E_0}\right] = 4D_b. \end{aligned}$$

Finally, we have

$$D_b = \frac{1}{4}(D_c + D_s).$$

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